Topological Data Analysis in Python

organized by:
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Heidelberg University

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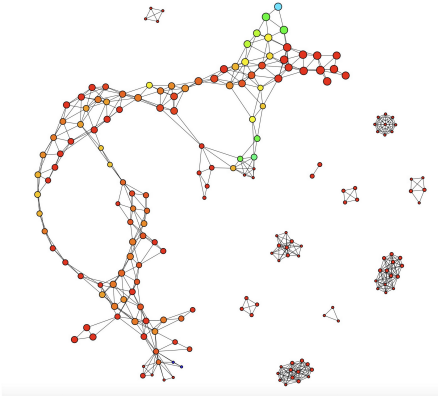

scikit-tda libraries

- Kepler Mapper

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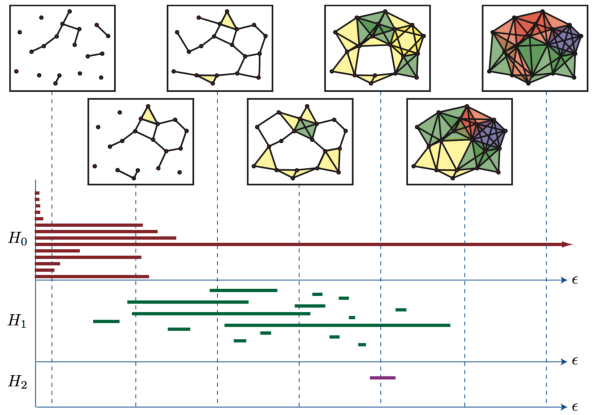

Melissa McGuirl, Lecture Notes, ICERM 2017

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- Ripser.py
- Persim
- CechMate

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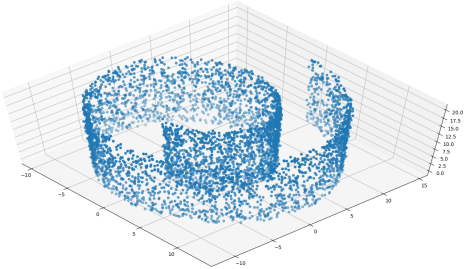

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	Monday	Tuesday	Wednesday
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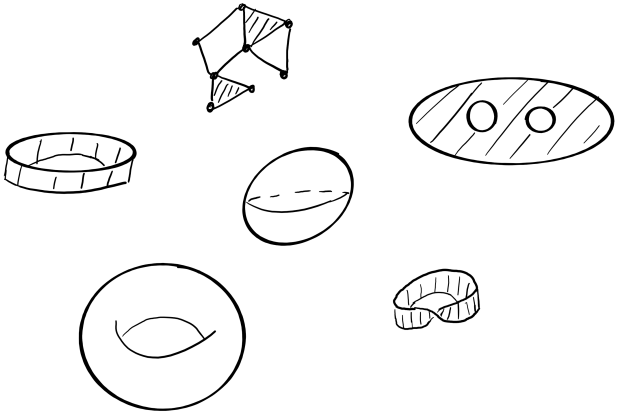
Topology

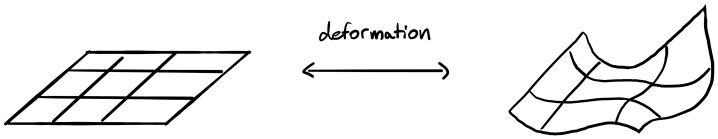
Topology is about studying shapes



Topology

Topology is about studying shapes

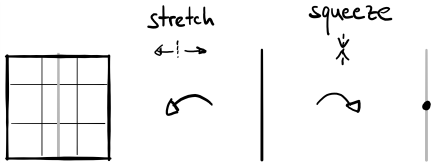
- up to deformations,



Topology

Topology is about studying shapes

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



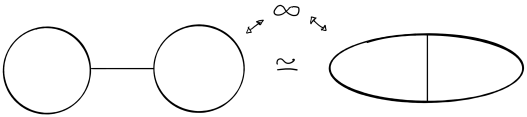
Topology

Topology is about studying shapes

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

Examples

Examples



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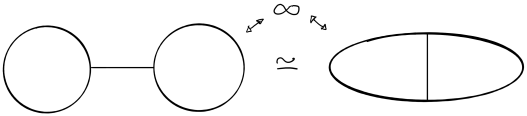

