



STRUCTURES  
CLUSTER OF  
EXCELLENCE



UNIVERSITÄT  
HEIDELBERG  
ZUKUNFT  
SEIT 1386

# Topological Data Analysis in Python

organized by:

Michael Bleher, Maximilian Schmahl and Daniel Spitz

Heidelberg University

26<sup>th</sup> - 28<sup>th</sup> of October 2020

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Programme / scikit-tda

Topological Data Analysis

The Mapper Algorithm

Kepler Mapper

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Topological Data Analysis

The Mapper Algorithm

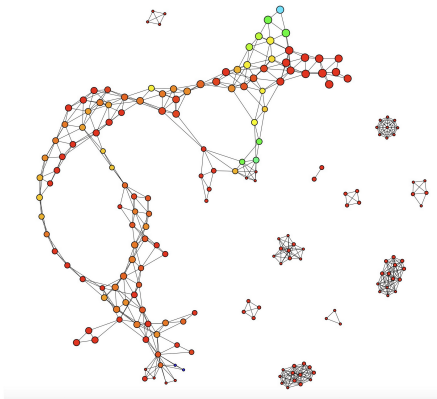
Kepler Mapper

# Overview scikit-tda and Programme



**scikit-tda libraries**

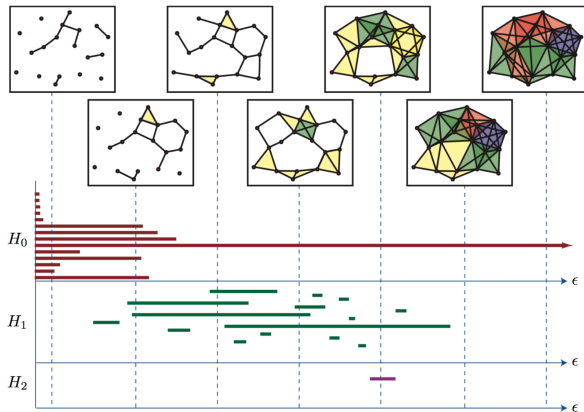
# Overview scikit-tda and Programme



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► Kepler Mapper

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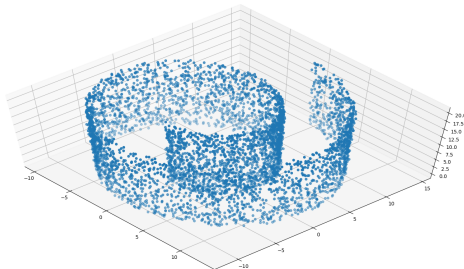


