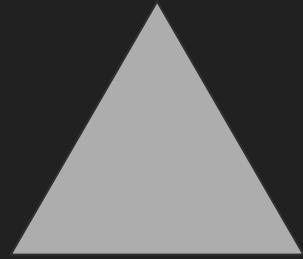
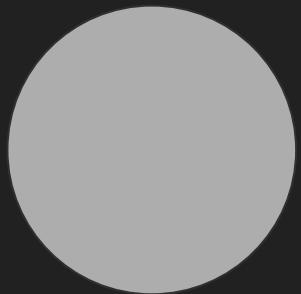


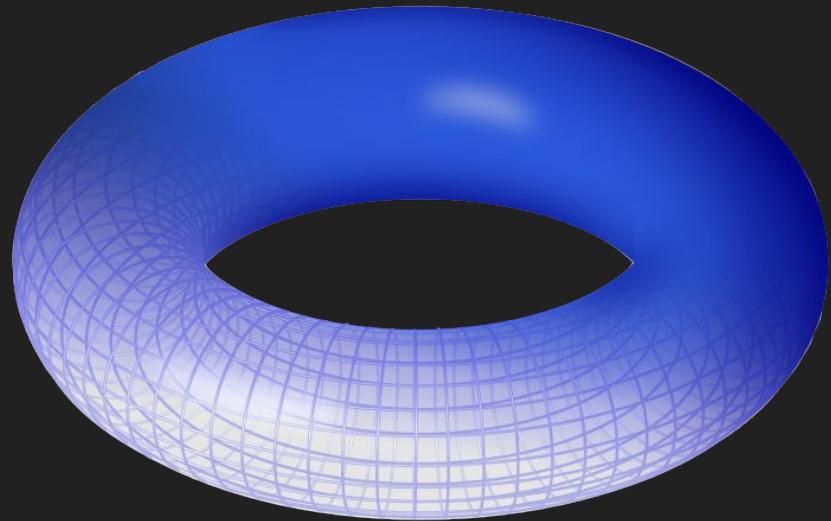
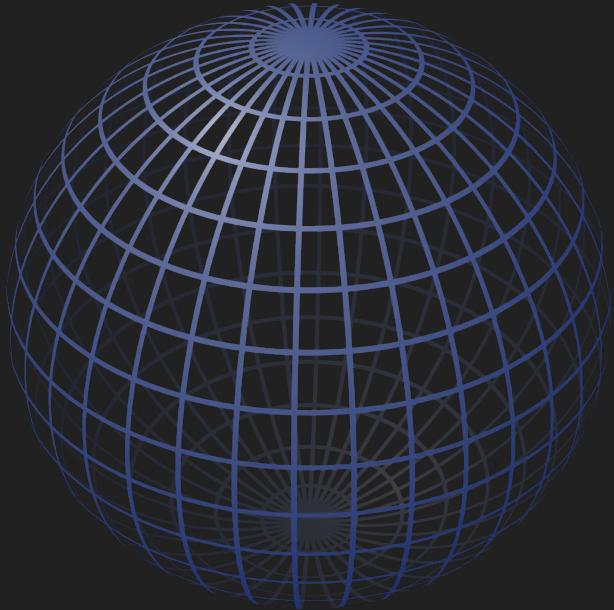
# Topological Data Analysis to understand Convolutional Neural Networks

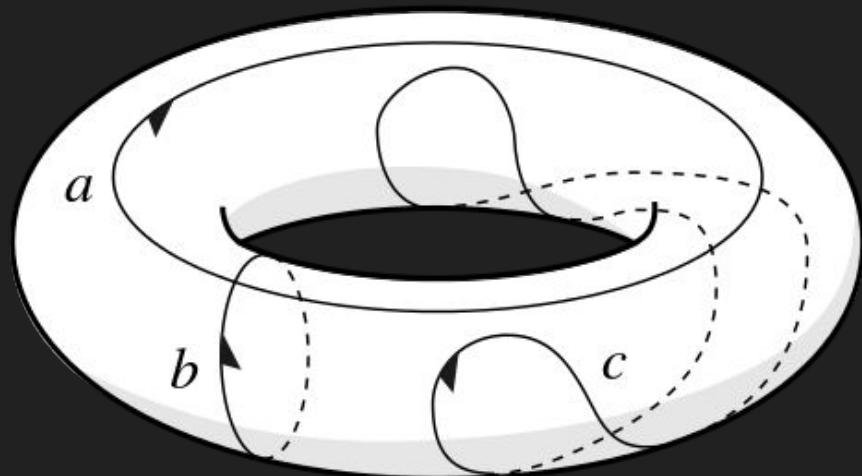
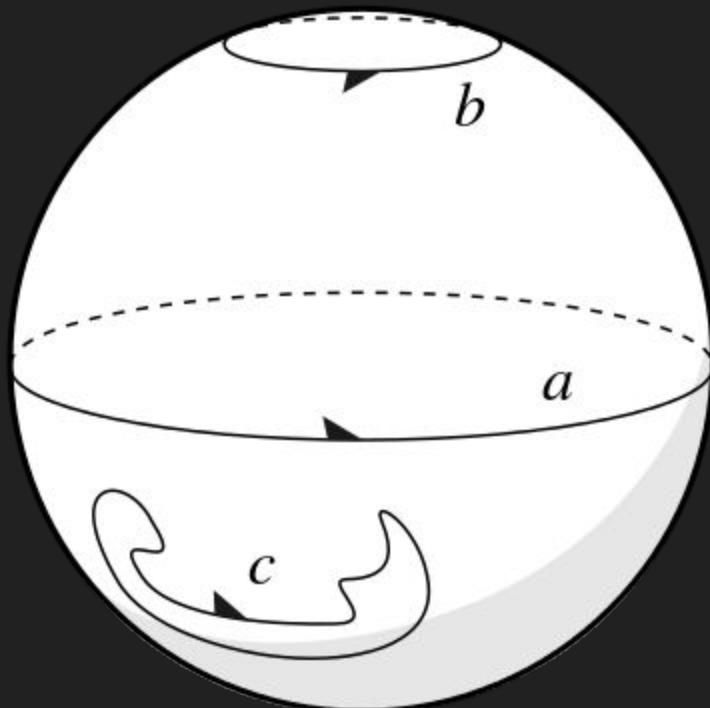
Aleksei Prokopev, SeoulAI, 2018

# Shape



# Topology





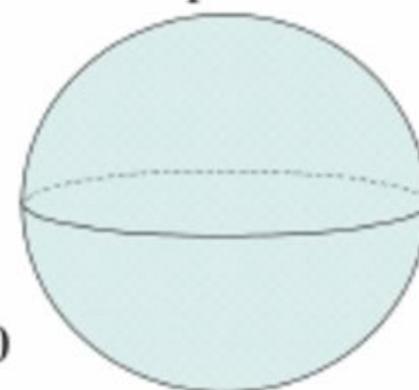
A solid 2-dimensional blob



$$\beta_0 = 1$$

$$\beta_{i>0} = 0$$

A sphere



$$\beta_0 = 1$$

$$\beta_1 = 0$$

$$\beta_2 = 1$$

$$\beta_{i>2} = 0$$

A 2D blob with three holes



$$\beta_0 = 1$$

$$\beta_1 = 3$$

$$\beta_{i>1} = 0$$

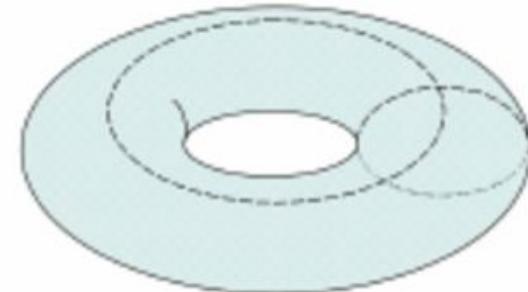
$$\beta_0 = 1$$

$$\beta_1 = 2$$

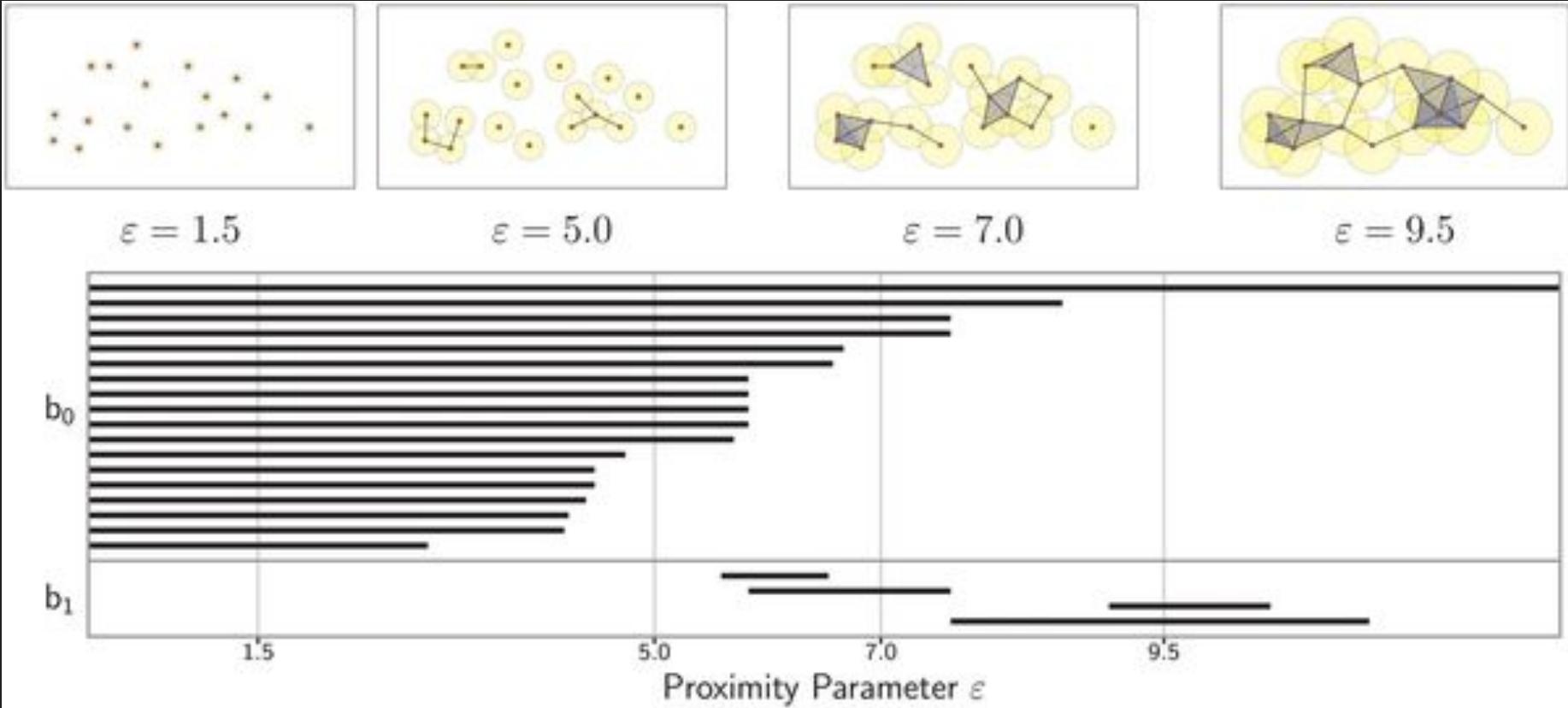
$$\beta_2 = 1$$

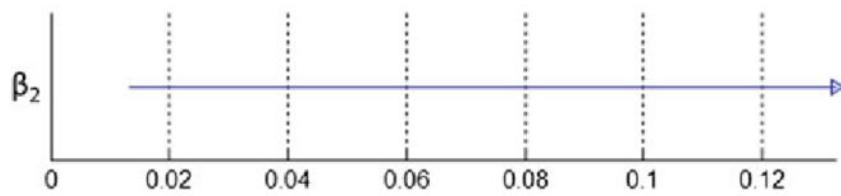
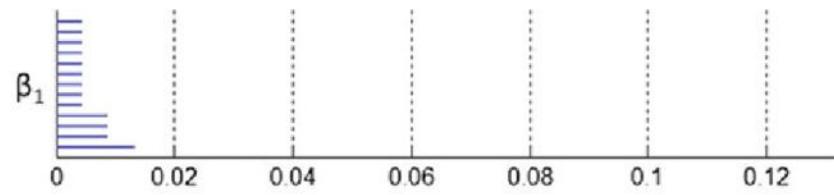
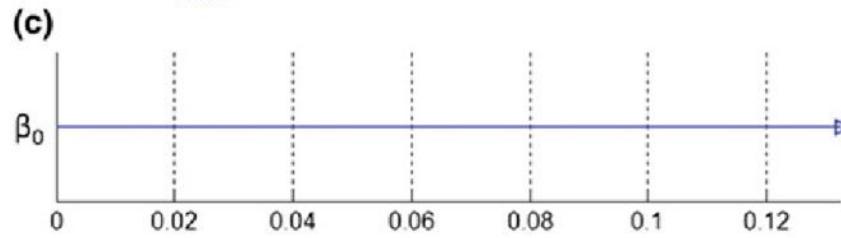
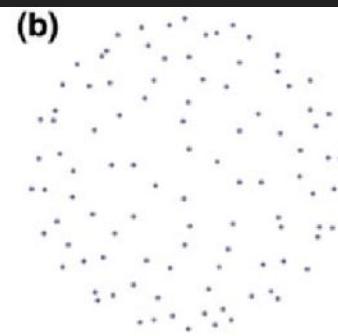
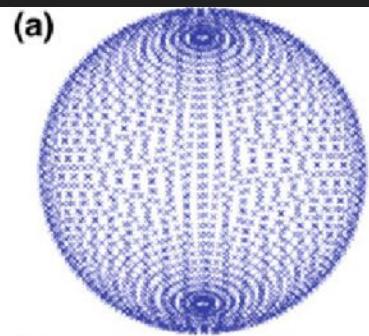
$$\beta_{i>2} = 0$$

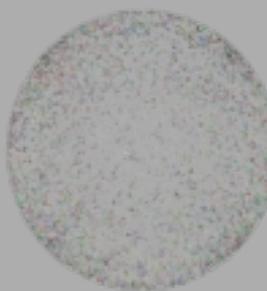
A torus

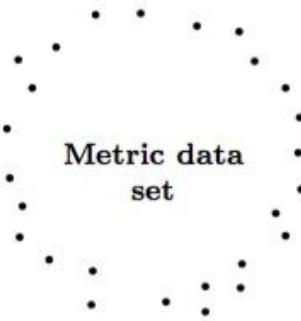


# Topological Data Analysis



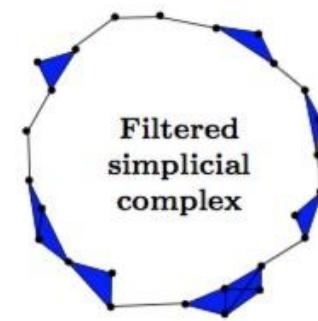






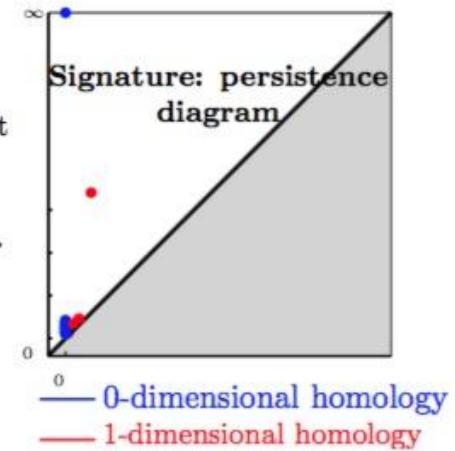
Metric data set

Build geometric  
filtered complex on  
top of data

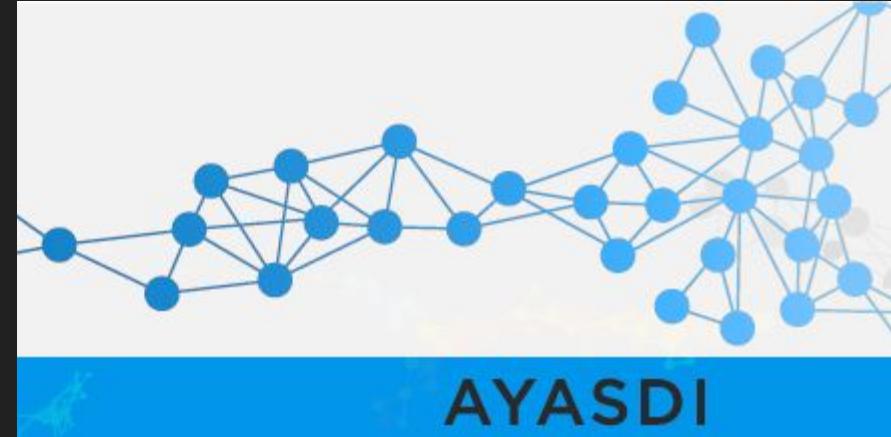
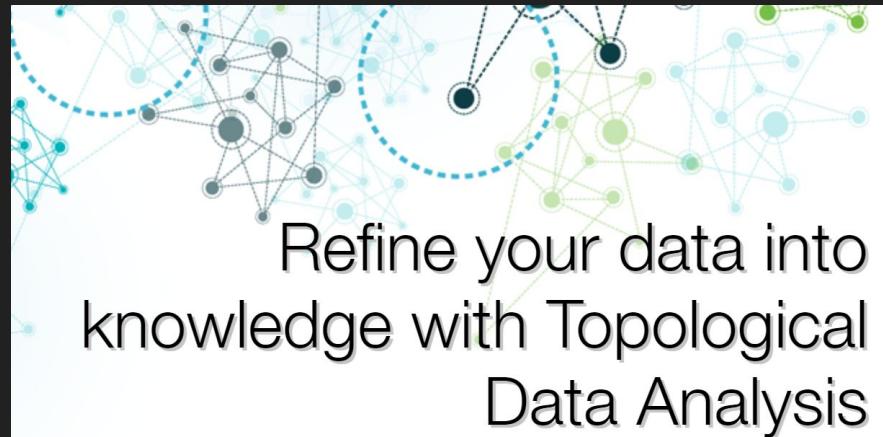


Filtered  
simplicial  
complex

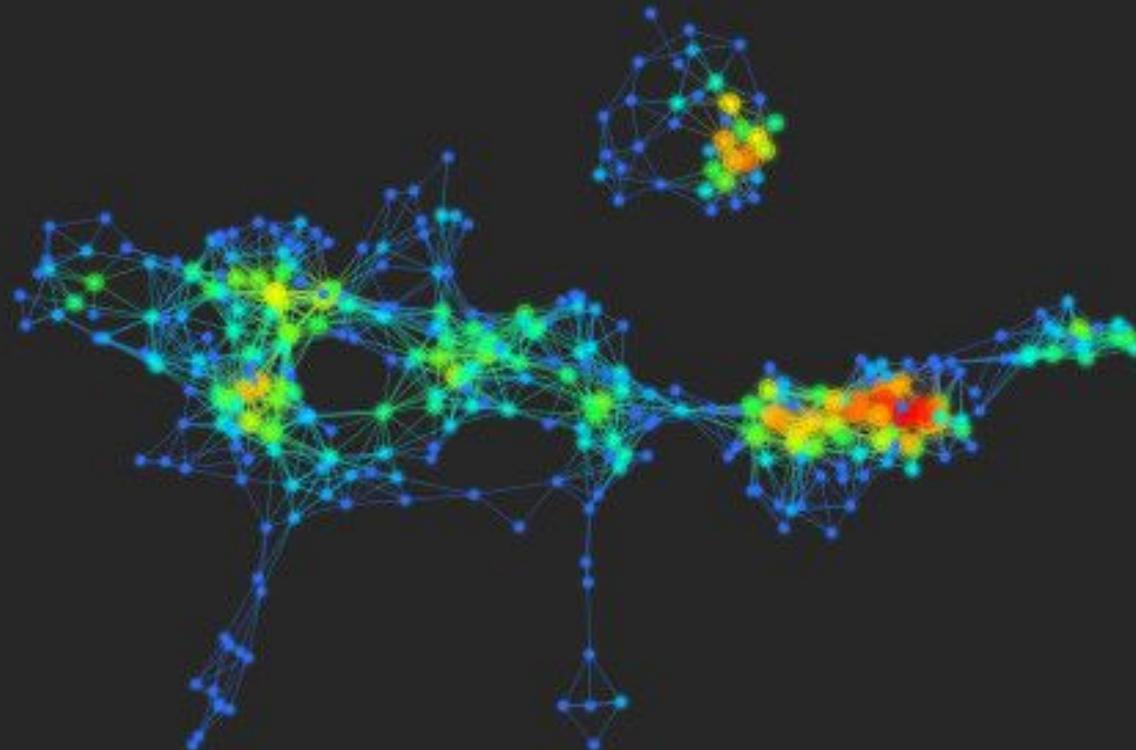
Compute persistent  
homology of the  
complex.