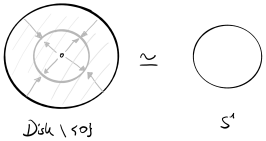

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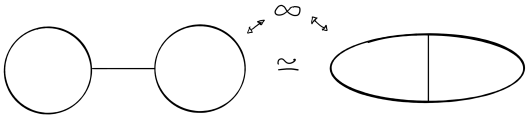

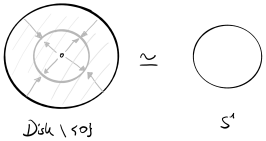

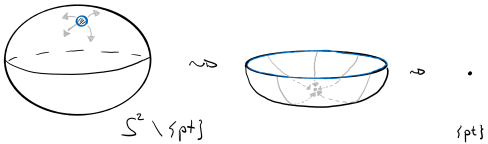

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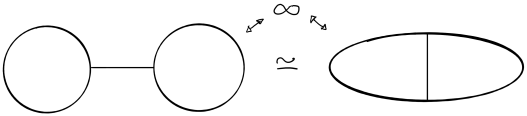
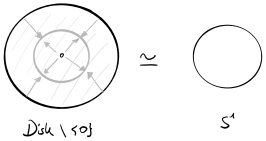
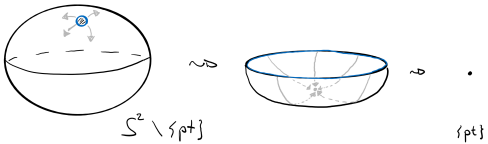
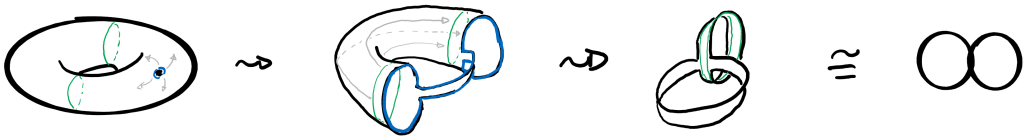


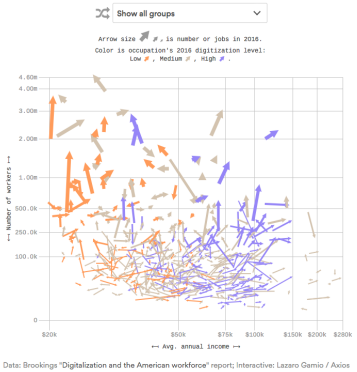






Data Analysis

Understanding data is complicated!

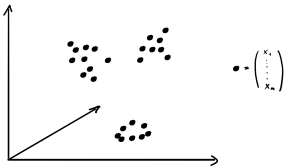


Challenges of data science: complexity, size, curse of dimensionality

Data Analysis

Data Analysis

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



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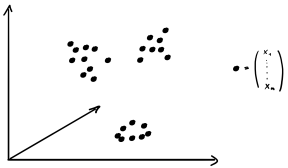
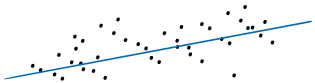
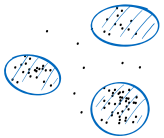


Classical Data Analysis:

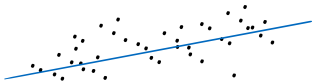


Correlation Methods



Clustering Methods

Topological Data Analysis



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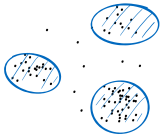

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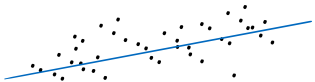

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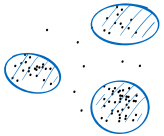
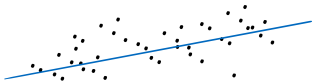


Clustering Methods

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



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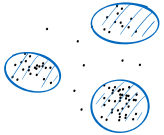

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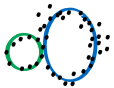
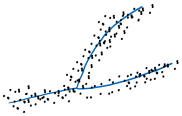


Loops
(and higher dim. generalizations)



Bifurcations

Topological Data Analysis

Promises of Topological Data Analysis:

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- model independent, non-parametric analysis.

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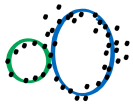
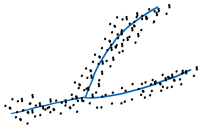
The Mapper algorithm provides a way to extract non-trivial properties from high-dimensional data.