## scikit-tda libraries

- Kepler Mapper
- Ripser.py
- Persim
- CechMate

Melissa McGuirl, Lecture Notes, ICERM 2017

# Overview scikit-tda and Programme



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- ▶ TaDAsets

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Programme / scikit-tda

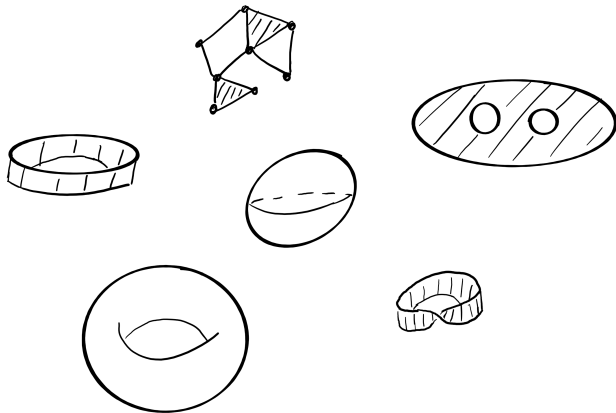
Topological Data Analysis

The Mapper Algorithm

Kepler Mapper

# Topology

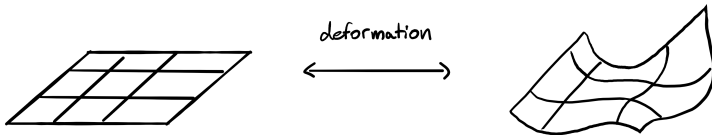
Topology is about studying shapes



# Topology

Topology is about studying shapes

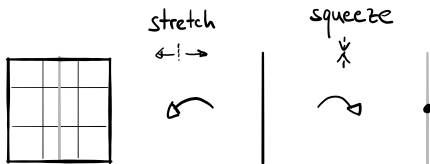
- up to deformations,



# Topology

Topology is about studying shapes

- ▶ up to deformations,
- ▶ and up to stretching and squeezing,



# Topology

Topology is about studying shapes

- ▶ up to deformations,
- ▶ and up to stretching and squeezing,
- ▶ **without** cutting or gluing.

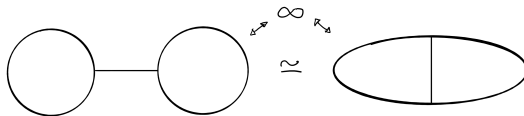




## Examples

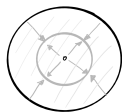
# Topology

## Examples



# Topology

## Examples

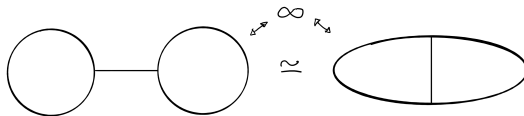


$Disk \setminus \{0\}$

$\cong$

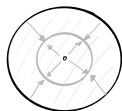
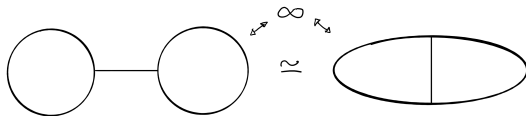


$S^1$



# Topology

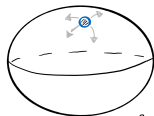
## Examples



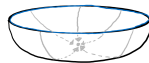
$\mathbb{R}$



$S^1$



$\mathbb{R}$



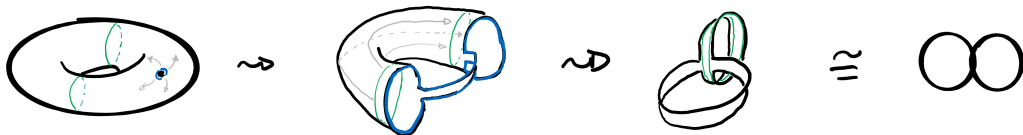
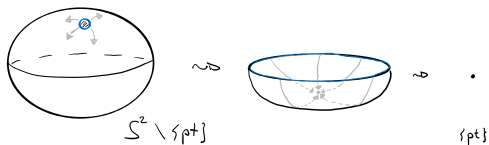
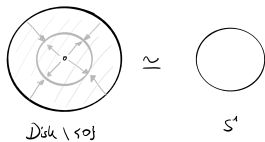
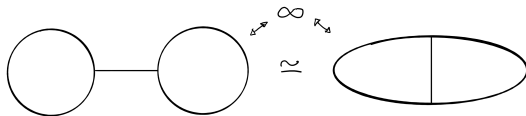
$\mathbb{R}$

$\cdot$

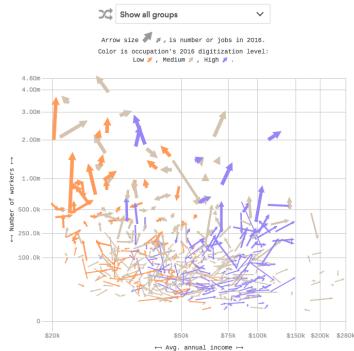
$\{pt\}$

# Topology

## Examples



Understanding data is complicated!