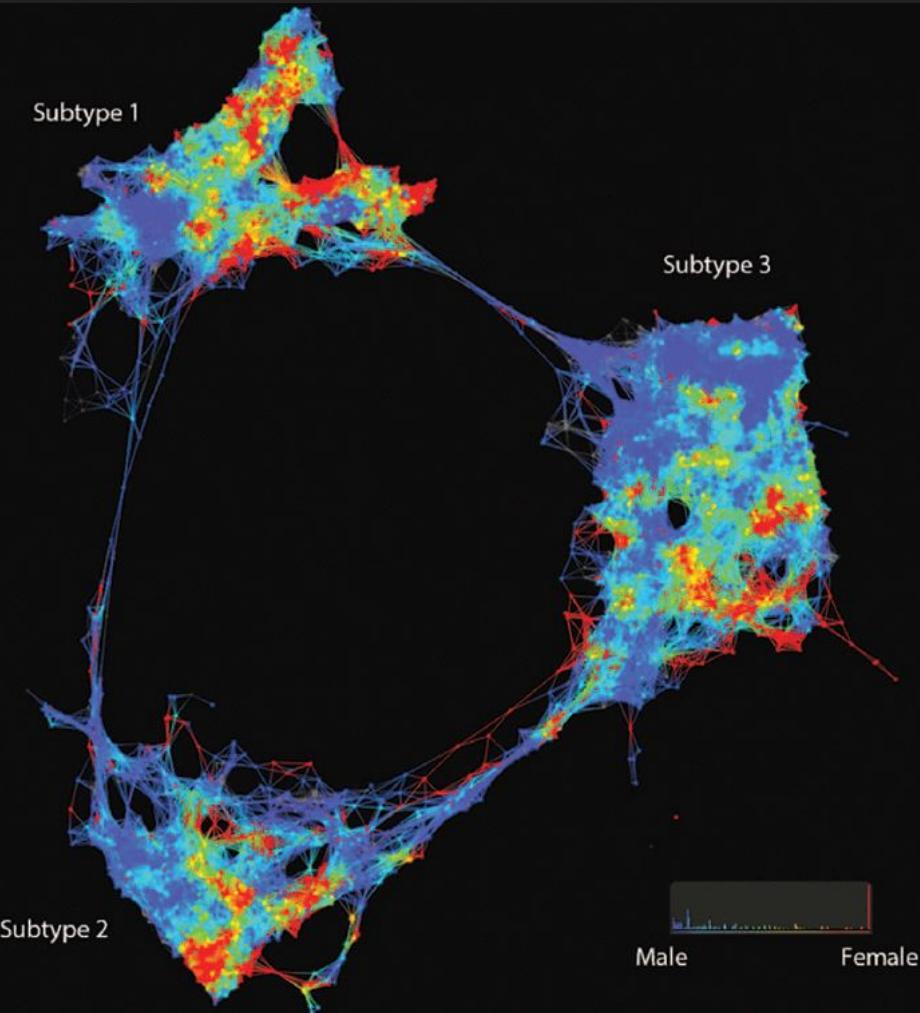
— 0-dimensional homology  
— 1-dimensional homology



# Examples



AYASDI

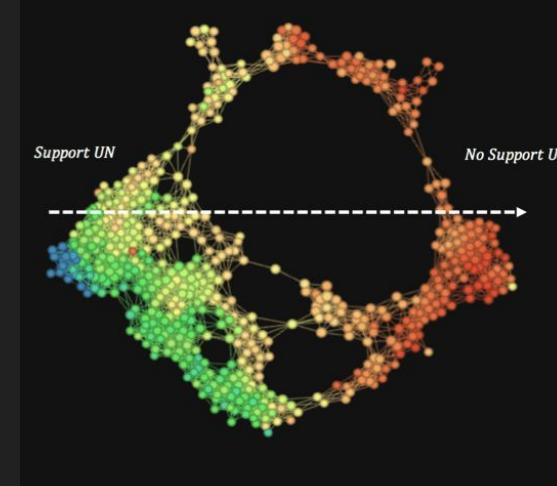
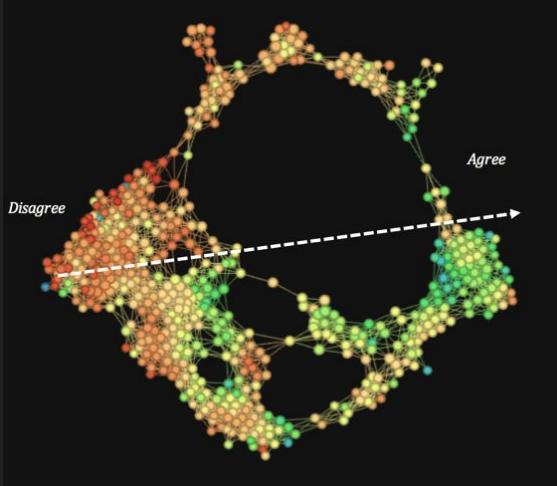
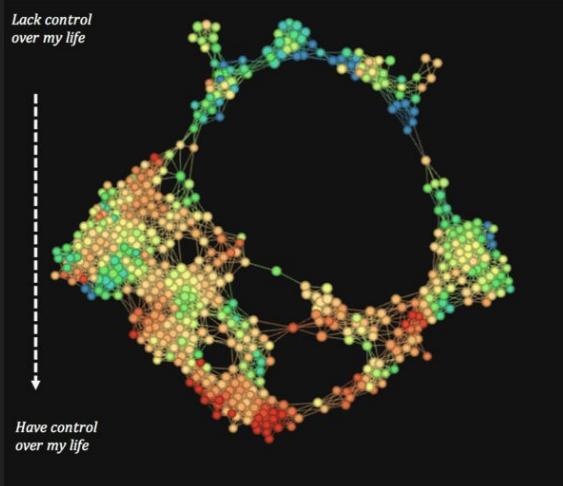
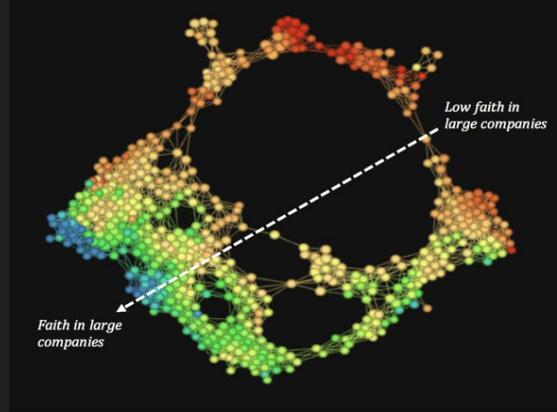
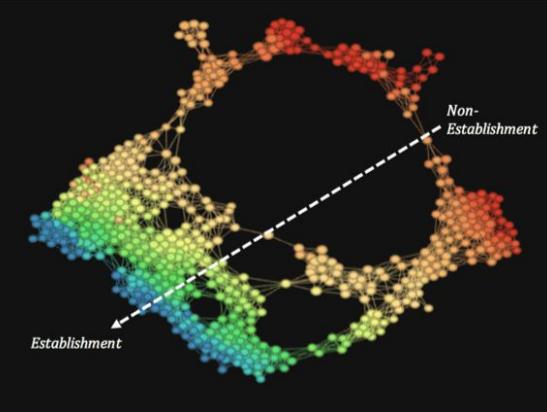
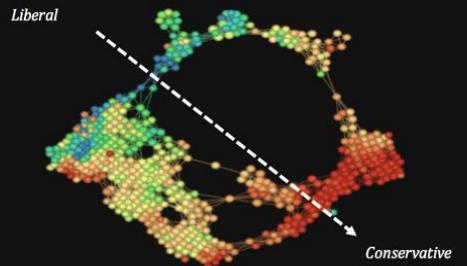
**B**

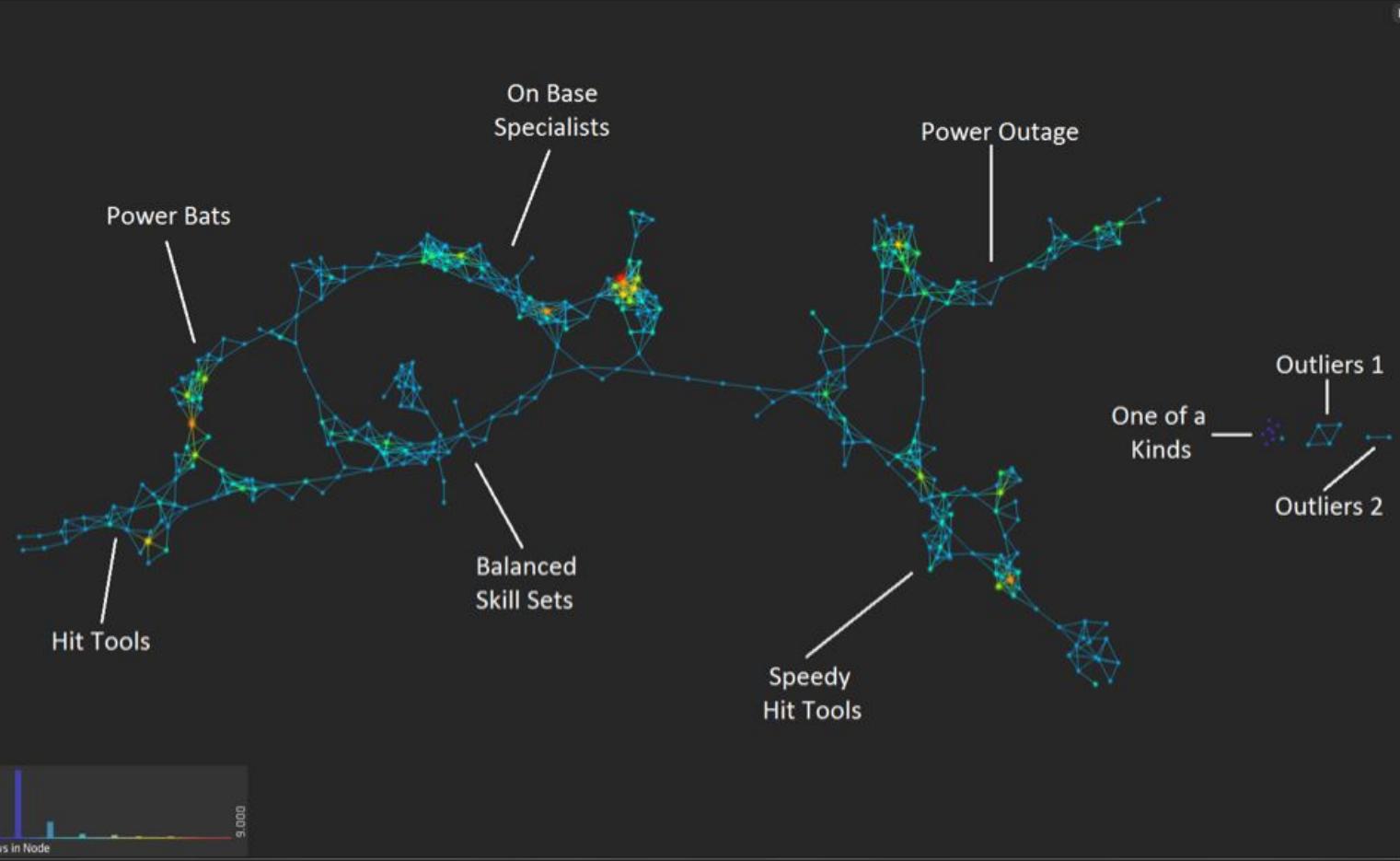
**Nodes** are groups of similar data points

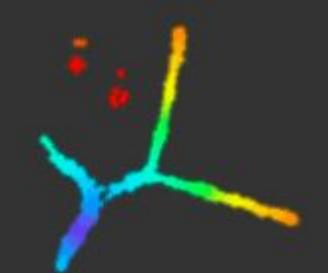
**Edges** connect similar nodes

**Colors** let you see values of interest

**Position** of a node on the screen doesn't matter

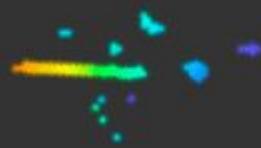






Breast invasive carcinoma

Kidney renal clear cell carcinoma



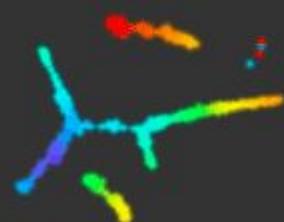
Cervical squamous cell carcinoma  
and endocervical adenocarcinoma



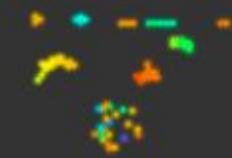
Bladder Urothelial Carcinoma



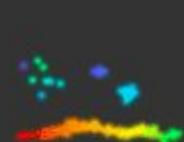
Lung squamous cell carcinoma



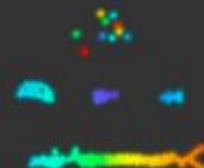
Ovarian serous cystadenocarcinoma



Uterine Corpus  
Endometrioid Carcinoma



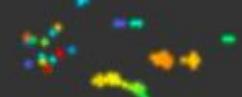
Colon adenocarcinoma



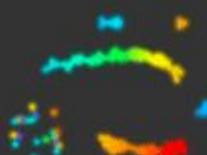
Glioblastoma multiforme



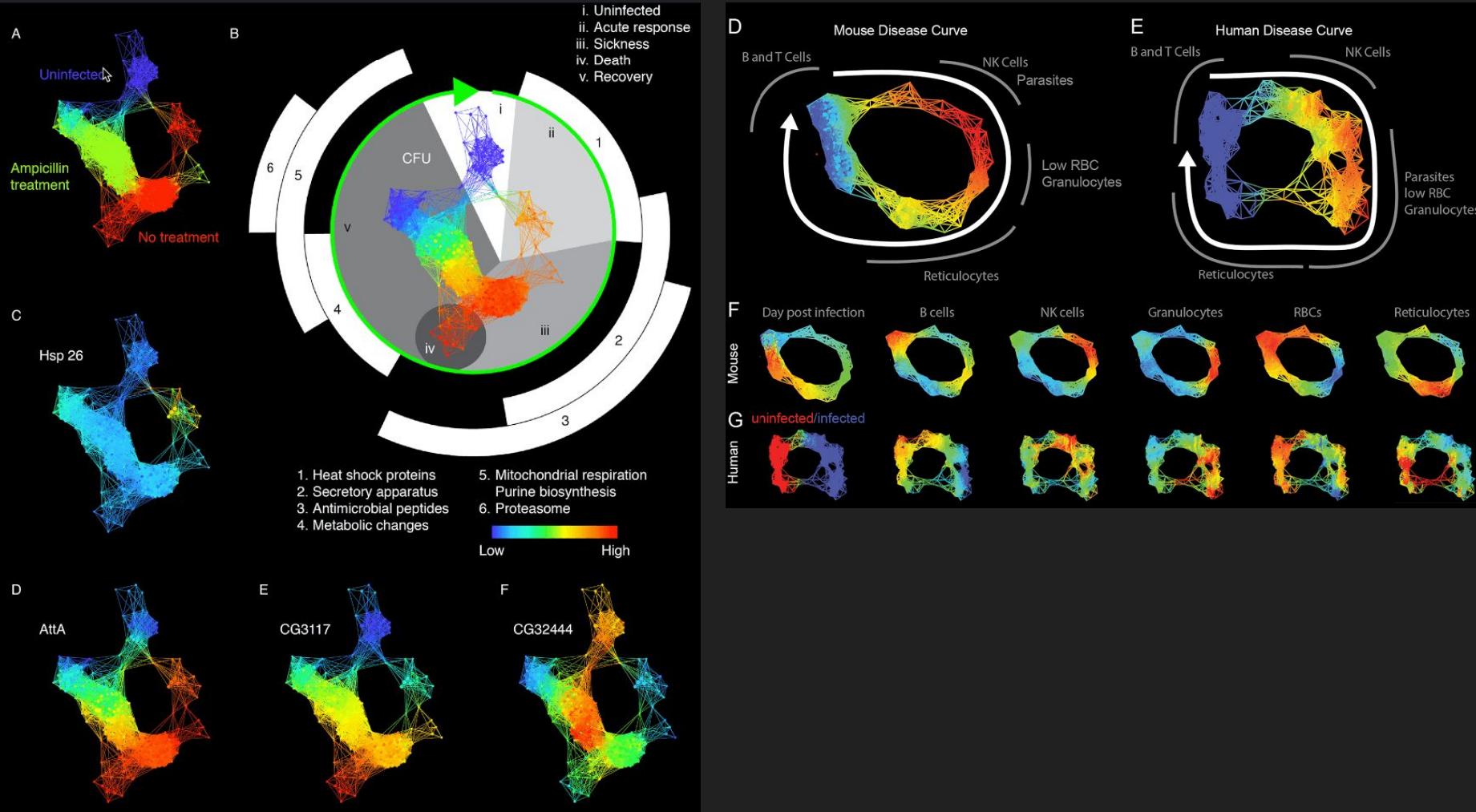
Prostate adenocarcinoma



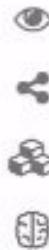
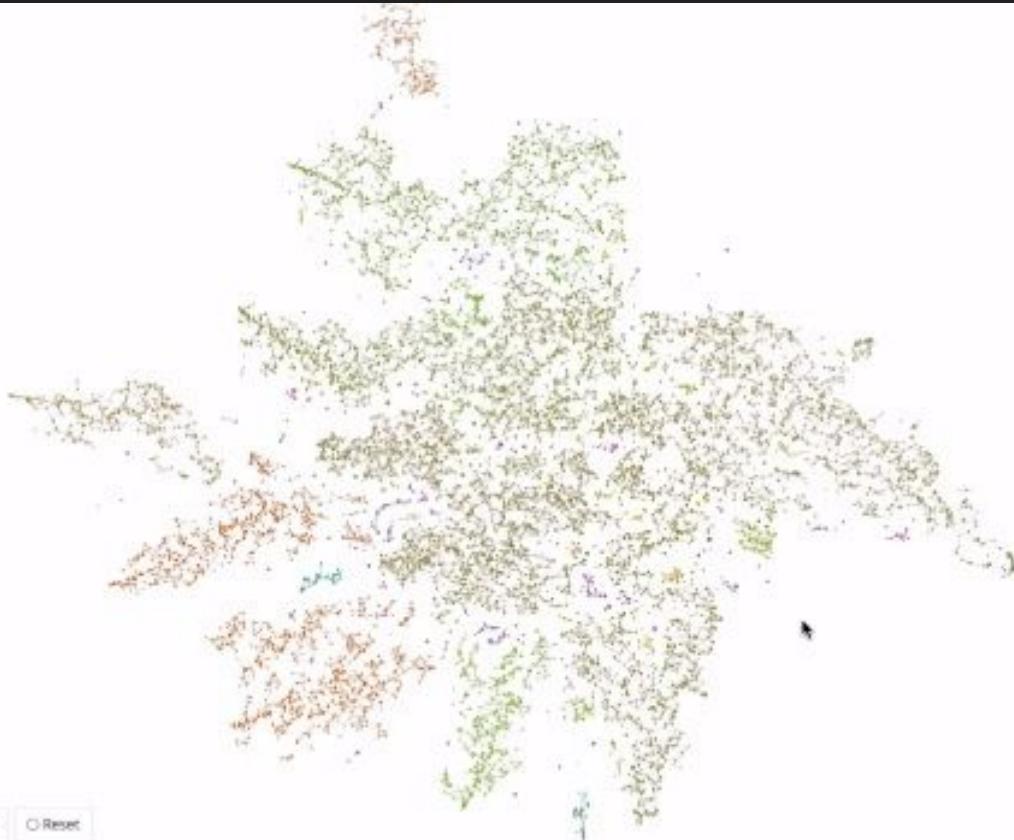
Rectum adenocarcinoma



Acute Myeloid Leukemia



## DATAREFINER

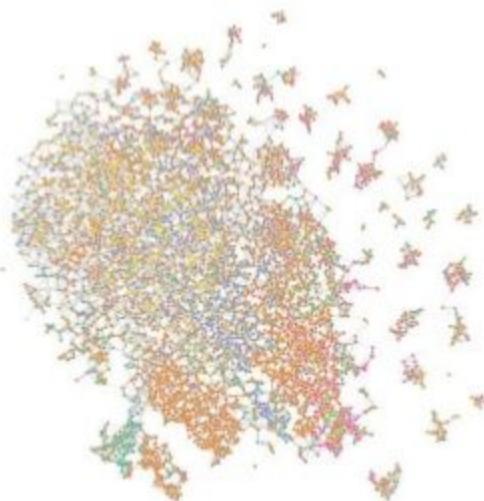


Drag    Select    Unselect    Reset

# Case study: Yelp Dataset Challenge

Result comparison: TDA with other techniques

Topological Data Analysis  
(275 sec)



PCA  
(0.19 sec)



Spectral  
Embedding  
(806 sec)



Modified LLE  
(1206 sec)