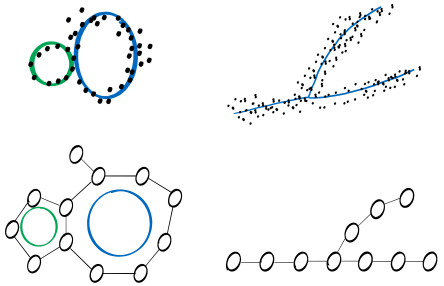




The Mapper Algorithm - Intro

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

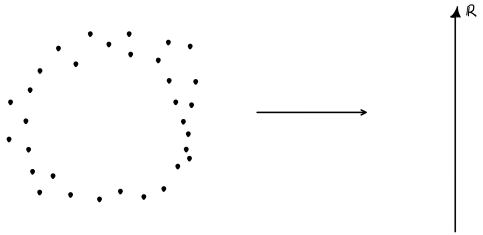
Mapper produces a graph that captures connectedness and topological properties of the data.



The Mapper Algorithm

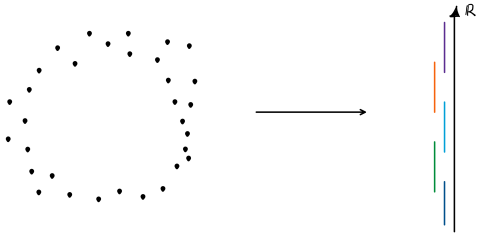
The Mapper Algorithm

1. **Project** (filter dependency)



The Mapper Algorithm

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



The Mapper Algorithm

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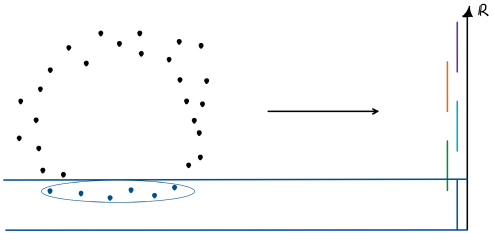
3. **Cluster** (metric & cluster algorithm)



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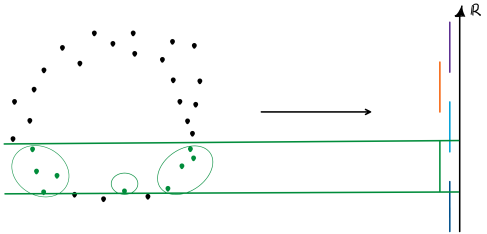

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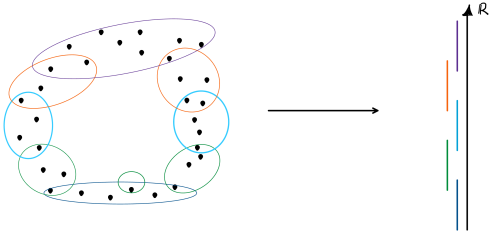

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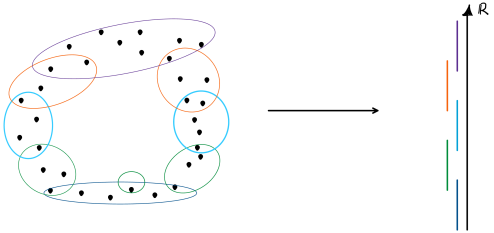

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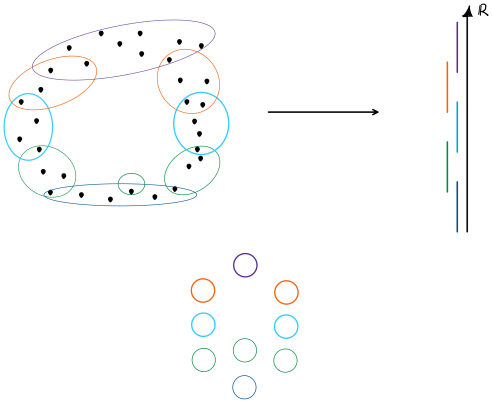
   - Draw a **node** for each **cluster**