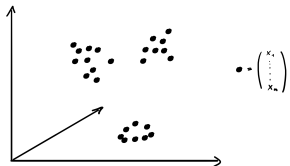
Data: Brookings "Digitalization and the American workforce" report; Interactive: Lazaro Gamio / Axios

Challenges of data science: complexity, size, curse of dimensionality



# Data Analysis

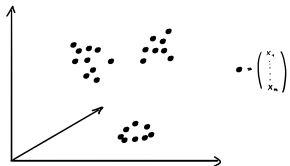
Data = sample of points in  $\mathbb{R}^n$



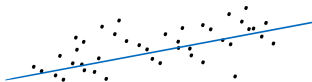


# Data Analysis

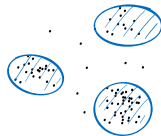
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## Classical Data Analysis:

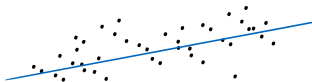


Correlation Methods

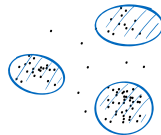


Clustering Methods

# Topological Data Analysis

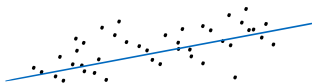


Correlation Methods

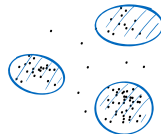


Clustering Methods

# Topological Data Analysis



Correlation Methods



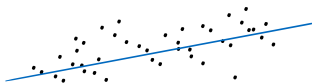
Clustering Methods

## Premise of Topological Data Analysis

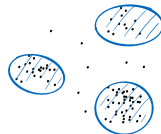
Data is noisy sample of some subspace in  $\mathbb{R}^n$ .

The “topology” of this subspace captures abstract (cor)relations in the data.

# Topological Data Analysis



Correlation Methods



Clustering Methods

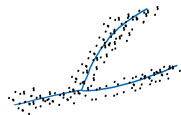
## Premise of Topological Data Analysis

Data is noisy sample of some subspace in  $\mathbb{R}^n$ .

The “topology” of this subspace captures abstract (cor)relations in the data.



Loops  
(and higher dim. generalizations)



Bifurcations

Promises of Topological Data Analysis:

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- ▶ model independent, non-parametric analysis.

# Topological Data Analysis

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- ▶ Compressed representation of global properties in highly complex data sets.

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## Promises of Topological Data Analysis:

- ▶ model independent, non-parametric analysis.
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- ▶ Resistance to noise and missing data. TDA retains significant features of the data.



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- ▶ Solid theoretical foundation, e.g. robustness with respect to change of choices.

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- ▶ Invariance. Only 'relations' matter. The skew, size, or orientation of data does not fundamentally change that data.

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## Promises of Topological Data Analysis:

- ▶ model independent, non-parametric analysis.
- ▶ Compressed representation of global properties in highly complex data sets.
- ▶ Resistance to noise and missing data. TDA retains significant features of the data.
- ▶ Solid theoretical foundation, e.g. robustness with respect to change of choices.
- ▶ Invariance. Only 'relations' matter. The skew, size, or orientation of data does not fundamentally change that data.
- ▶ A data exploration tool. Get answers to questions you haven't even asked yet.

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**Break**  
Continue at:

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Programme / scikit-tda

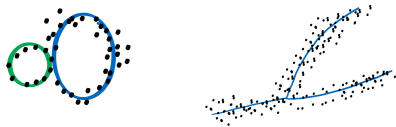
Topological Data Analysis

The Mapper Algorithm

Kepler Mapper

# The Mapper Algorithm - Intro

The Mapper algorithm provides a way to extract non-trivial properties from high-dimensional data.

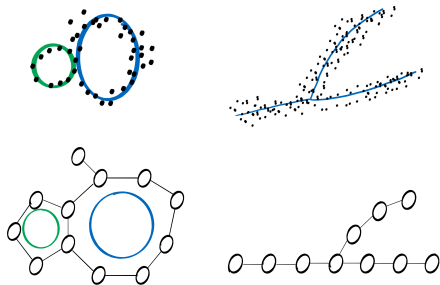




# The Mapper Algorithm - Intro

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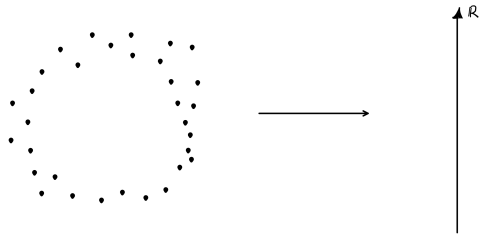
Mapper produces a graph that captures connectedness and topological properties of the data.