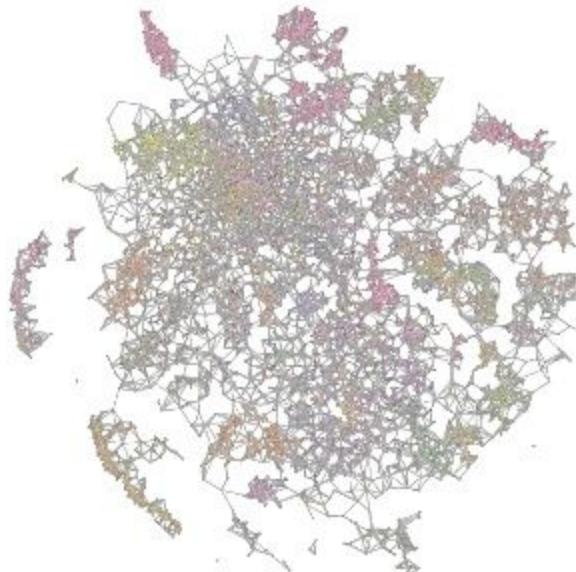
LLE  
(366 sec)



# Case study: Netflix competition

Result comparison: TDA with other techniques

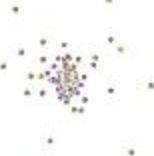
Topological Data Analysis



LLE



LTSA



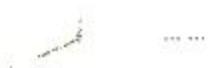
PCA



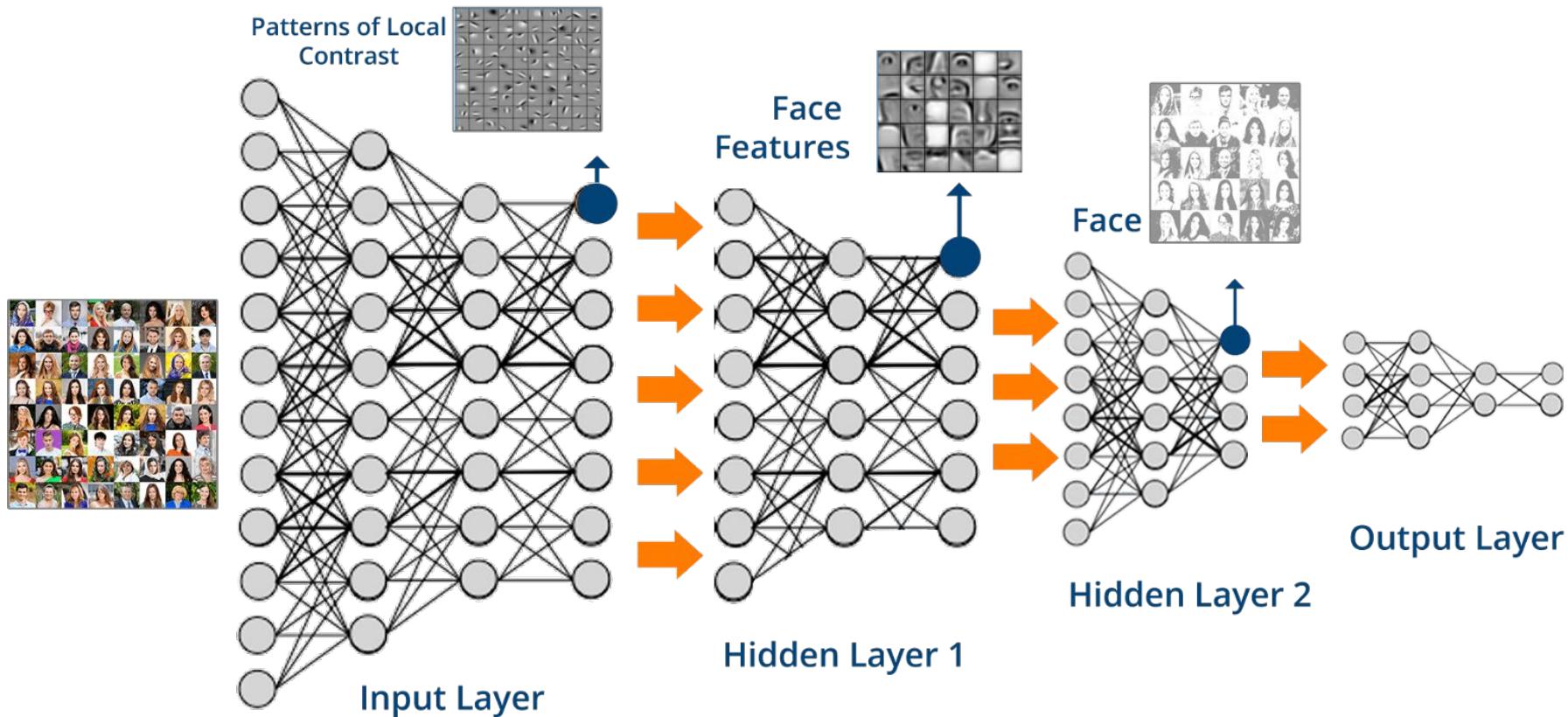
Hessian LLE



Spectral Embedding



# Convolutional Neural Networks





# Convolution

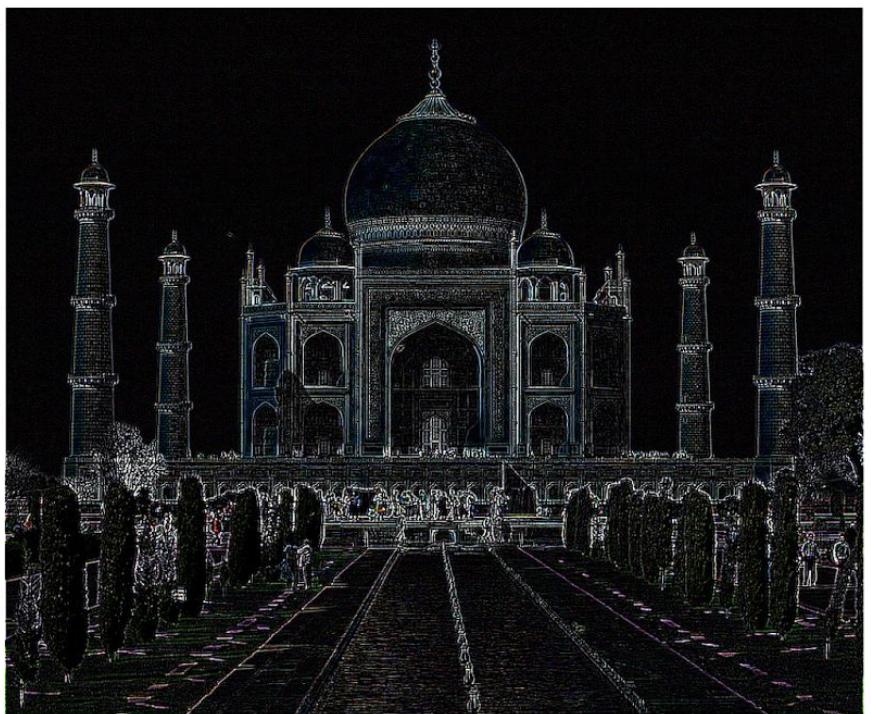
35	40	41	45	50
40	40	42	46	52
42	46	50	55	55
48	52	56	58	60
56	60	65	70	75



0	1	0		
0	0	0		
0	0	0		




0	0	0	0	0	0	0
0	0	0	0	0	0	0
0	0	-2	-2	-2	0	0
0	0	-2	16	-2	0	0
0	0	-2	-2	-2	0	0
0	0	0	0	0	0	0
0	0	0	0	0	0	0



<i>Original</i>	<i>Gaussian Blur</i>	<i>Sharpen</i>	<i>Edge Detection</i>
$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$\frac{1}{16} \begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix}$	$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 5 & -1 \\ 0 & -1 & 0 \end{bmatrix}$	$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$
			

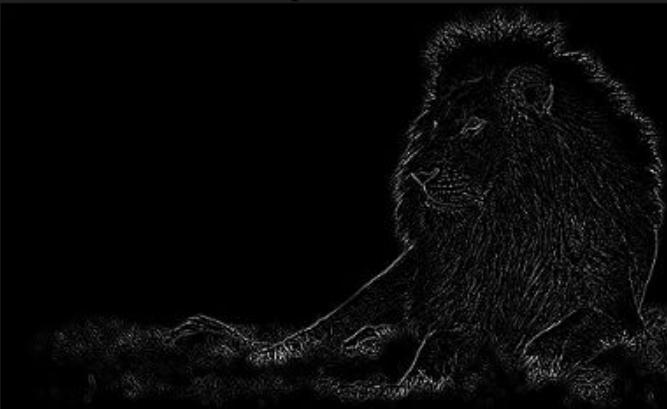
Original Image



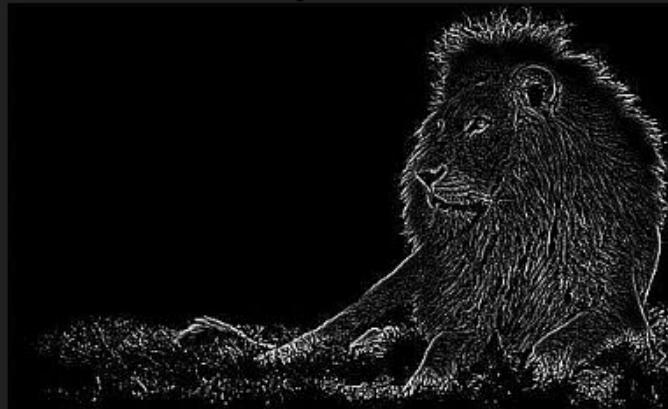
Edge Kernel 1



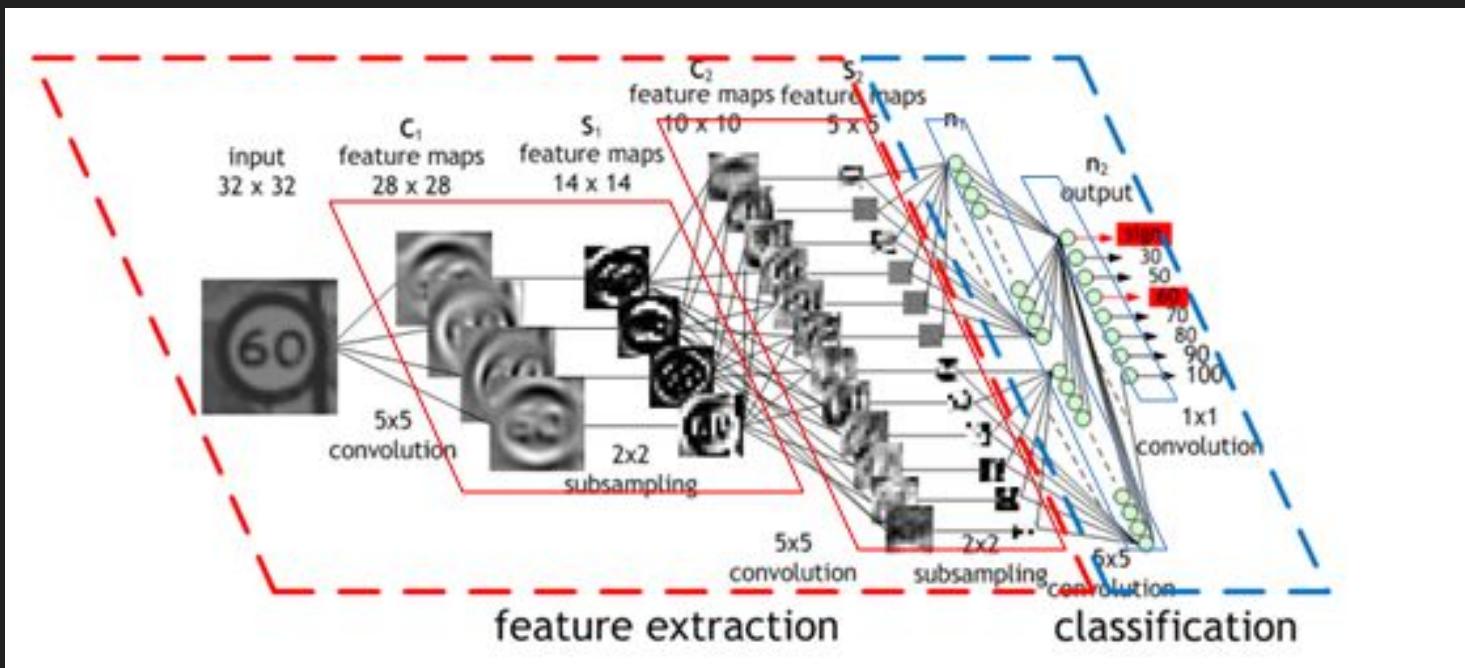
Edge Kernel 2



Edge Kernel 3



# Weights





0.19	0.8	0.7	0.34	0.23	0.11	0.01
0.05	0.18	0.47	0.09	0.45	0.27	0.07
0.09	0.23	0.78	0.17	0.34	0.22	0.12
0.17	0.2	0.09	0.21	0.67	0.99	0.54
0.21	0.09	0.17	0.45	0.43	0.78	0.35
0.01	0.17	0.41	0.67	0.44	0.29	0.19
0.02	0.21	0.27	0.56	0.22	0.33	0.05
0.01	0.04	0.36	0.55	0.31	0.04	0.02

1.3	0.91	2.4
0.88	4.7	0.67
0.62	0.06	0.01

0.77	0.98	0.01
0.78	1.7	0.45
0.45	0.32	0.12

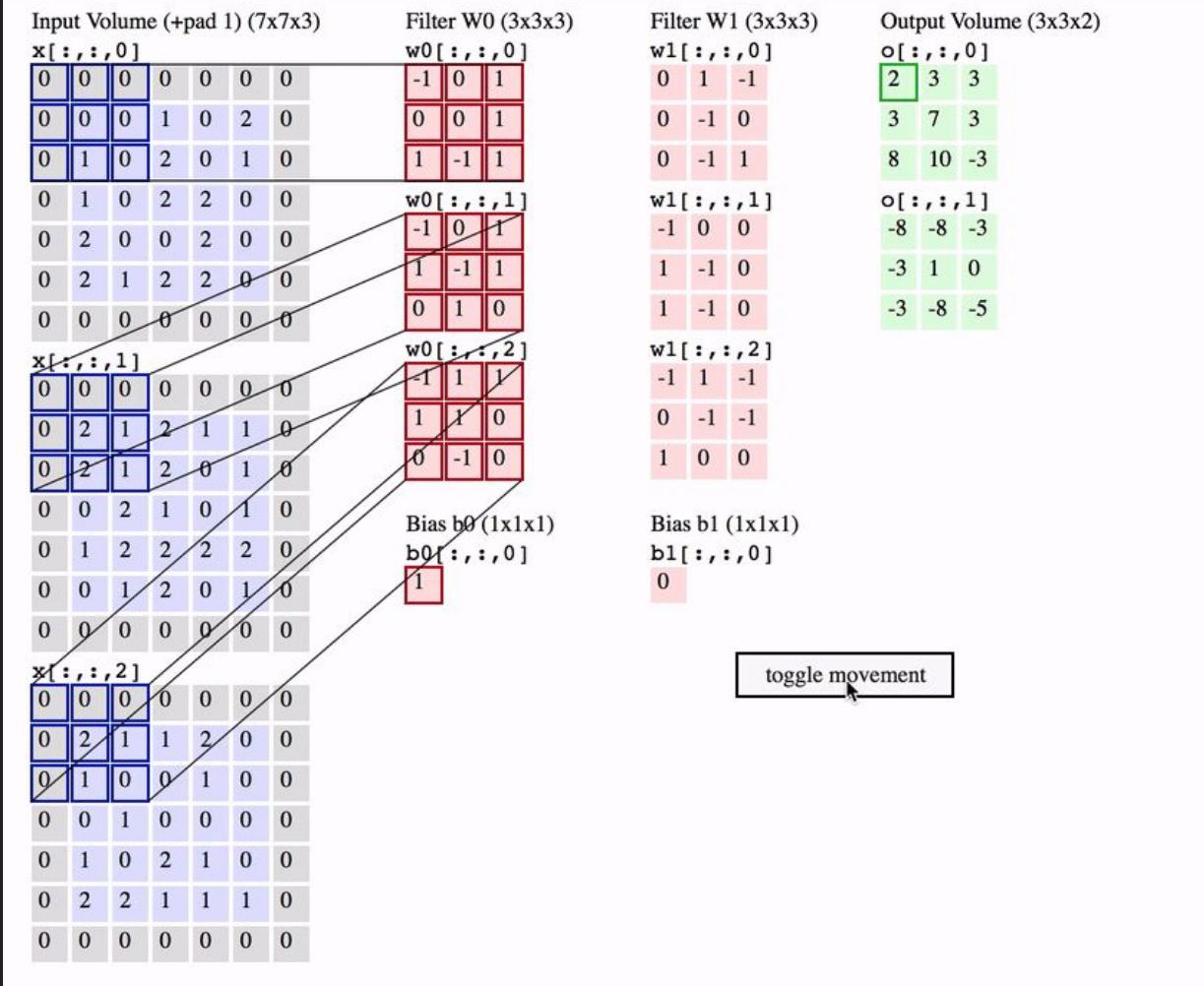
3.3	2.7
4.1	1.3

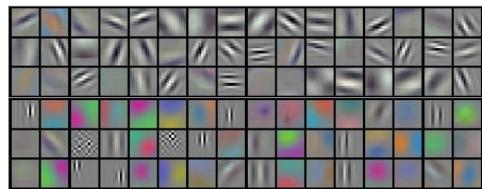
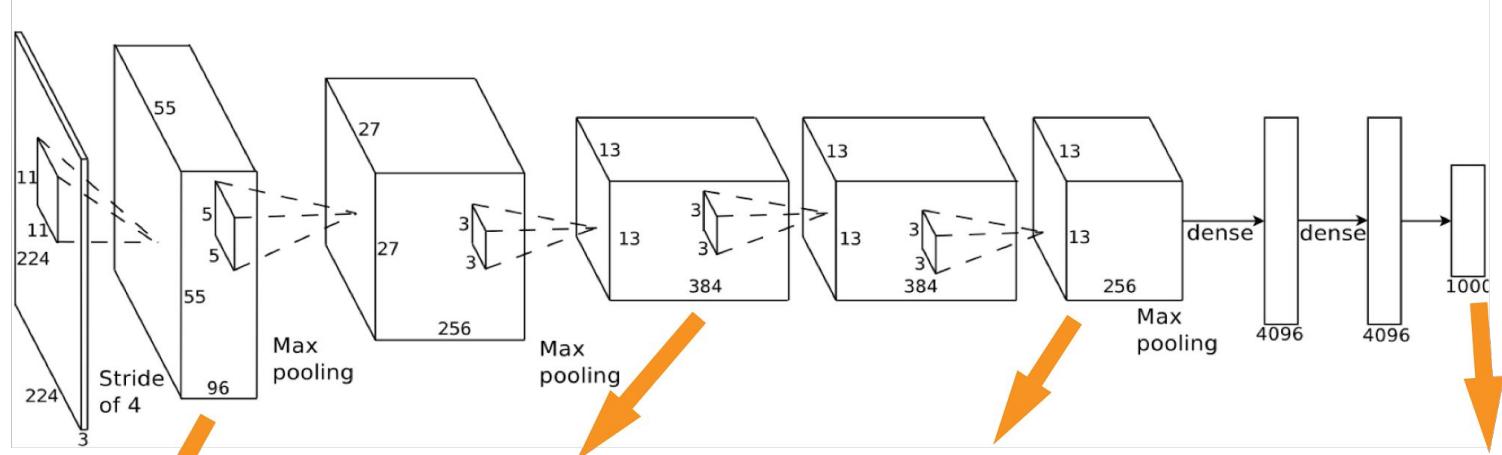
1.7	3.7
2.9	4.2