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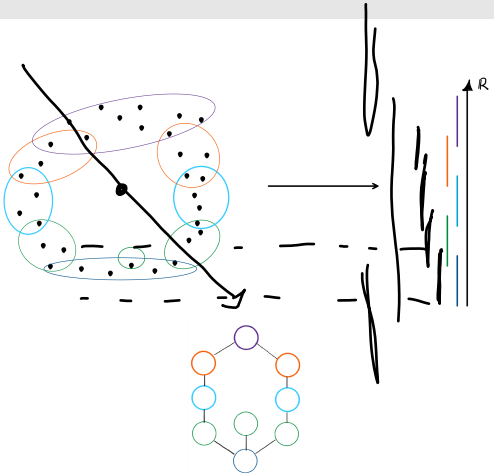
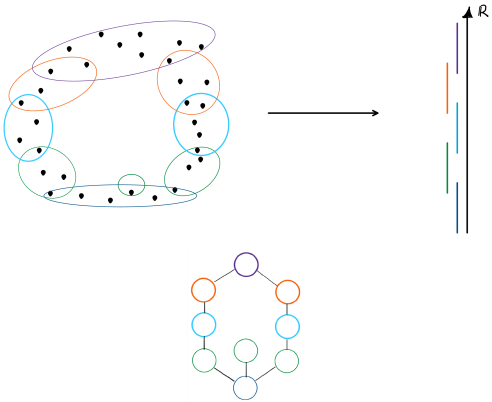
4. **Graph**
   - Draw a **node** for each **cluster**
   - Draw an **edge** when clusters **interesect**

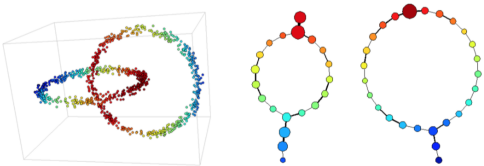


The Mapper Algorithm

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 **interesect**
5. Prettify (e.g. node size, edge length, node colour, graph shape) and Analyze



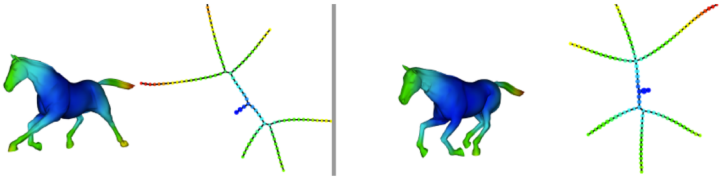
The Mapper Algorithm - Examples



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

The Mapper Algorithm - Examples

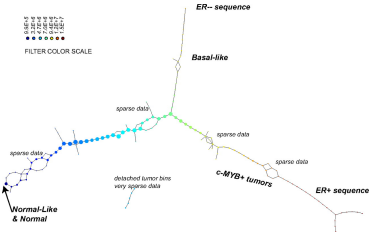
The Mapper graph is preserved throughout the animated movement of a 3d model of a horse.
(filter = eccentricity)



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

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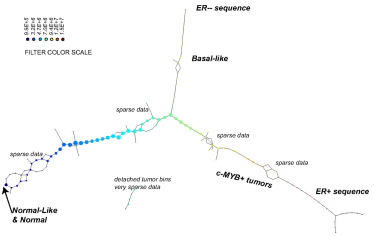


M. Nicolau et al, PNAS 108:17 (2011)

- 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

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()

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.

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.

```
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

kmapper.Cover()

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

kmapper.KeplerMapper.visualize()

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

Kepler Mapper - kmapper visualize

kmapper.KeplerMapper.visualize()

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

km.KeplerMapper.visualize(graph, args)

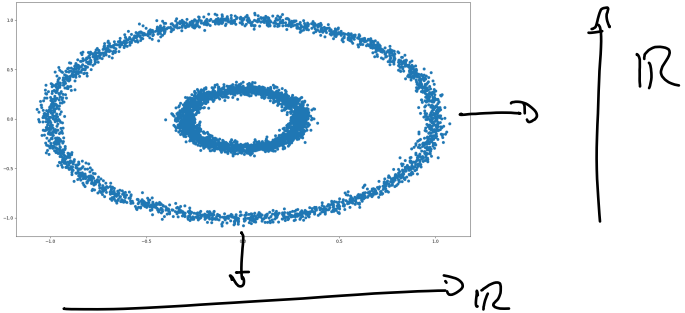
**see `help(km.KeplerMapper.visualize)` for details.

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)'
    )
```

Kepler Mapper - Example

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import kmapper as km
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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

- 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.