# The Mapper Algorithm

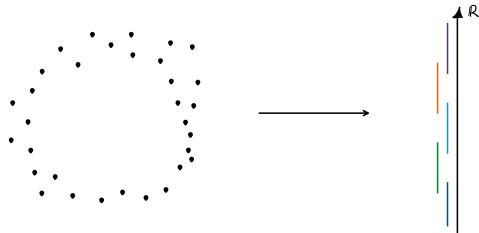
# The Mapper Algorithm

## 1. **Project** (filter dependency)



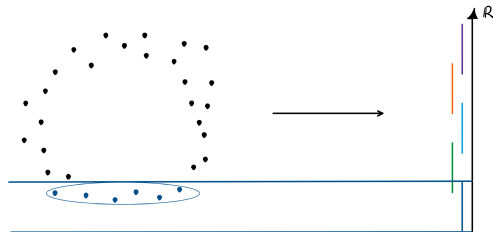
# The Mapper Algorithm

1. Project (filter dependency)
2. **Cover** (cover dependency)



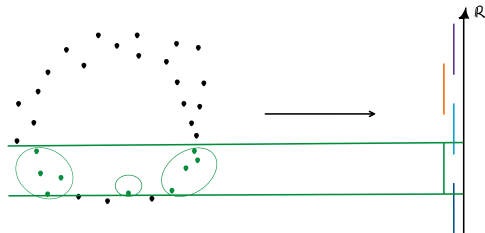
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1. Project (filter dependency)
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3. **Cluster** (metric & cluster algorithm)



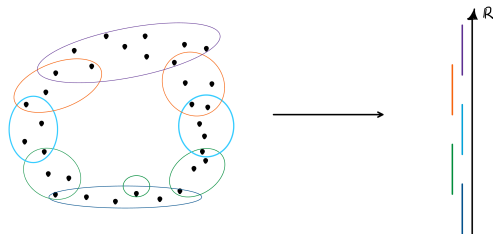
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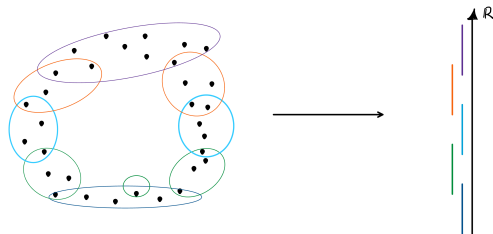
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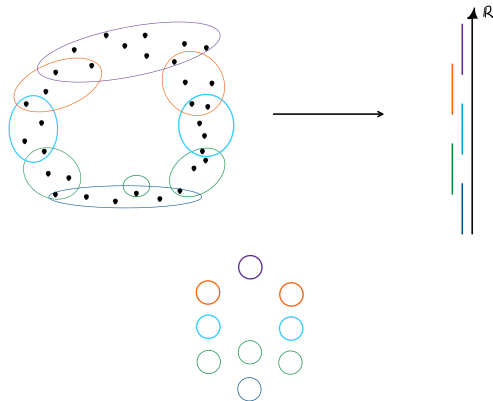
1. Project (filter dependency)
2. Cover (cover dependency)
3. Cluster (metric & cluster algorithm)
4. **Graph**





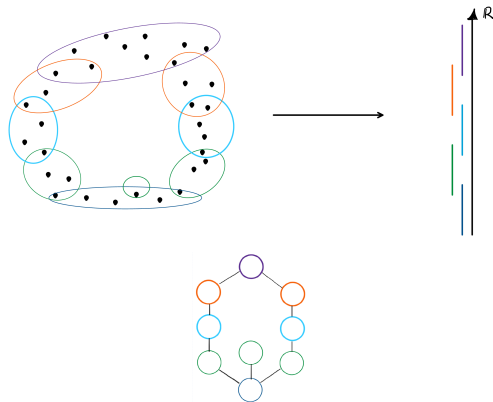
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1. Project (filter dependency)
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4. **Graph**
  - Draw a **node** for each **cluster**