1.1	4.5
2.9	3.6

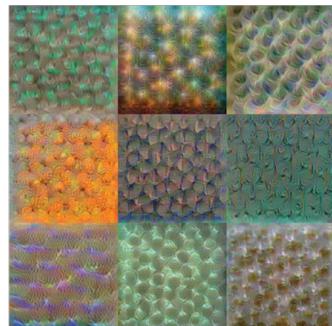
1.9	2.5
3.4	2.1

City  
Beach

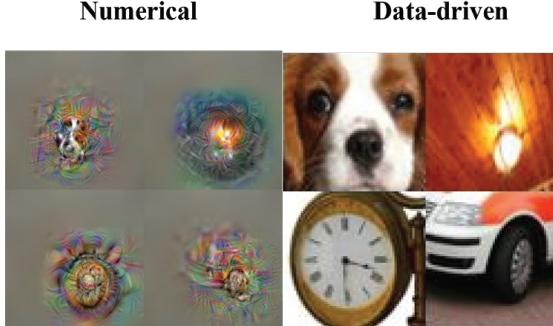




**Conv 1: Edge+Blob**



**Conv 3: Texture**



**Conv 5: Object Parts**



**Fc8: Object Classes**

clock

ship

dimming table

grocery store

Faces



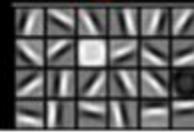
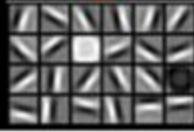
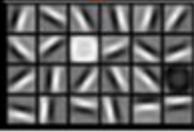
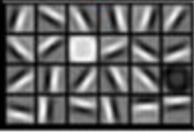
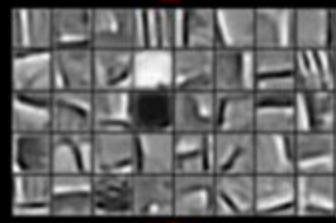
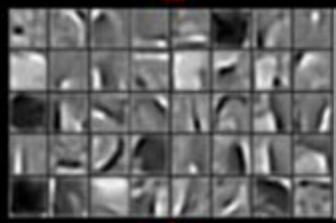
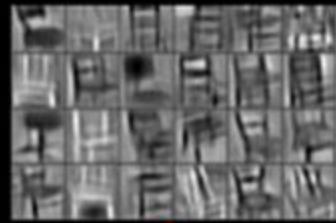
Cars



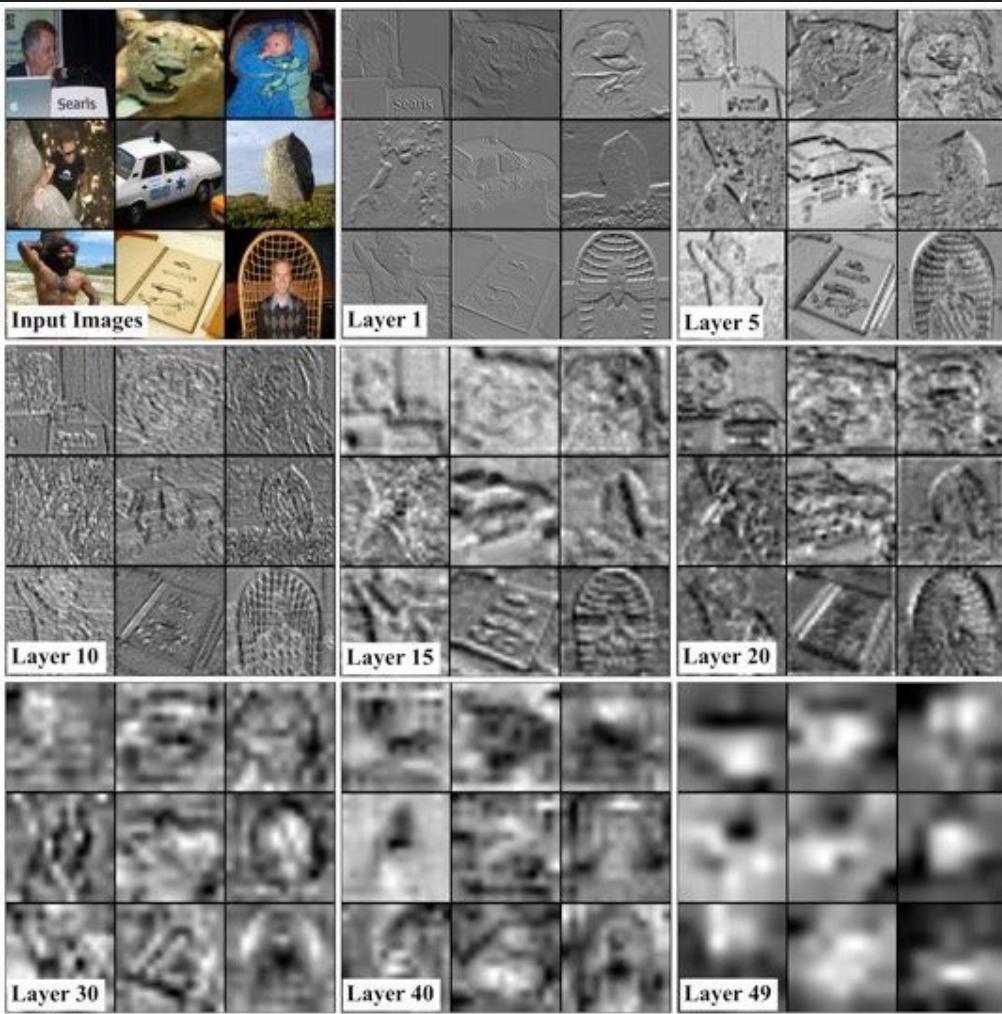
Elephants

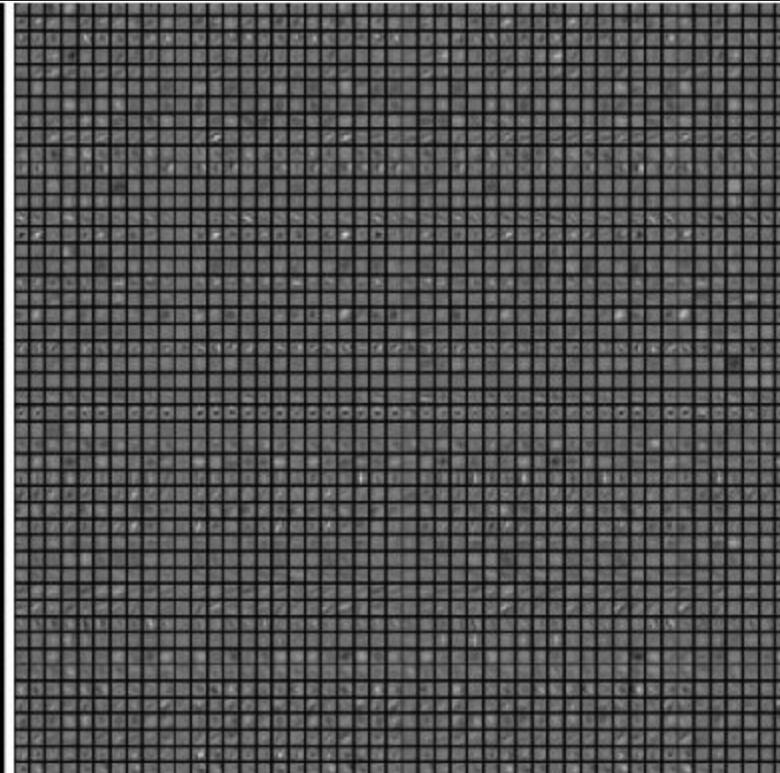
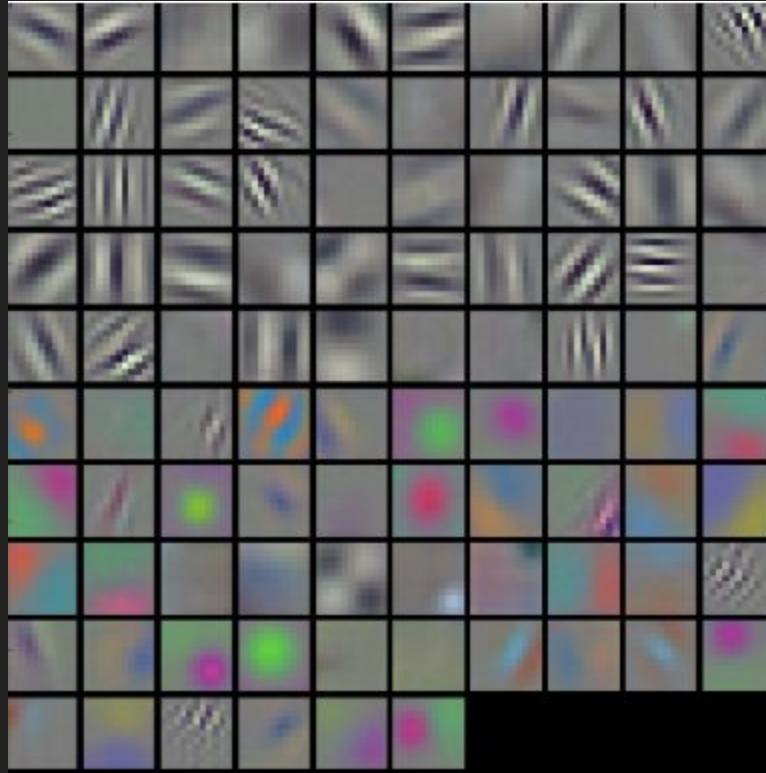


Chairs



# Problems







conv1/weights0 conv1/biases0 conv2/weights0 conv2/biases0 conv3/weights0 conv3/biases0 conv4/weights0 conv4/biases0 conv5/weights0 conv5/biases0 fc6/weights0 fc6/biases0 fc7/weights0 fc7/biases0 fc8/weights0 fc8/biases0

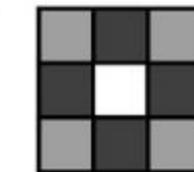
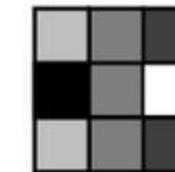
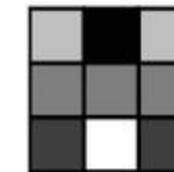
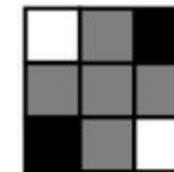
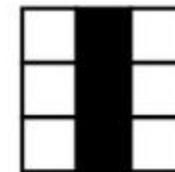
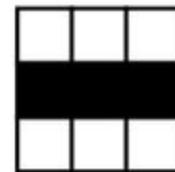
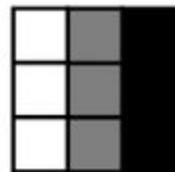
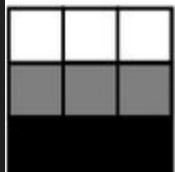
Loss: 2.1670868544

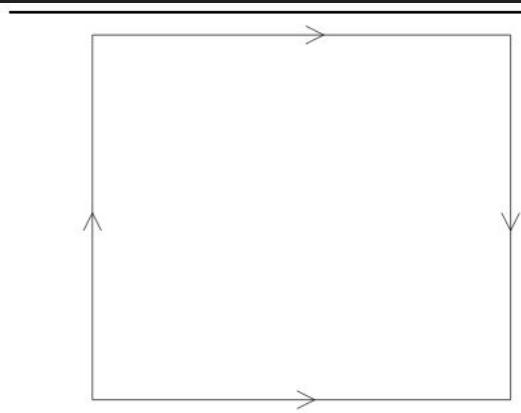
# TDA for CNN

# On the Local Behavior of Spaces of Natural Images

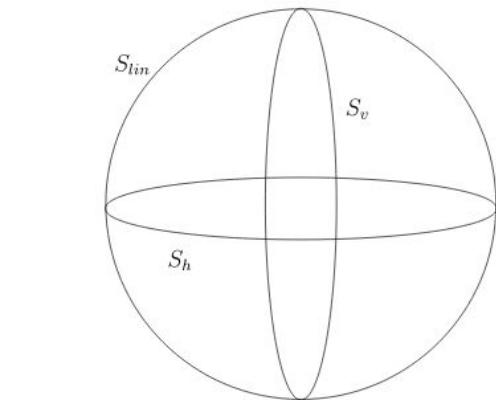
**Gunnar Carlsson · Tigran Ishkhanov · Vin de Silva ·  
Afra Zomorodian**

Received: 19 May 2006 / Accepted: 27 March 2007 / Published online: 30 June 2007  
© Springer Science+Business Media, LLC 2007

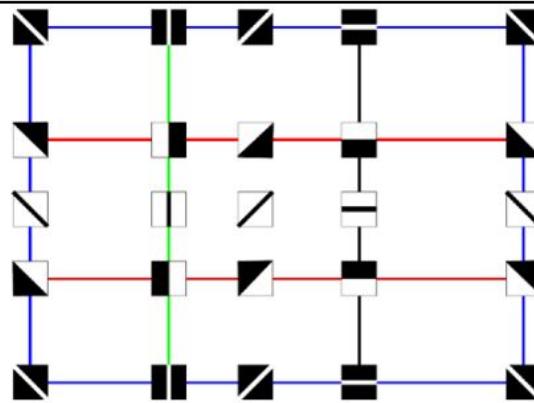




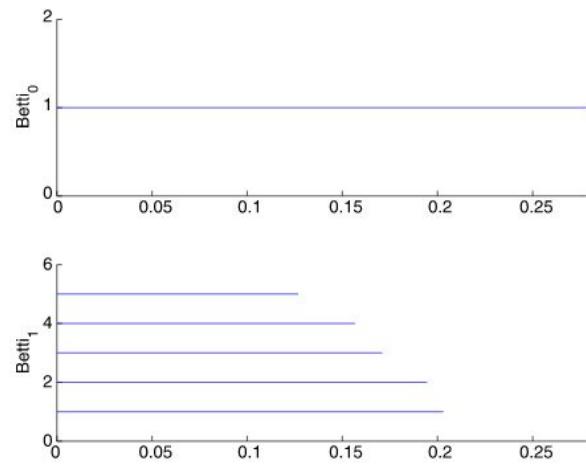
**Fig. 4** Klein bottle representation as a rectangle with opposite edges identified



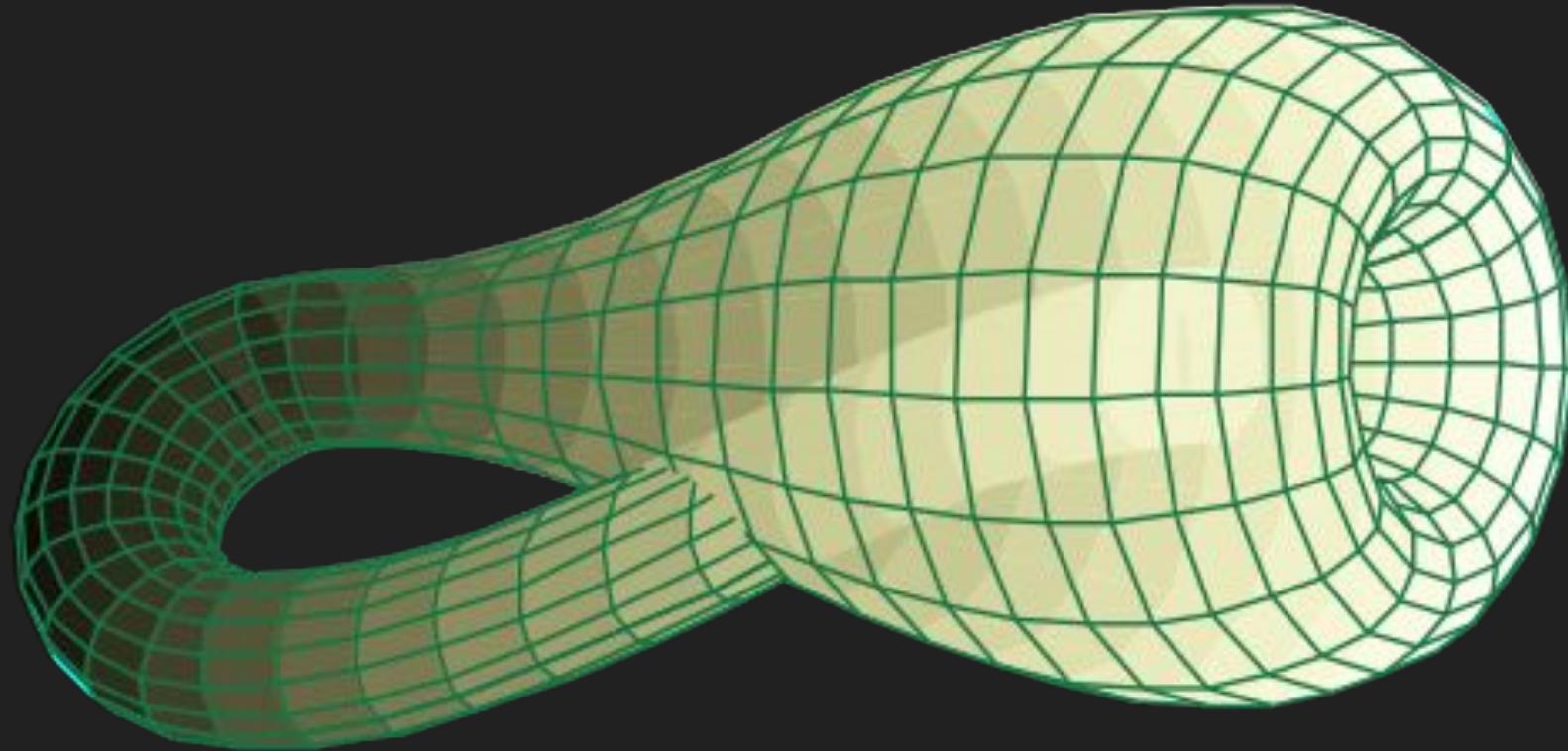
**Fig. 5** The ‘three circle’ space



**Fig. 6** 3 by 3 patches parametrized by the Klein bottle

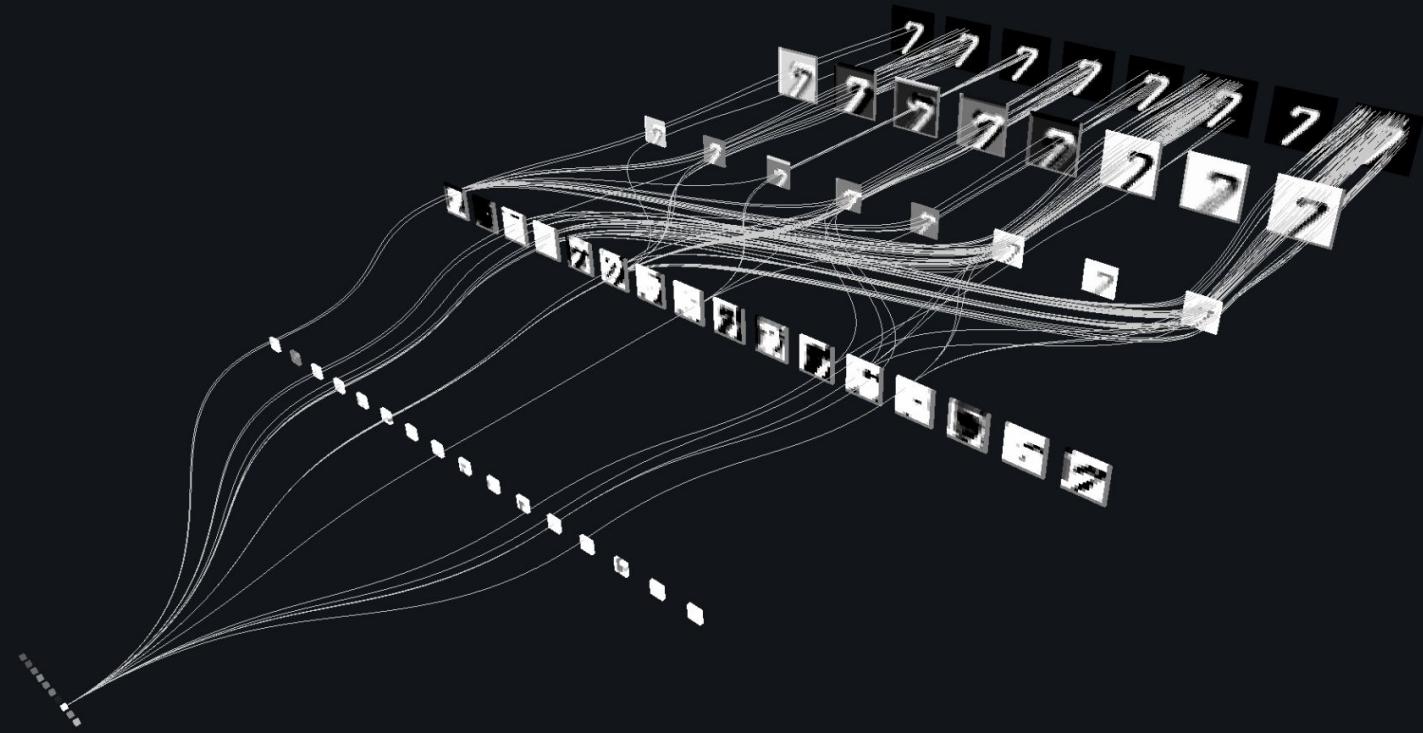


**Fig. 7** PLEX results for  $X(15, 30)$

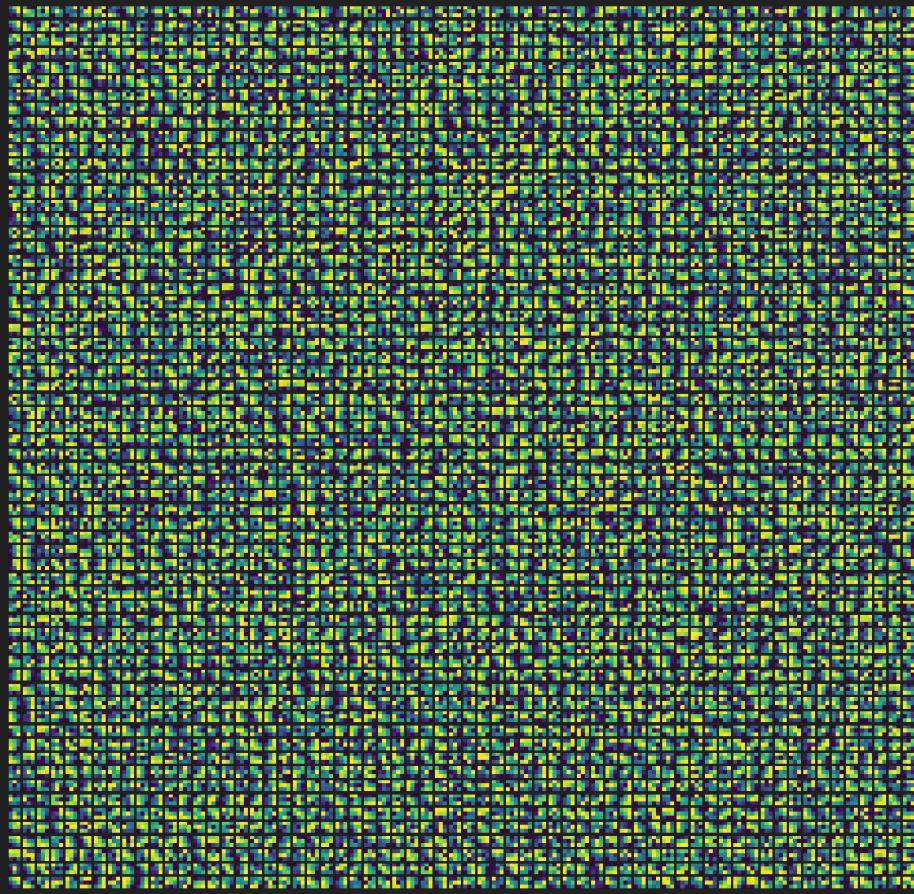


763403618197846730616523528784659374246192751139773948549394949405542  
2067899034081479349452474364649722091366491923892994406688686810698103  
151135674425812868256841432621857668652537552916359545729651641961014  
0412828746590263173755830290151711761620062610213418816890387032987925  
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193043778299315737764343277158928097180811289932221270002998174250647  
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915703643189262731004054777034572639488577859768036750224952736719369  
592483604341639093006328335684799377520826650098815600128335379117119970  
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675071053714190432053882135608771592290089638005748519668518320293503  
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1127313626112246536615624967024124517851689113358702930791093486205447  
264878524312110203148274990624936919137421758134673872833106648116548

The diagram illustrates a neural network architecture for image classification. It starts with an **Input Image** of size  $28 \times 28$ , which is processed by a **Convolutional Layer** with **Kernels** numbered 1 through 5. This layer produces **Five Images of Size  $14 \times 14$** . These images are then flattened into a **Vector of Size 980**, which is passed through an **Activation Layer** (ReLU). The resulting vector is then processed by two **Fully Connected** layers, each with **FC weights** and a **ReLU** activation. The final output is a **Vector of Size 10**, which is passed through an **Activation Layer** (ReLU) and an **arg max** operation to produce the **Output Label**. The **Client Output** is the final result.



0  
50419213143536172869409112432738  
69056076187939859330749809414460  
45670017163021178026783904674680  
78315717116302931104920020271864  
163439\33854)7428586734619960372  
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87413110239492168417449287244219  
72876922381651102645831519274448  
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1610301182039405061778(920512273  
54971839403112635768395857411317  
55525870977509008924816165183405  
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40659309347129426189066799801446  
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79237324162755740263640426000031  
62231415461728792051428324154607  
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86168940904159753749858638699183  
58659725087110918670930889678475  
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51415517364325644044672433800322  
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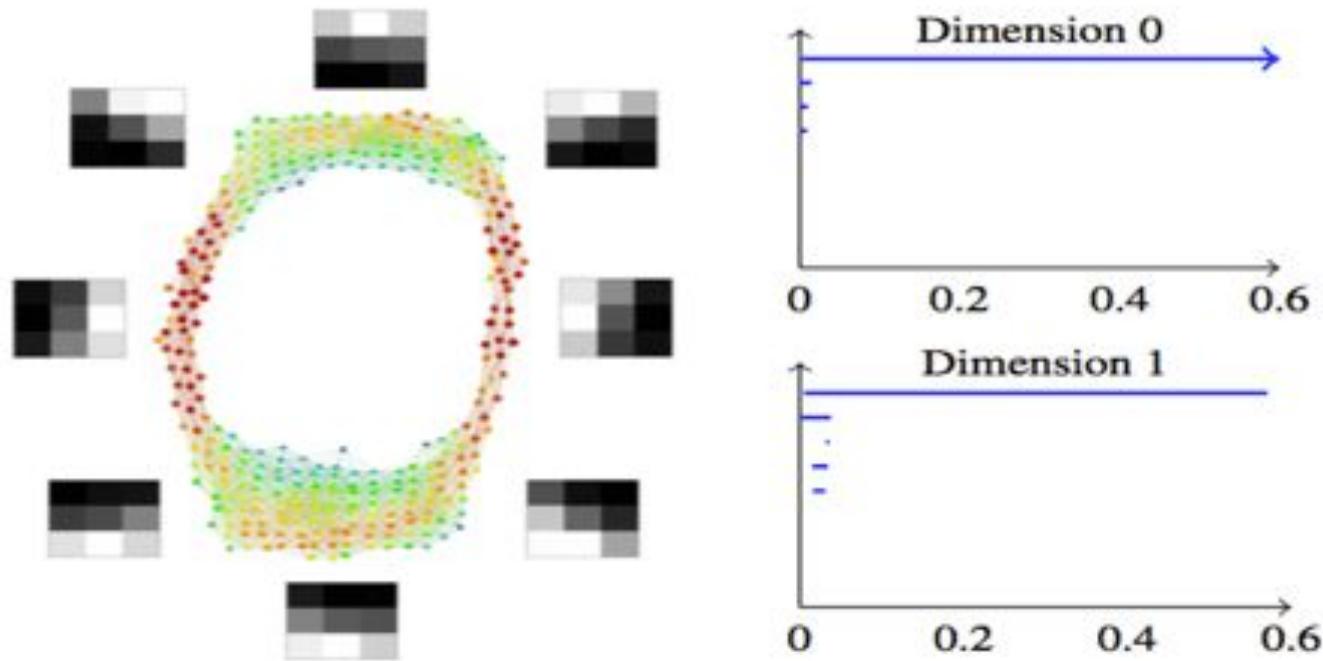
# Using Topological Data Analysis to Understand the Behavior of Convolutional Neural Networks

By [Gunnar Carlsson](#)

June 21, 2018

[ARTIFICIAL INTELLIGENCE](#), [MACHINE INTELLIGENCE](#), [MACHINE LEARNING](#), [TOPOLOGY](#)

TLDR: Neural Networks are powerful but complex and opaque tools. Using [Topological Data Analysis](#), we can describe the functioning and learning of a convolutional neural network in a compact and understandable way. The implications of the findings are profound and will accelerate the development of a wide range of applications from self-driving cars and drones to complying with things like GDPR.

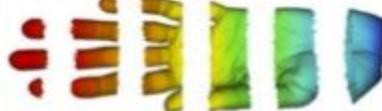


# MAPPER IV

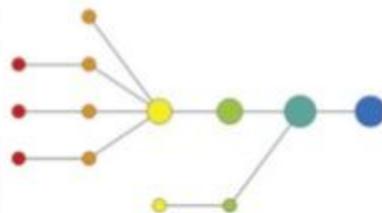
B Coloring by filter value



C Binning by filter value



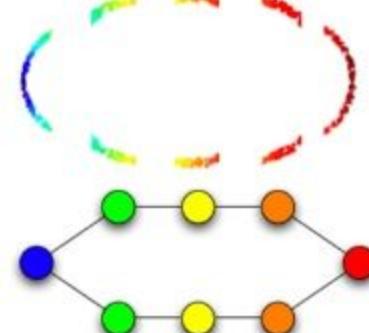
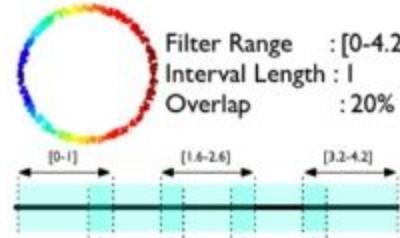
D Clustering and network construction



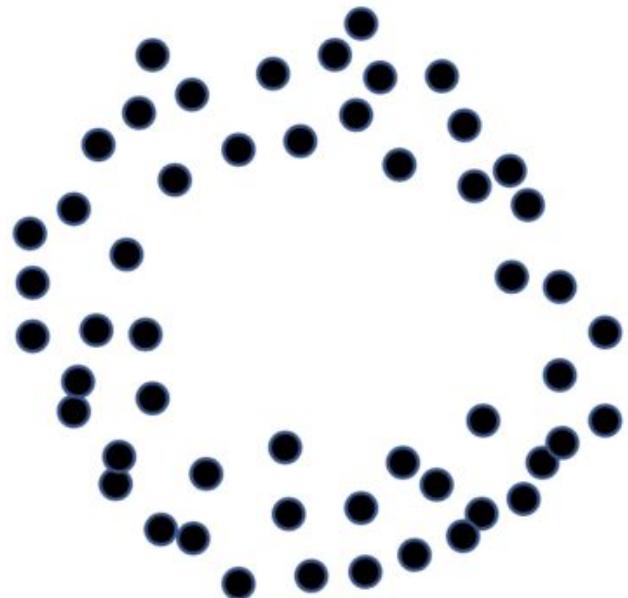
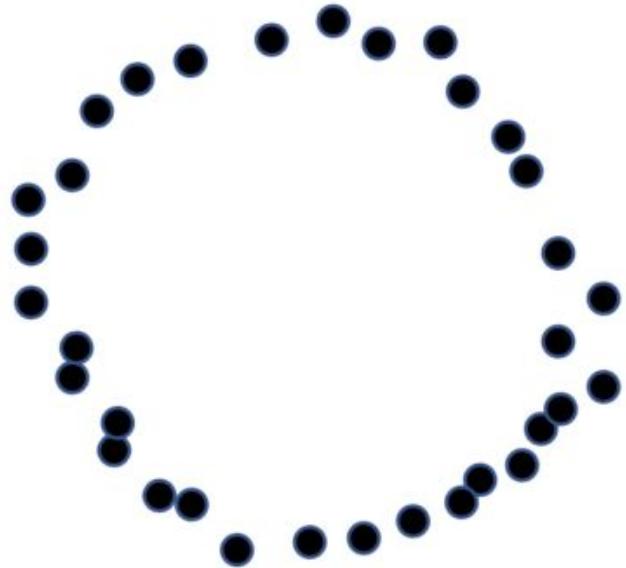
Filter Range : [0-4.2]

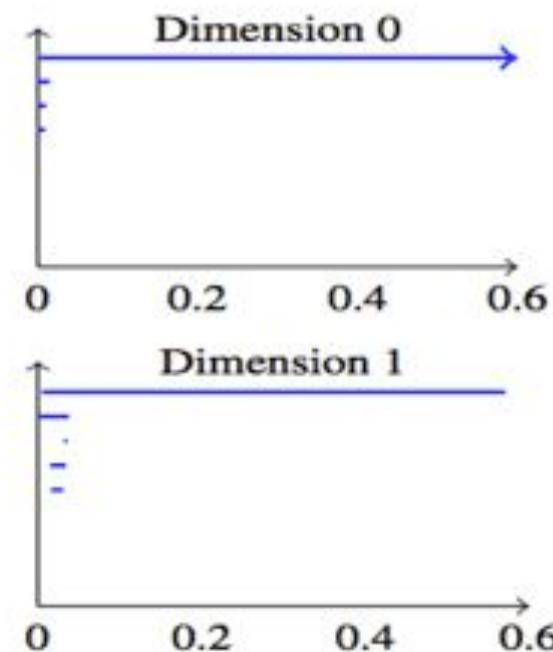
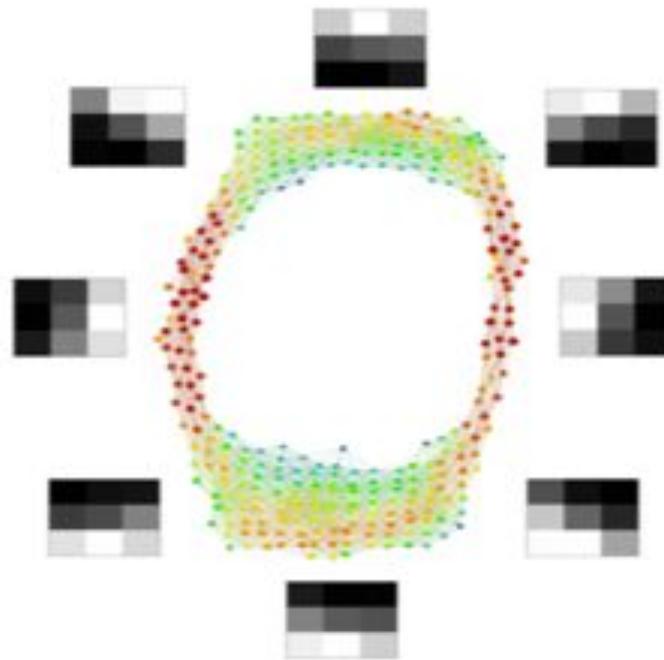
Interval Length : 1