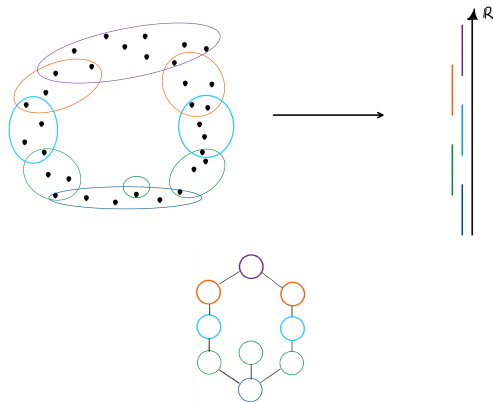
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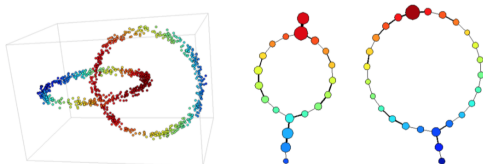


# The Mapper Algorithm

1. Project (filter dependency)
2. Cover (cover dependency)
3. Cluster (metric & cluster algorithm)
4. **Graph**
  - ▶ Draw a **node** for each **cluster**
  - ▶ Draw an **edge** when clusters **intersect**
5. Prettify (e.g. node size, edge length, node colour, graph shape) and Analyze



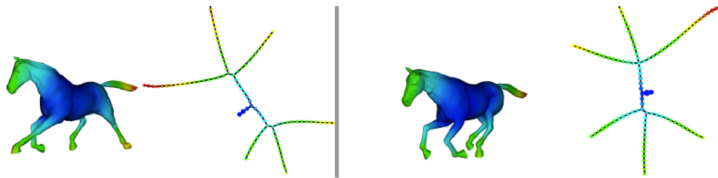
# The Mapper Algorithm - Examples



The Mapper graph of two linked circles recognizes two distinct connected components and their shapes.  
(filter = SVD)

# The Mapper Algorithm - Examples

The Mapper graph is preserved throughout the animated movement of a 3d model of a horse.  
(filter = eccentricity)

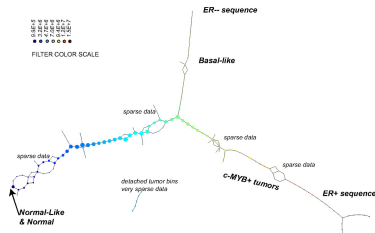


# The Mapper Algorithm - Examples

Application to breast cancer data

data = gene expressions of tumor cells

filter  $\sim$  deviation from normal cells



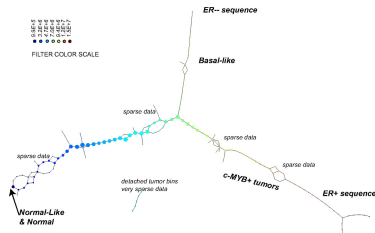
M. Nicolau et al, PNAS 108:17 (2011)

# The Mapper Algorithm - Examples

Application to breast cancer data

data = gene expressions of tumor cells

filter  $\sim$  deviation from normal cells



M. Nicolau et al, PNAS 108:17 (2011)

- ▶ most filters reproduce known classification of clustering methods
- ▶ special filters: graph suggests existence of previously unknown cluster c-MYB+
- ▶ further analysis shows 100% overall survival rate in this cluster

# Contents

Programme / scikit-tda

Topological Data Analysis

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Kepler Mapper



# Kepler Mapper - Install

## Install

```
$ pip install kmapper  
$ python3  
Python 3.8  
> import kmapper
```

# Kepler Mapper - The Main Function

```
kmapper.KeplerMapper.map()
```

Applies Mapper algorithm on a given projection and returns a graph.

# Kepler Mapper - The Main Function

```
kmapper.KeplerMapper.map()
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Applies Mapper algorithm on a given projection and returns a graph.