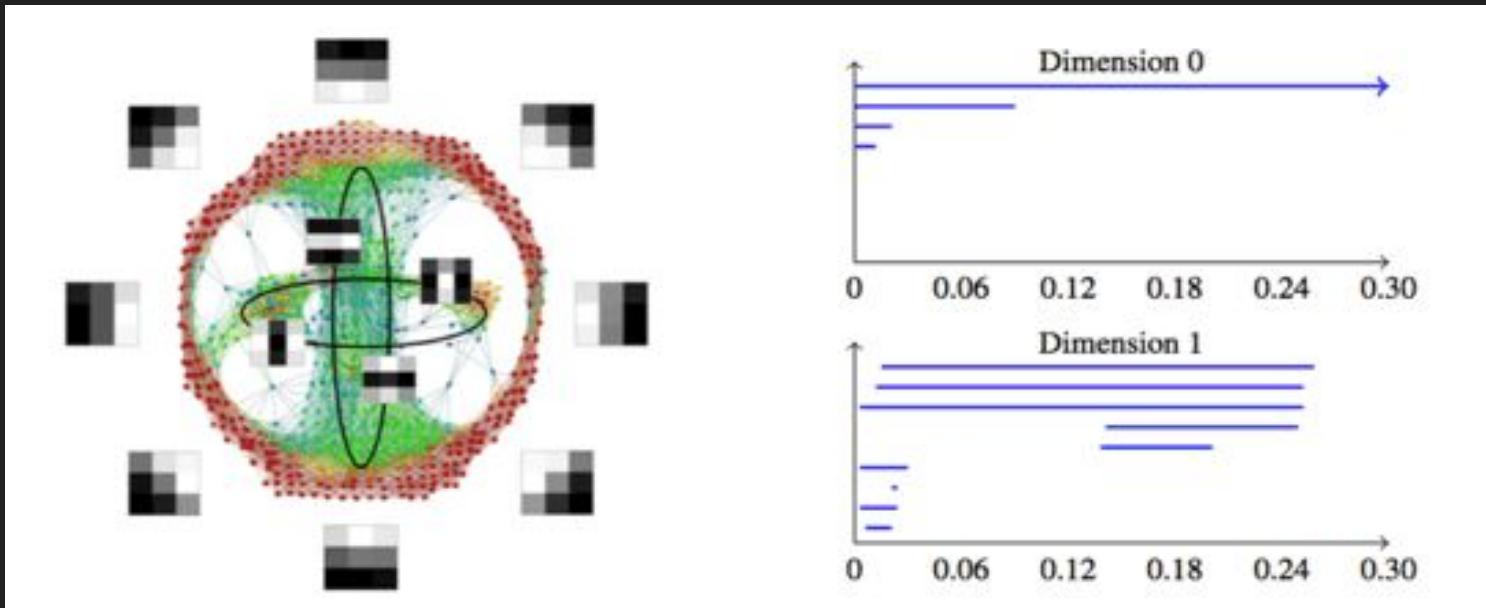
Overlap : 20%

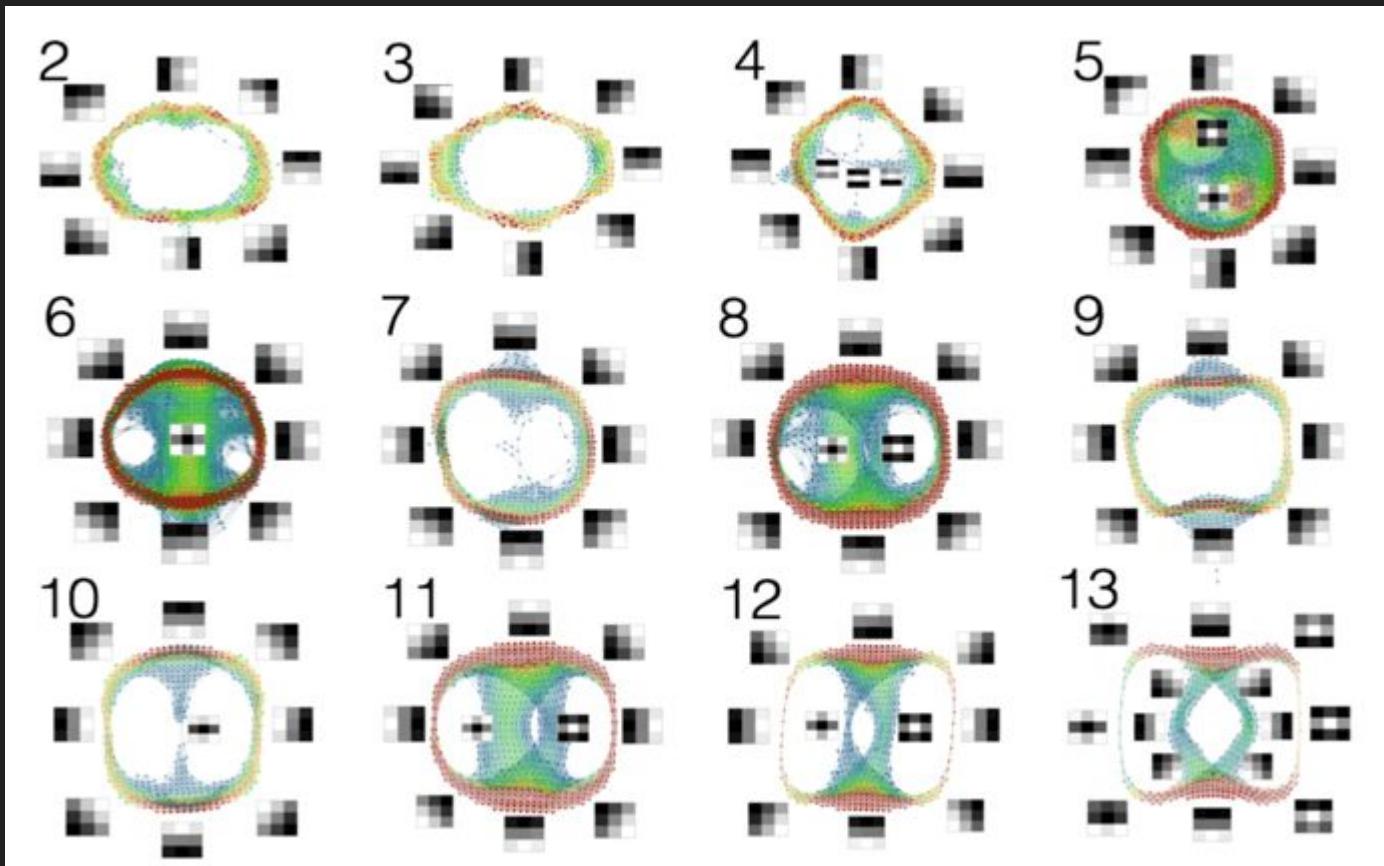


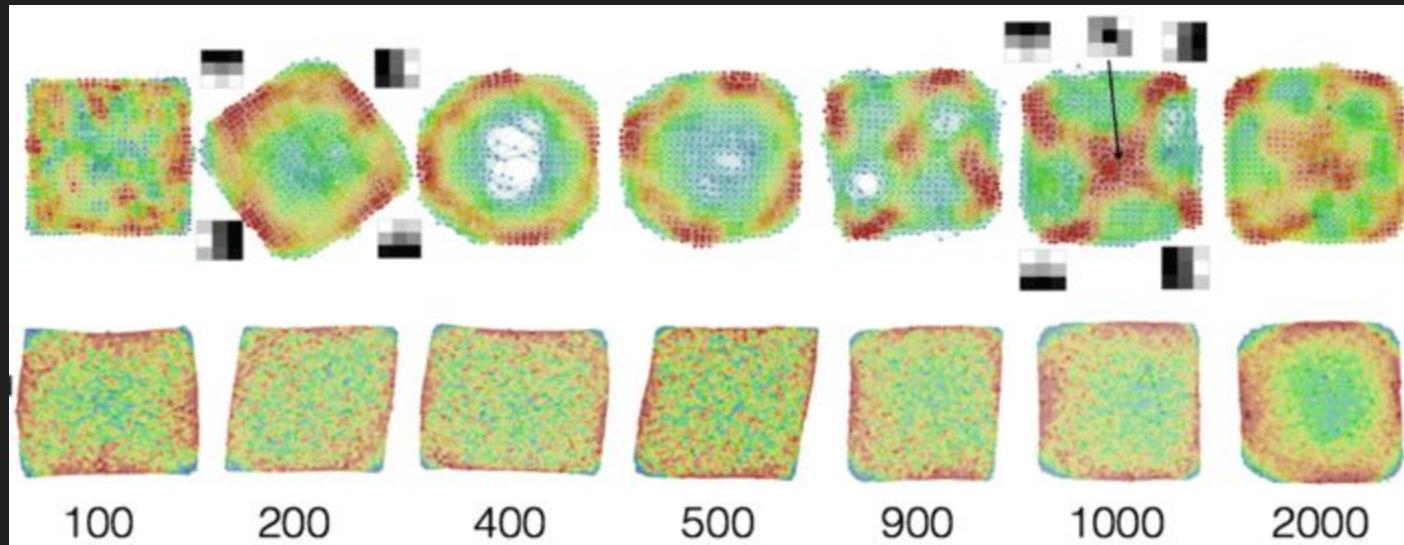












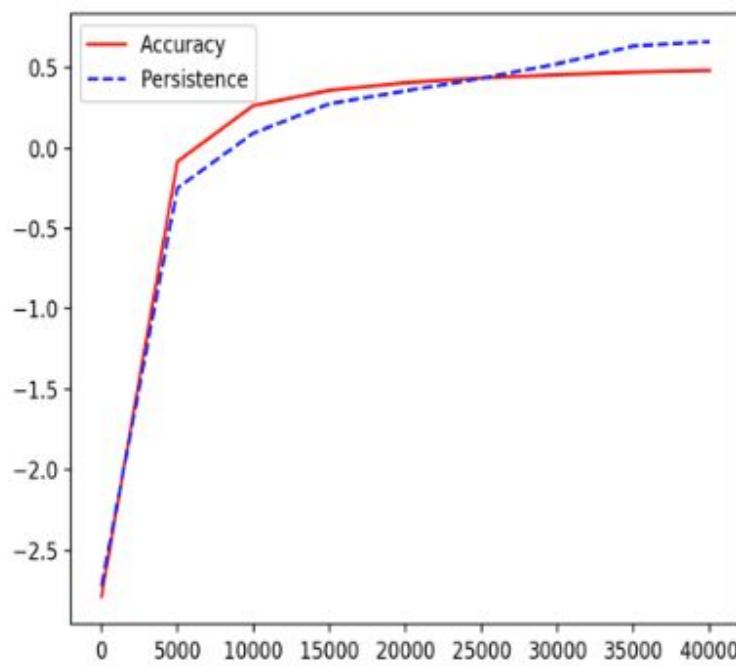
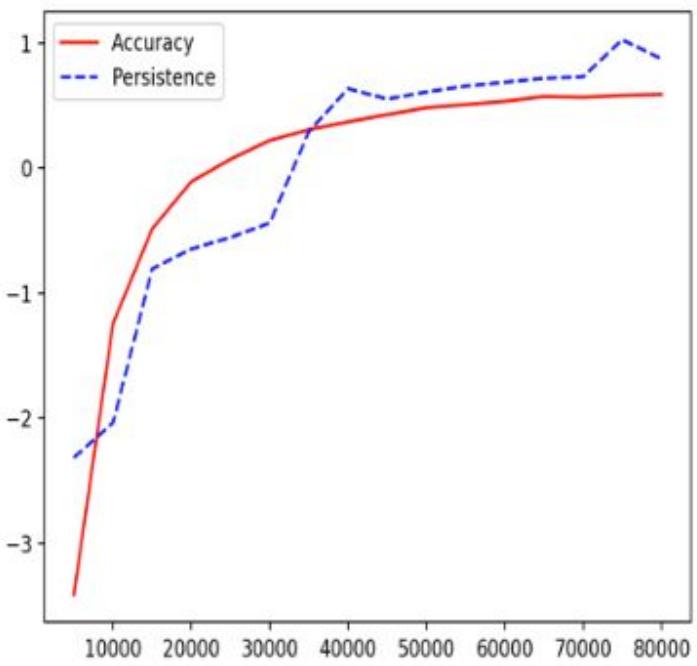
# Going Deeper: Understanding How Convolutional Neural Networks Learn Using TDA

By [Gunnar Carlsson](#)

August 9, 2018

[ARTIFICIAL INTELLIGENCE](#), [MACHINE INTELLIGENCE](#), [MACHINE LEARNING](#), [TOPOLOGY](#)

In my earlier [post](#) I discussed how performing [topological data analysis](#) on the weights learned by convolutional neural nets (CNN's) can give insight into what is being learned and how it is being learned.



# Mathematical Acceleration: Incorporating Prior Information to Make Neural Nets Learn 3.5X Faster

By [Gunnar Carlsson](#)

August 30, 2018

**ARTIFICIAL INTELLIGENCE, MACHINE LEARNING, TOPOLOGY**

Validation Accuracy	# Batch iterations Boosted	# Batch iterations standard
.8	187	293
.9	378	731
.95	1046	2052
.96	1499	2974
.97	2398	4528
.98	5516	8802
.985	9584	16722

Validation Accuracy	# Batch iterations Boosted	# Batch iterations standard
.25	303	1148
.5	745	2464
.75	1655	5866
.8	2534	8727
.83	4782	13067
.84	6312	15624
.85	8426	21009

Thank you !

**PLEASE STAND BY**

?

Weapon of choice

# ગુઢી GUDHI Geometry Understanding in Higher Dimensions

The GUDHI library is a generic open source [C++ library](#), with a [Python interface](#), for Topological Data Analysis (TDA) and Higher Dimensional Geometry Understanding. The library offers state-of-the-art data structures and algorithms to construct simplicial complexes and compute persistent homology.

The library comes with data sets, demos, examples and test suites.

The GUDHI library is developed as part of the [GUDHI project](#) supported by the [European Research Council](#).

## NEW RELEASE

### GUDHI version 2.2.0

As a major new feature, the GUDHI library now offers a Čech complex module, a sparse version of the Rips complex and a utility to build the Rips complex from a correlation matrix (no Python interface yet).

## More Articles

---

New release · [GUDHI version 2.1.0 Debian package](#)

---

New release · [GUDHI version 2.1.0](#)

---

New release · [GUDHI version 2.0.1](#)

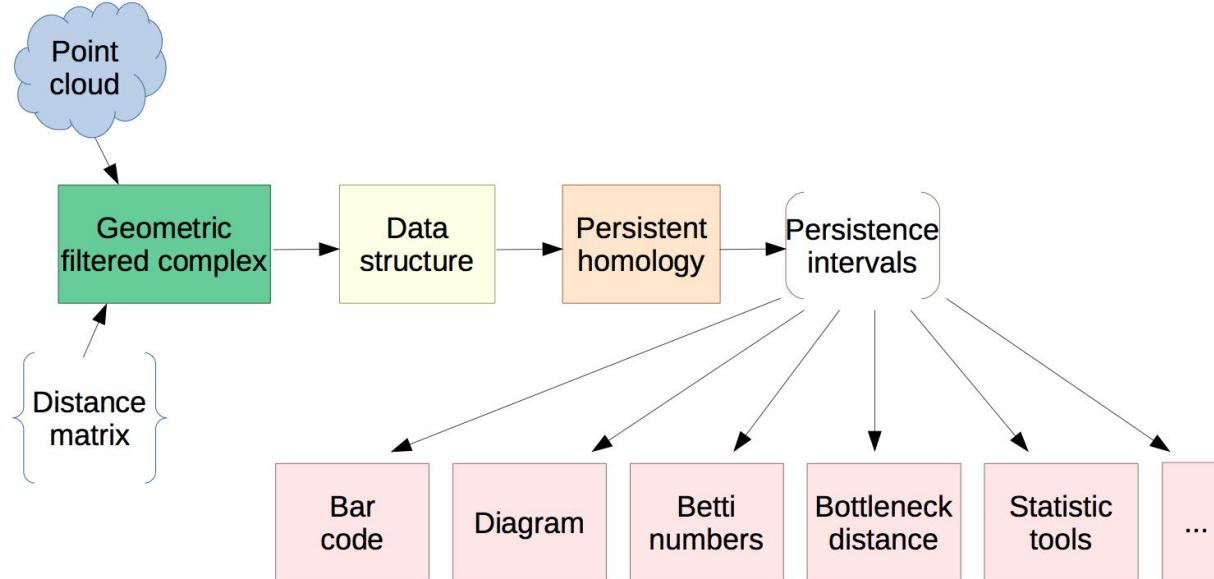
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[More ›](#)

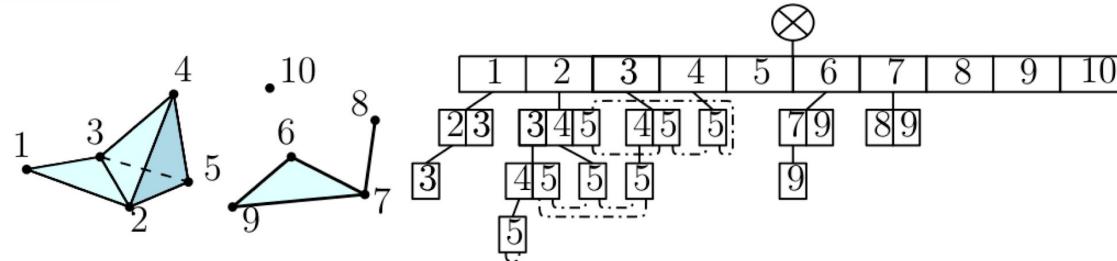
# ગુઢી GUDHI

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informatics for mathematics

Geometric Understanding in Higher Dimensions



## Filtered simplicial complexes – Simplex tree



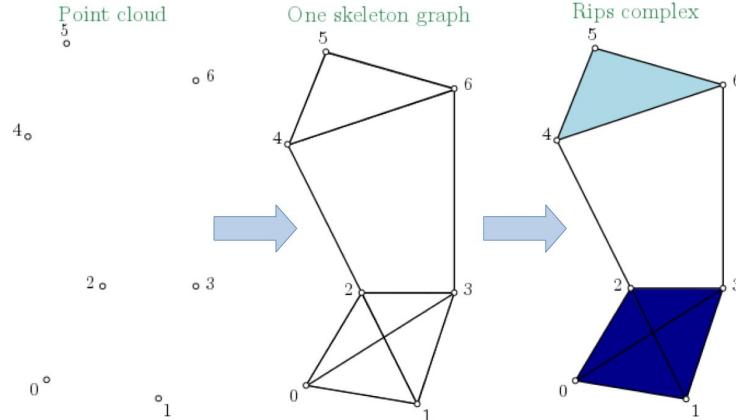
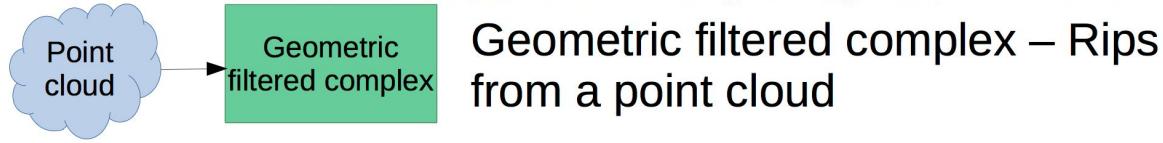
- Memory and time-efficient data structure to store simplicial complexes.
- Every simplex is a word stored in the tree.
- The nodes corresponding to simplices of the same dimension having the same maximal vertex are stored in a cyclic list.
- It is a base of all algorithms to compute persistence of weighted simplicial complexes in GUDHI.

by Clément Maria



inria  
informatics for mathematics

Geometric Understanding in Higher Dimensions



by Clément Maria

# mapper 0.1.17



Latest version

pip install mapper



Last released: Apr 19, 2017

Python Mapper: an open source tool for exploration, analysis and visualization of data.

## Navigation

Project description

Release history

Download files

## Project links

Homepage

## Project description

See the project home page <http://danifold.net/mapper> for a detailed description and documentation.

This package features both a GUI and a Python package for custom scripts. The Python package itself works with Python 2 and 3. The GUI, however, depends on wxPython, which is available for Python 2 only. Therefore, the setup script will install the GUI only if it is executed by Python 2.

See also <https://pypi.python.org/pypi/cmappertools> for the companion package with fast C++ algorithms.

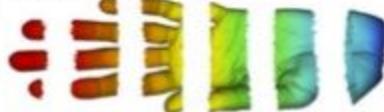
The authors of Python mapper are [Daniel Müllner](#) and [Aravindakshan Babu](#). (PyPI apparently suppresses everything but the first name in the “author” field, hence only one author is displayed below.)

# MAPPER IV

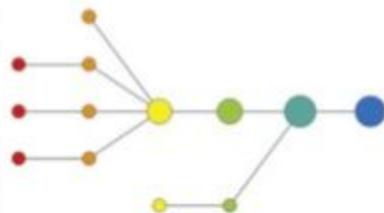
B Coloring by filter value



C Binning by filter value



D Clustering and network construction



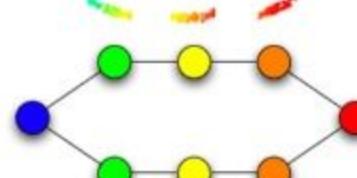
Filter Range : [0-4.2]

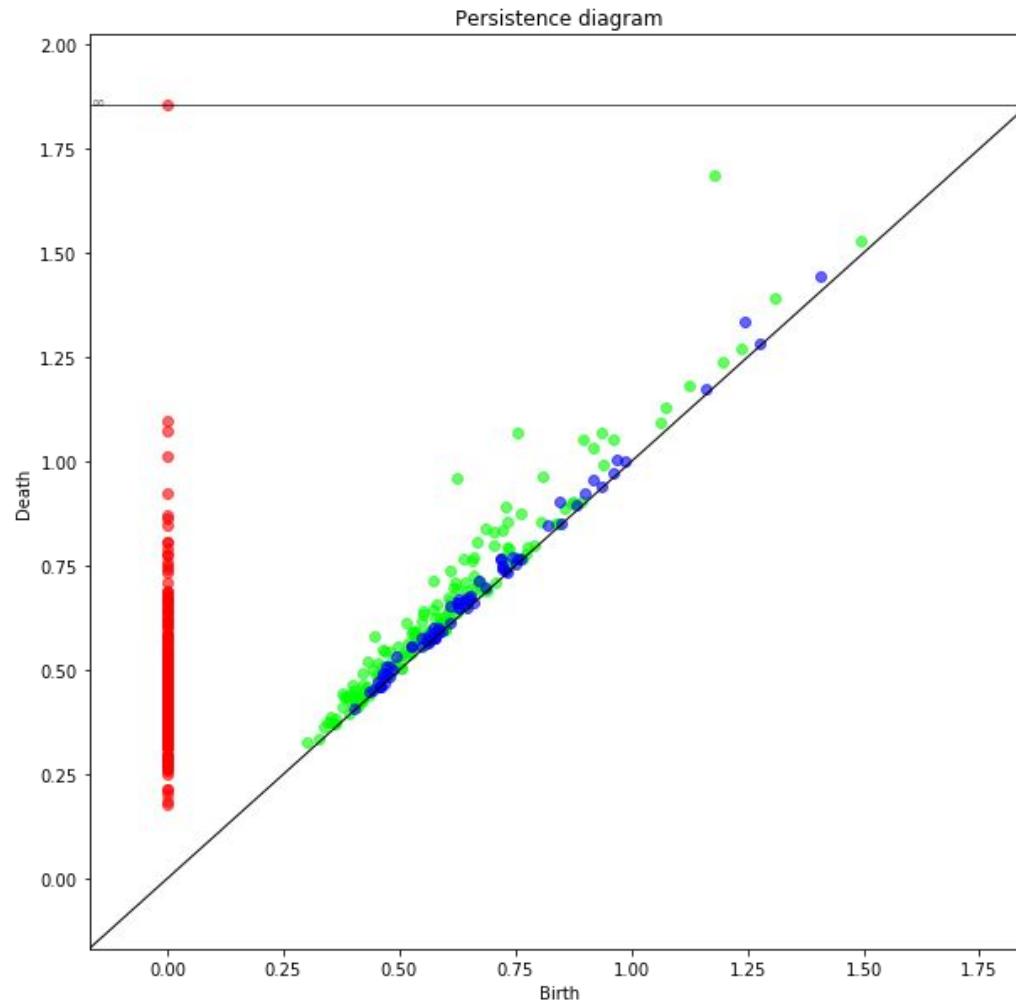
Interval Length : 1

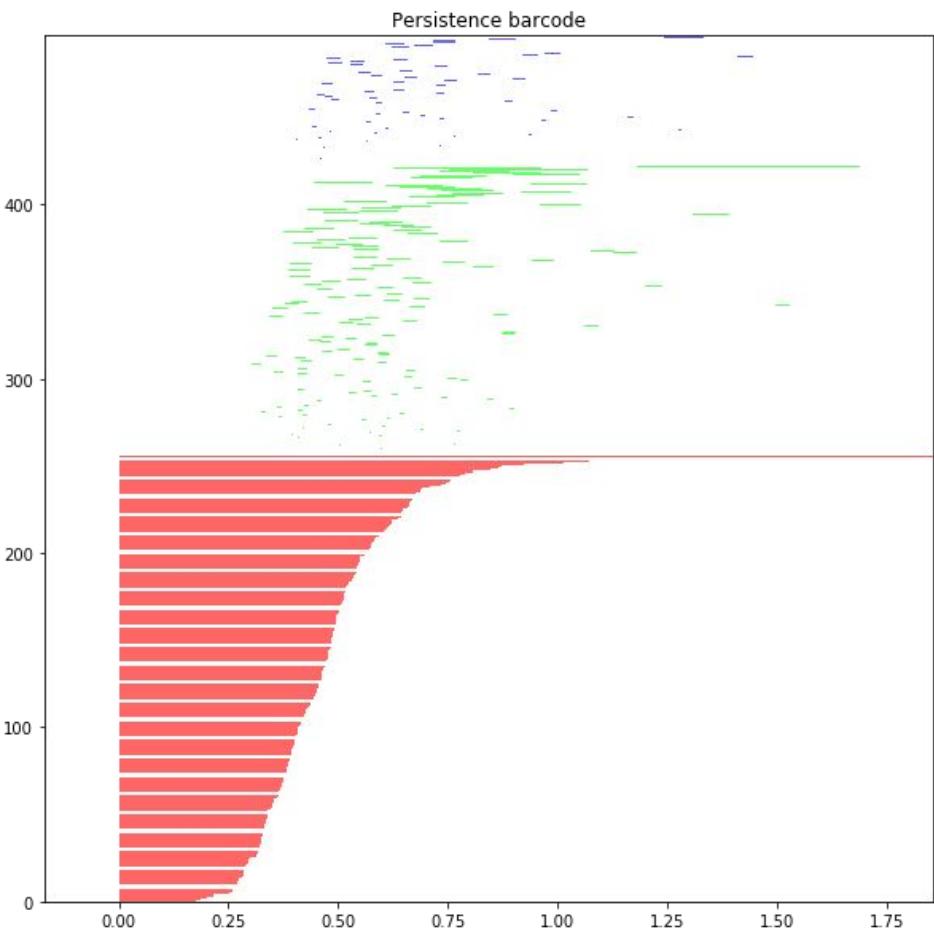
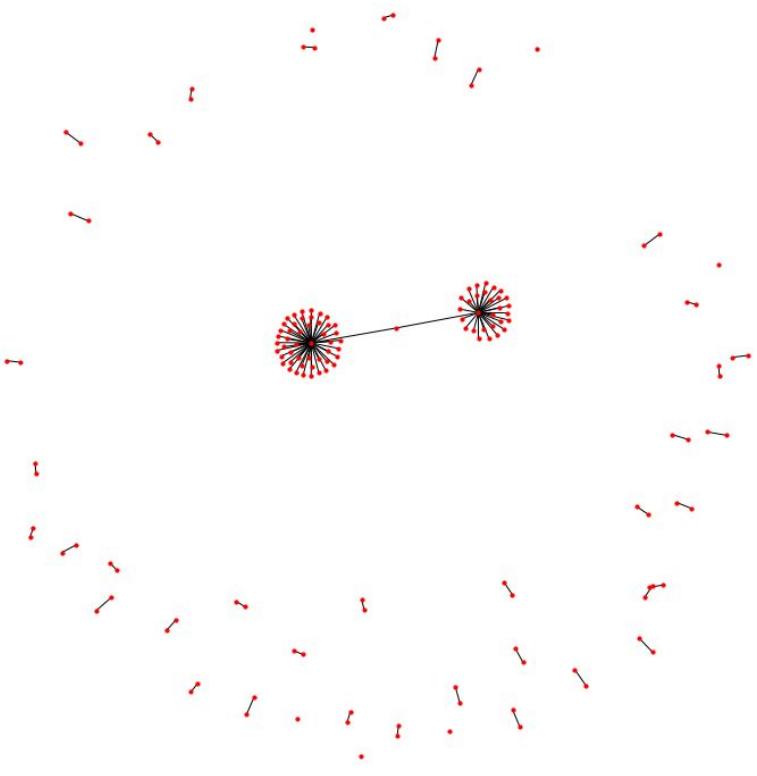
Overlap : 20%

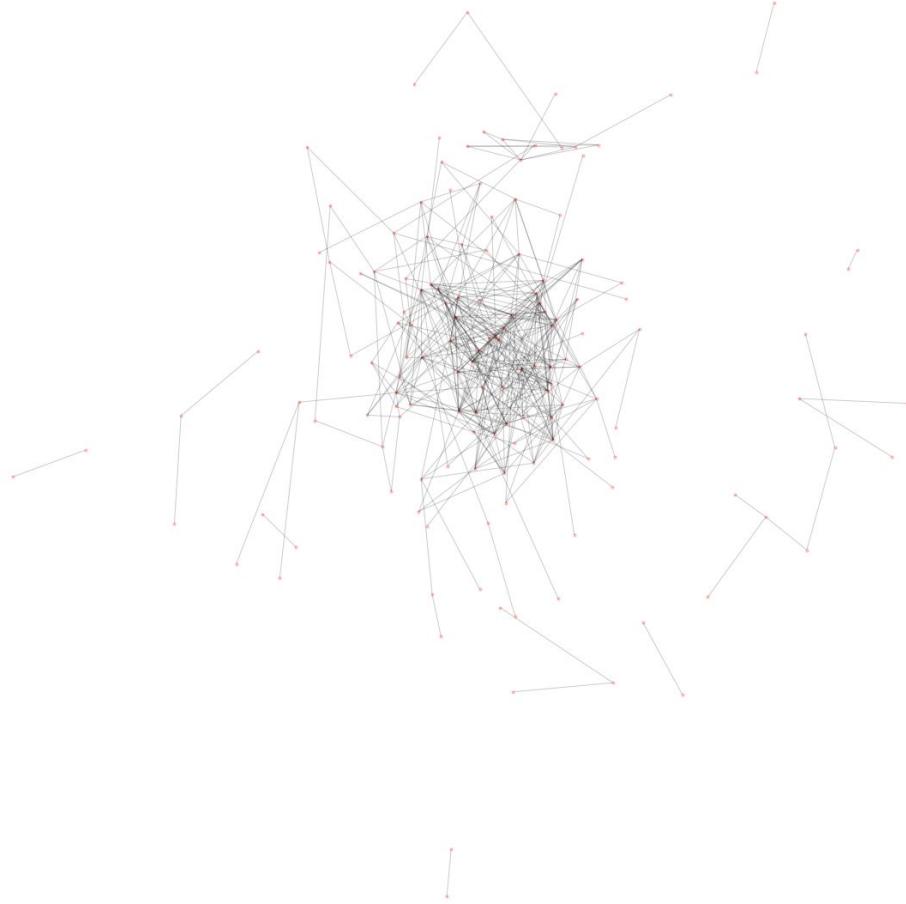
[0-1] [1.6-2.6] [3.2-4.2]

[0.8-1.8] [2.4-3.4]

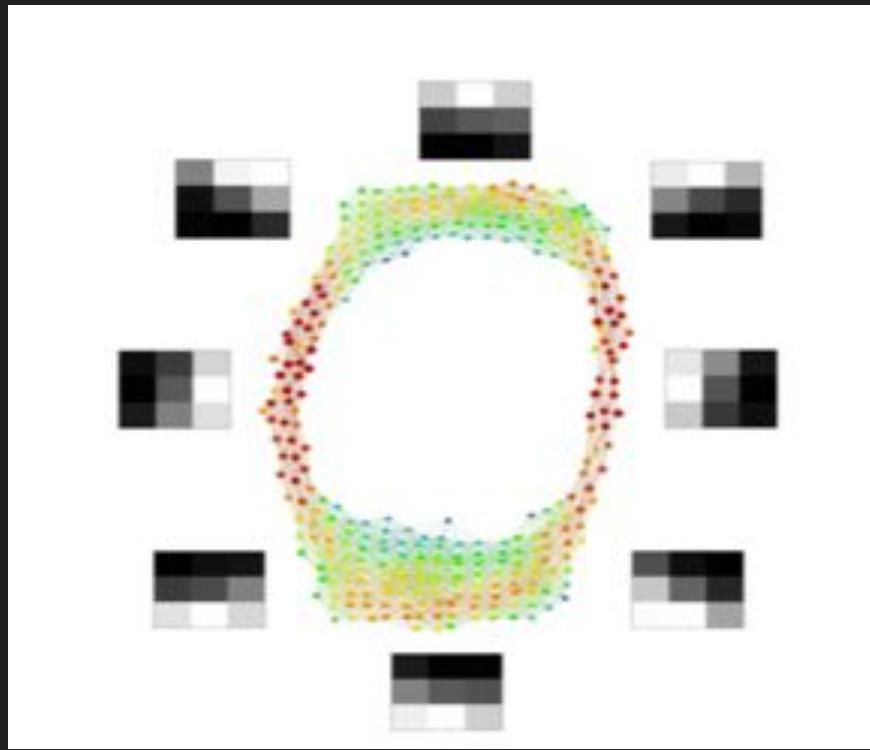








???



```
model.summary()
```

Layer (type)	Output Shape	Param #
<hr/>		
conv2d_5 (Conv2D)	(None, 64, 26, 26)	640
max_pooling2d_5 (MaxPooling2D)	(None, 32, 13, 26)	0
conv2d_6 (Conv2D)	(None, 16, 12, 25)	2064
max_pooling2d_6 (MaxPooling2D)	(None, 8, 6, 25)	0
flatten_3 (Flatten)	(None, 1200)	0
dense_3 (Dense)	(None, 10)	12010
<hr/>		
Total params: 14,714		
Trainable params: 14,714		
Non-trainable params: 0		
<hr/>		

Train on 60000 samples, validate on 10000 samples

Epoch 1/8

60000/60000 [=====] - 3s 53us/step - loss: 0.4136 - acc: 0.8756 - val\_loss: 0.1806 - val\_acc : 0.9449

Epoch 2/8

60000/60000 [=====] - 3s 47us/step - loss: 0.1528 - acc: 0.9548 - val\_loss: 0.1083 - val\_acc : 0.9674

Epoch 3/8

60000/60000 [=====] - 3s 48us/step - loss: 0.1086 - acc: 0.9673 - val\_loss: 0.0814 - val\_acc : 0.9741

Epoch 4/8

60000/60000 [=====] - 3s 48us/step - loss: 0.0862 - acc: 0.9739 - val\_loss: 0.0671 - val\_acc : 0.9795

Epoch 5/8

60000/60000 [=====] - 3s 48us/step - loss: 0.0702 - acc: 0.9788 - val\_loss: 0.0622 - val\_acc : 0.9797

Epoch 6/8

60000/60000 [=====] - 3s 48us/step - loss: 0.0605 - acc: 0.9822 - val\_loss: 0.0509 - val\_acc : 0.9828

Epoch 7/8

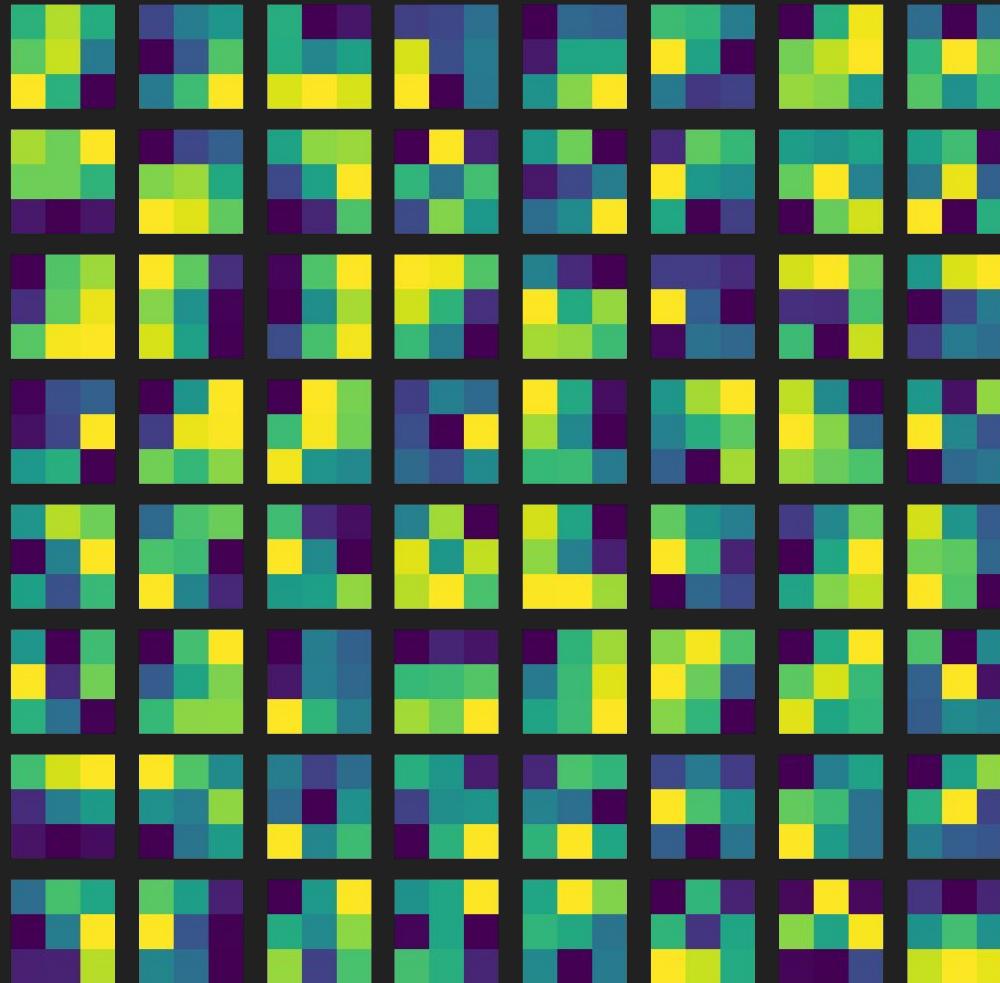
60000/60000 [=====] - 3s 48us/step - loss: 0.0540 - acc: 0.9837 - val\_loss: 0.0562 - val\_acc : 0.9826

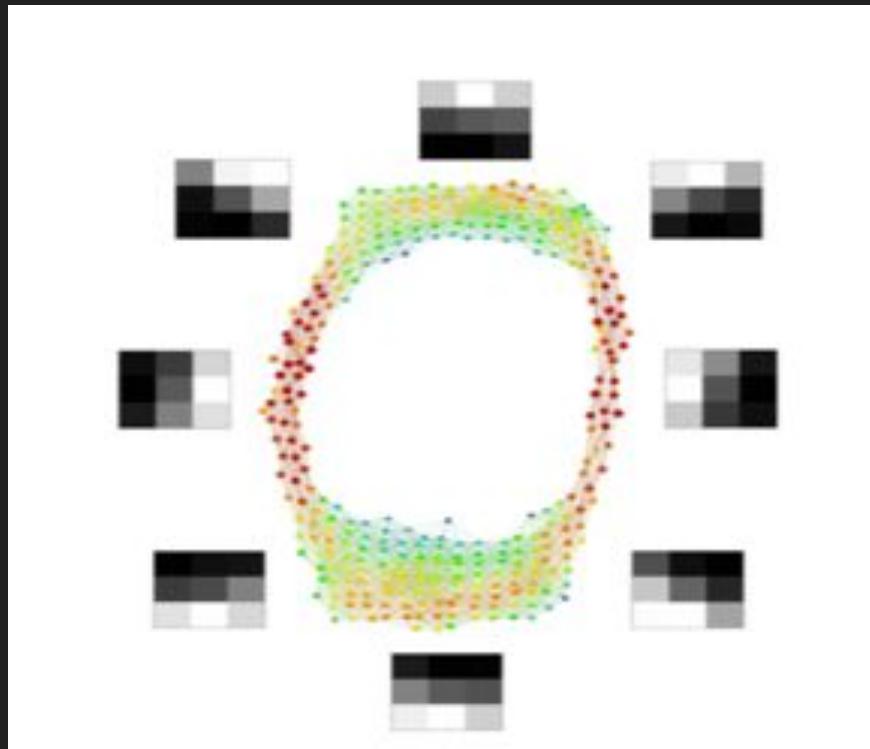
Epoch 8/8

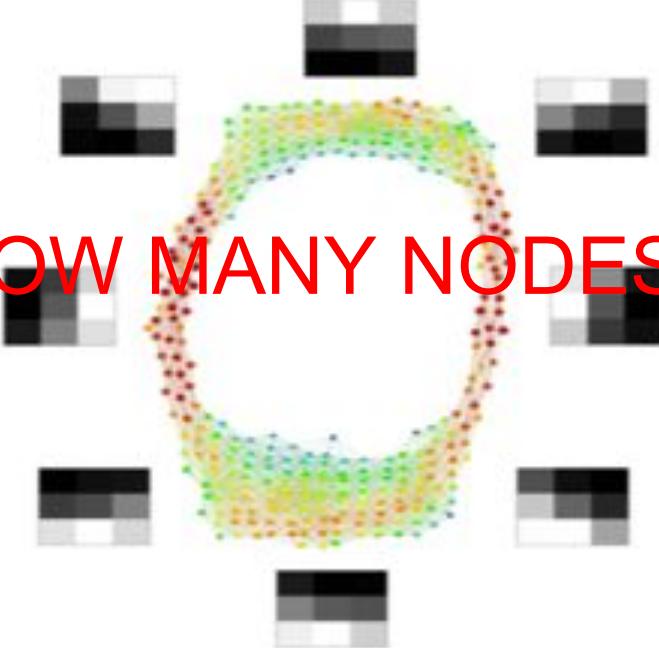
60000/60000 [=====] - 3s 47us/step - loss: 0.0486 - acc: 0.9850 - val\_loss: 0.0528 - val\_acc : 0.9829

Test loss: 0.05276332234479487

Test accuracy: 0.9829







HOW MANY NODES?

Ok

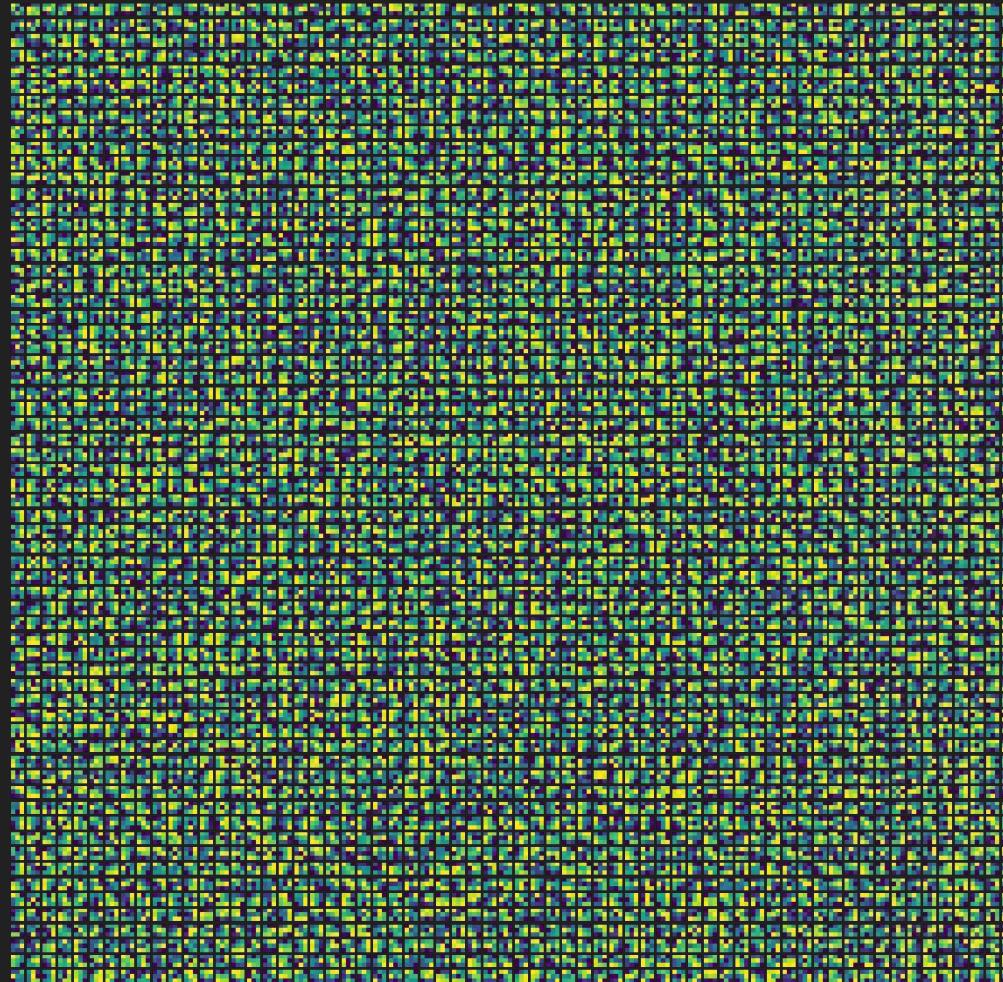
Layer (type)	Output Shape	Param #
conv2d_1 (Conv2D)	(None, 4096, 26, 26)	40960
max_pooling2d_1 (MaxPooling2D)	(None, 2048, 13, 26)	0
conv2d_2 (Conv2D)	(None, 16, 12, 25)	131088
max_pooling2d_2 (MaxPooling2D)	(None, 8, 6, 25)	0
flatten_1 (Flatten)	(None, 1200)	0
dense_1 (Dense)	(None, 10)	12010