```
import kmapper as km  
km.KeplerMapper.map(projected_data, data [,cover])
```

projected\_data: Numpy Array

data: Numpy Array

```
cover = kmapper.Cover(n_cubes=10, perc_overlap=0.1, limits=None, verbose=0)
```

# Kepler Mapper - The Main Function

## Output

```
import kmapper as km
graph = km.KeplerMapper.map(projected_data, data [,cover])

graph = {
    'nodes': {'cube0_cluster0': [points], ...},
    'links': {'cube0_cluster0': [linked clusters], ...},
    'simplices': {[nodes], ..., [edges], ...},
    'meta_data': {summary of choices}
    'meta_nodes': {?}
}
```

# Kepler Mapper - kmapper projections

`kmapper.KeplerMapper.project()` and `fit_transform()`

Create a projection from a dataset.

Input the data set. Specify a projection. Output the projected data.

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```
km.KeplerMapper.project(data,  
    projection='sum',  
    scaler=MinMaxScaler(copy=True, feature_range=(0, 1)),  
    distance_matrix=None)
```

`projection`: `str**`, or a Scikit-learn class with `fit_transform`, or a list of dimension indices.

`scaler`: Scikit-Learn API compatible scaler.

`distance_matrix`: `str**` or `None`. If `None` do nothing, else compute distance matrix with chosen metric, before applying the projection.

`**see help(kmapper.KeplerMapper.project) for more details.`

# Kepler Mapper - kmapper Cover

`kmapper.Cover()`

Calculates a cover based on number of cubes and the percentage of their overlap.

# Kepler Mapper - kmapper Cover

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Calculates a cover based on number of cubes and the percentage of their overlap.

`km.Cover(n_cubes=10, perc_overlap=0.5, limits=None)`

`n_cubes`: int. Number of hypercubes along each dimension.

`perc_overlap`: float. Amount of overlap between adjacent cubes.

`limits`: Numpy Array ( $n_{\text{dim}}, 2$ ).

- ▶ the value `np.float('inf')` corresponds to min/max value of the projection in this dimension.
- ▶ `limits == None` corresponds to min/max value of the projection for all dimensions.



## Kepler Mapper - kmapper visualize

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Generate a visualization of the simplicial complex mapper output. Turns the complex dictionary into a HTML/D3.js visualization.

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Generate a visualization of the simplicial complex mapper output. Turns the complex dictionary into a HTML/D3.js visualization.

```
km.KeplerMapper.visualize(graph, args)
```

**\*\*see `help(km.KeplerMapper.visualize)` for details.**

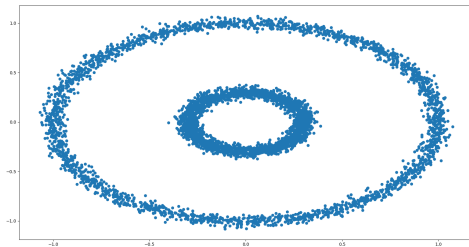


# Kepler Mapper - Example

# Kepler Mapper - Example

Import data

```
from sklearn import datasets  
data = datasets.make_circles(n_samples=5000, noise=0.03, factor=0.3)
```



# Kepler Mapper - Example

```
import kmapper as km
mapper = km.KeplerMapper

# Project data to x and y axis
projected_data = mapper.fit_transform(data, projection=[0,1])

# Create graph (using default nr_cubes=10)
graph = mapper.map(projected_data, data)

# Visualize it
mapper.visualize(
    graph,
    path_html='make_circles_keplermapper_output.html',
    title='make_circles(n_samples=5000,noise=0.03,factor=0.3)'
)
```

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```

projection=[0,1]: [example\\_xy.html](#)  
projection='sum': [example\\_sum.html](#)

# Breakout Rooms

Type a room ID in chat to get assigned to it.

## Room IDs

- ▶ **0** + '**group id**' create/join custom room
  - ▶ **1** Exercise 1
  - ▶ **2** Exercise 2
  - ▶ **3** Exercise 3
  - ▶ **4** Exercise 4
  - ▶ **9** Break Room
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- ▶ If you run into problems while in a room, hit the *contact moderator* button. This should summon a moderator into your room.
  - ▶ If you want to change rooms, simply get back to the main session and let us know.