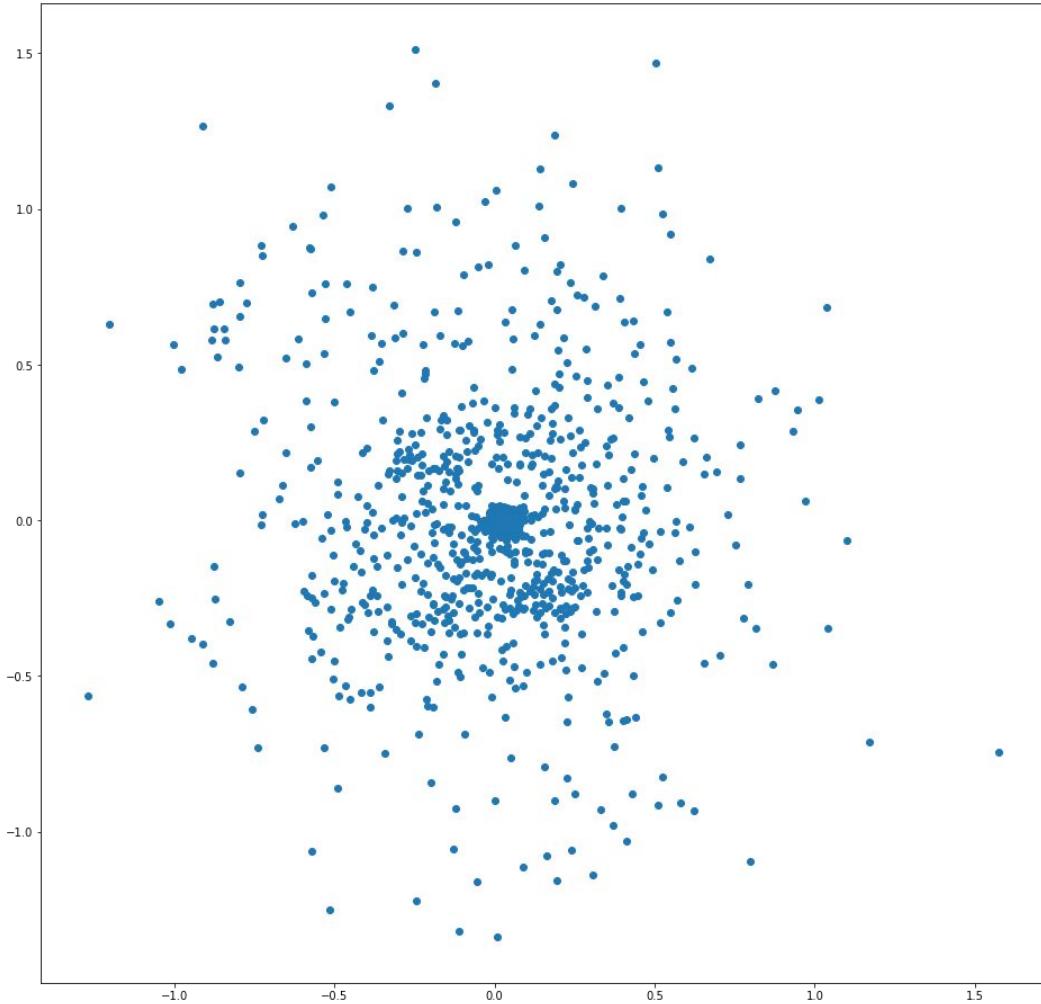
Total params: 184,058

Trainable params: 184,058

Non-trainable params: 0

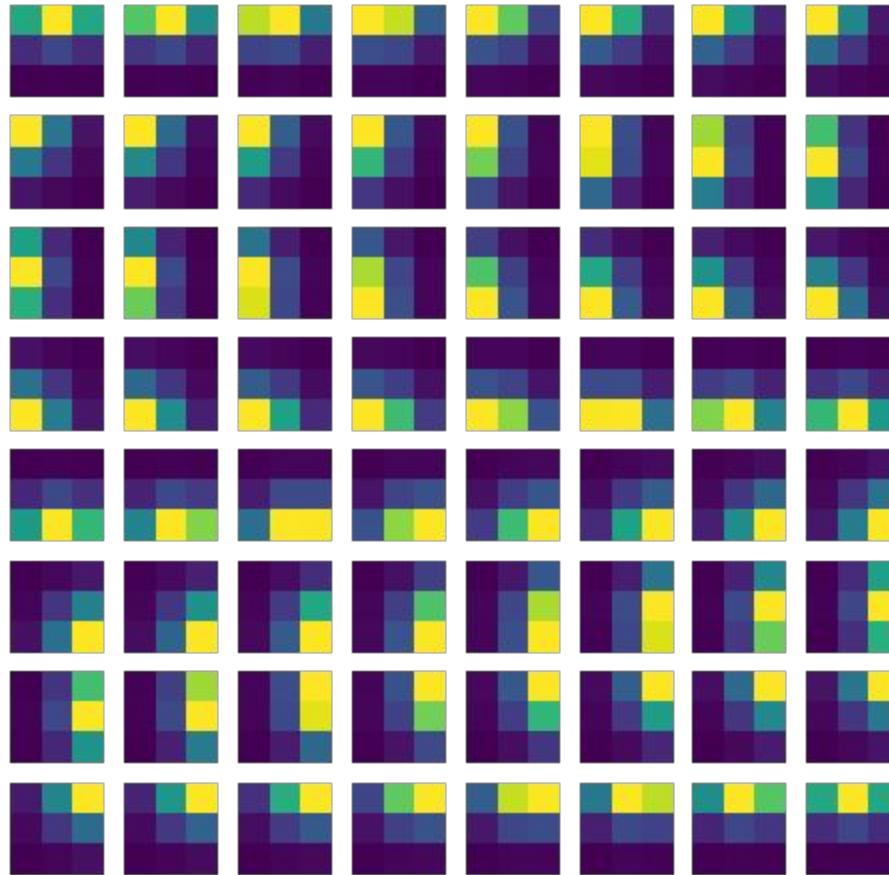
```
Train on 60000 samples, validate on 10000 samples
Epoch 1/16
60000/60000 [=====] - 78s 1ms/step - loss: 0.2617 - acc: 0.9183 - val_loss: 0.0865
val_acc: 0.9728
Epoch 2/16
60000/60000 [=====] - 77s 1ms/step - loss: 0.0858 - acc: 0.9737 - val_loss: 0.0637
val_acc: 0.9806
Epoch 3/16
60000/60000 [=====] - 77s 1ms/step - loss: 0.0650 - acc: 0.9804 - val_loss: 0.0517
val_acc: 0.9843
Epoch 4/16
60000/60000 [=====] - 77s 1ms/step - loss: 0.0547 - acc: 0.9827 - val_loss: 0.0522
val_acc: 0.9826
Epoch 5/16
60000/60000 [=====] - 77s 1ms/step - loss: 0.0481 - acc: 0.9846 - val_loss: 0.0658
val_acc: 0.9801
Epoch 6/16
60000/60000 [=====] - 77s 1ms/step - loss: 0.0436 - acc: 0.9860 - val_loss: 0.0460
val_acc: 0.9845
Epoch 7/16
60000/60000 [=====] - 77s 1ms/step - loss: 0.0376 - acc: 0.9882 - val_loss: 0.0539
val_acc: 0.9841
Epoch 8/16
60000/60000 [=====] - 77s 1ms/step - loss: 0.0347 - acc: 0.9891 - val_loss: 0.0480
val_acc: 0.9854
Epoch 9/16
60000/60000 [=====] - 76s 1ms/step - loss: 0.0310 - acc: 0.9900 - val_loss: 0.0512
val_acc: 0.9850
Epoch 10/16
60000/60000 [=====] - 76s 1ms/step - loss: 0.0296 - acc: 0.9903 - val_loss: 0.0621
val_acc: 0.9814
Epoch 11/16
60000/60000 [=====] - 76s 1ms/step - loss: 0.0264 - acc: 0.9913 - val_loss: 0.0484
val_acc: 0.9857
Epoch 12/16
60000/60000 [=====] - 75s 1ms/step - loss: 0.0247 - acc: 0.9916 - val_loss: 0.0486
val_acc: 0.9863
Epoch 13/16
60000/60000 [=====] - 75s 1ms/step - loss: 0.0229 - acc: 0.9923 - val_loss: 0.0623
val_acc: 0.9821
Epoch 14/16
60000/60000 [=====] - 75s 1ms/step - loss: 0.0200 - acc: 0.9935 - val_loss: 0.0592
val_acc: 0.9846
Epoch 15/16
60000/60000 [=====] - 75s 1ms/step - loss: 0.0200 - acc: 0.9933 - val_loss: 0.0719
val_acc: 0.9824
Epoch 16/16
60000/60000 [=====] - 75s 1ms/step - loss: 0.0176 - acc: 0.9944 - val_loss: 0.0634
val_acc: 0.9839
Test loss: 0.06344677277751035
Test accuracy: 0.9839
```

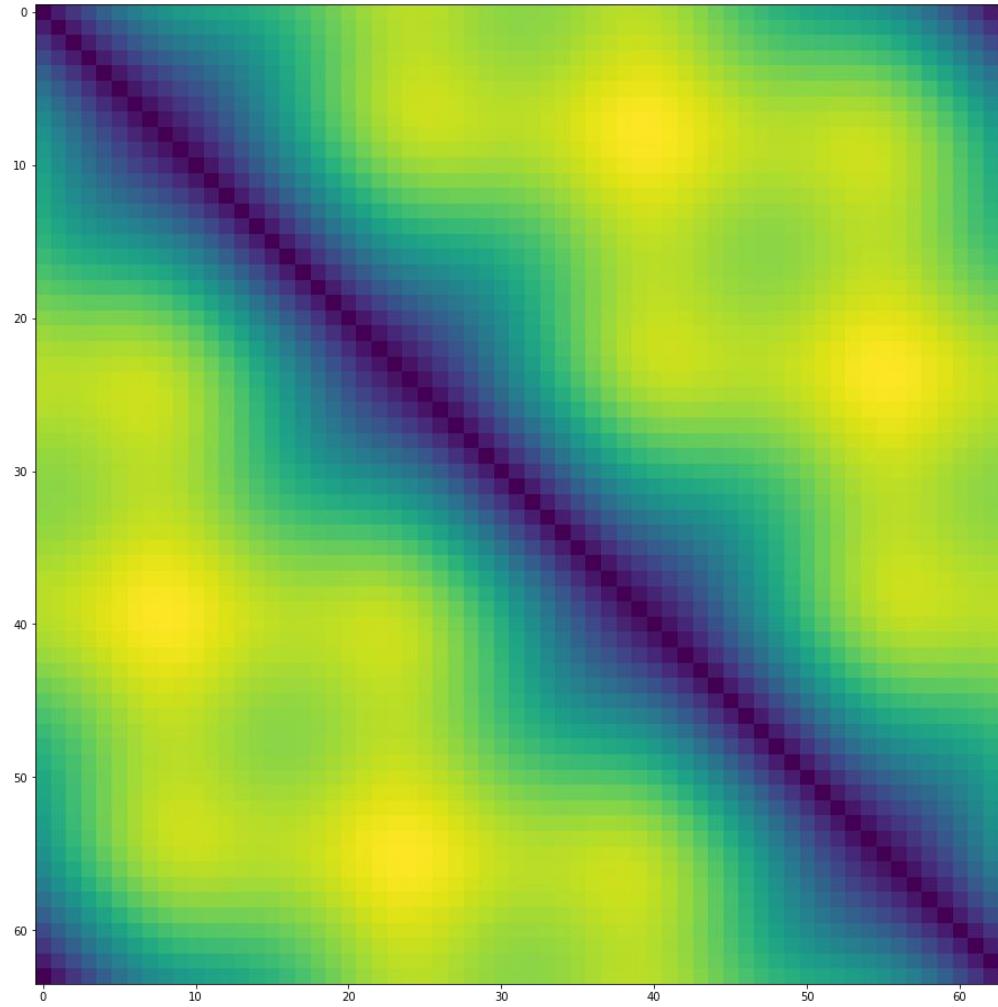


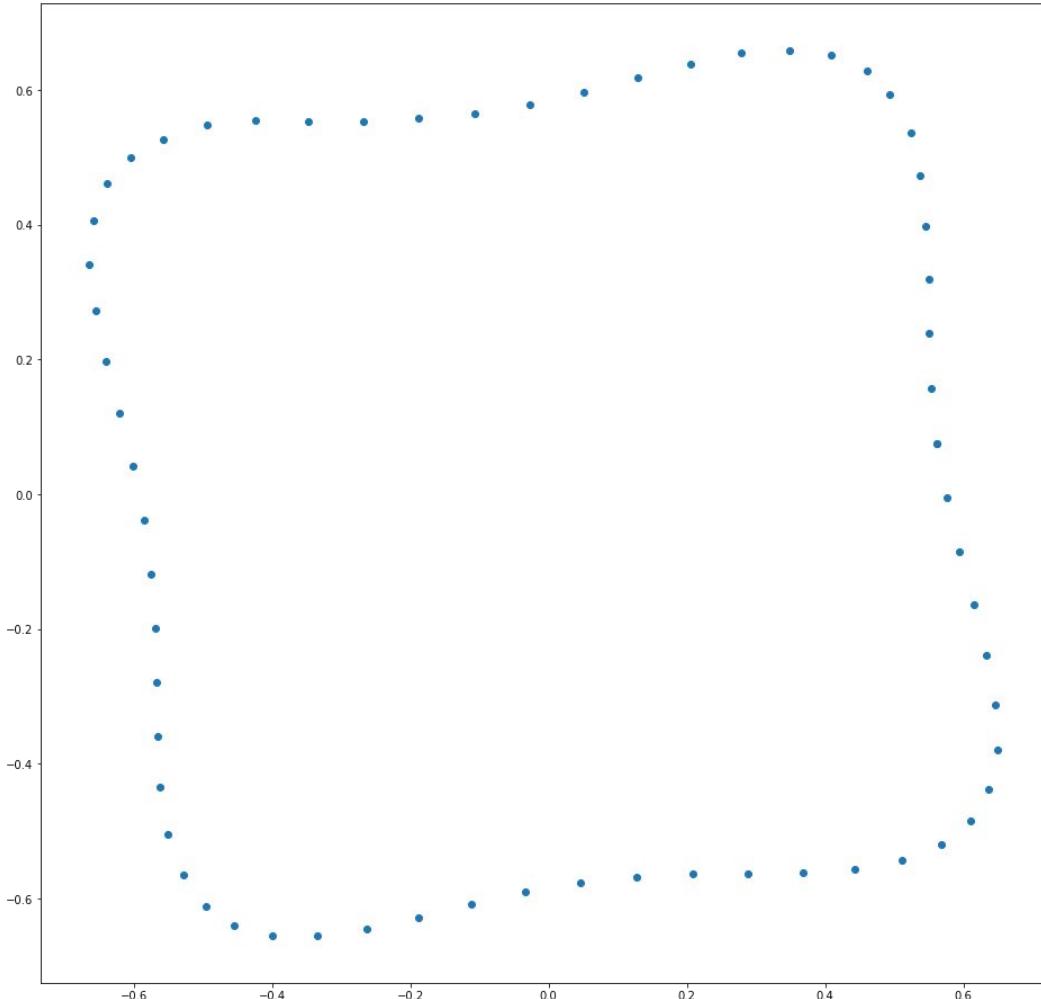




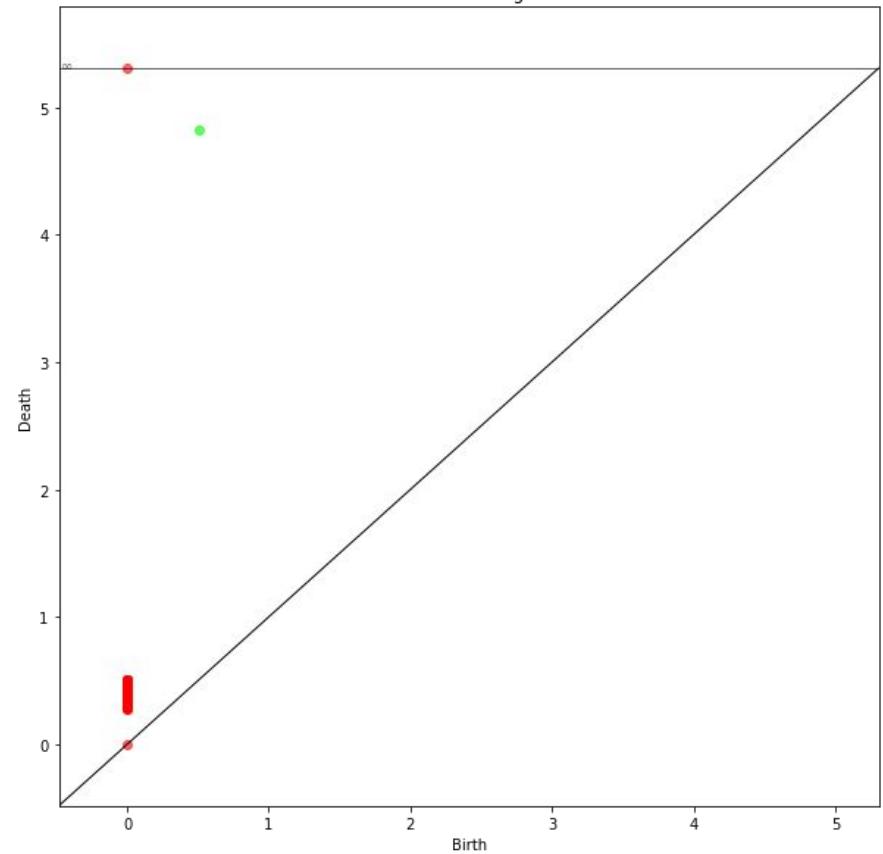
Does it make sense?



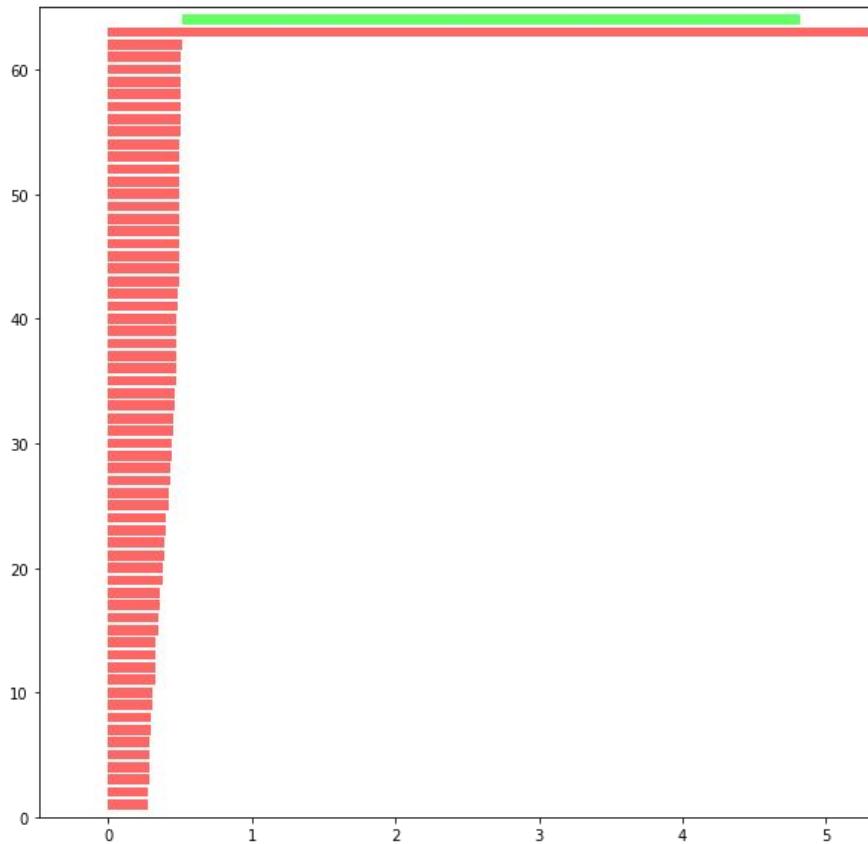




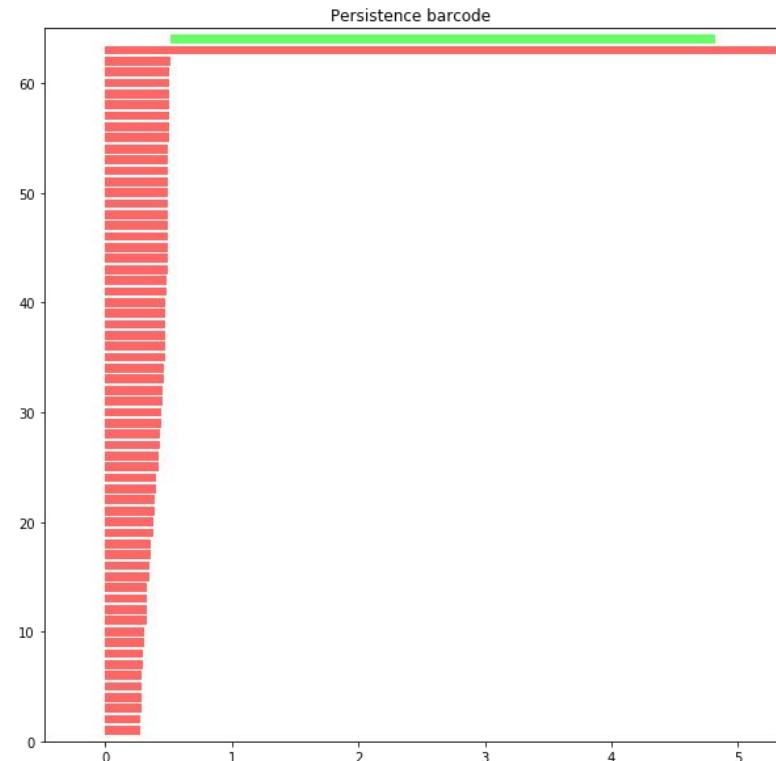
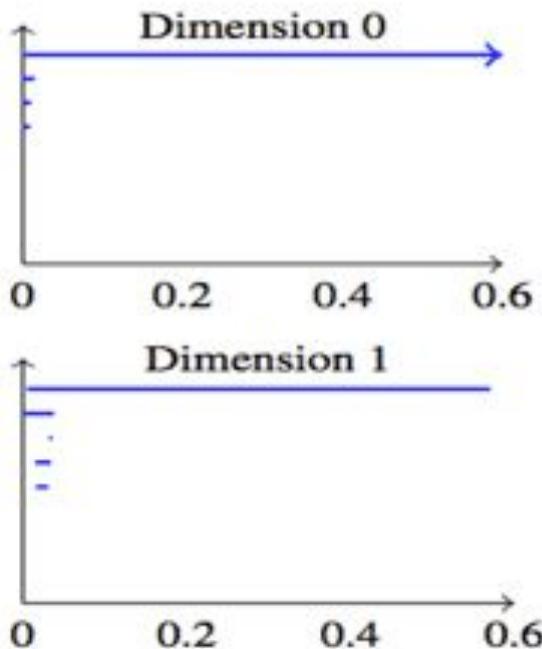
Persistence diagram



Persistence barcode







# Conclusion

# Challenges

- Mapper is confusing, too many parameters to tune
- Computations are very memory extensive
- Requires sophisticated preprocessing
- Toolkits are not perfect

Still very promising!

# Why TDA?

- No good understanding what is happening inside Neural Networks, despite of abundance of good research done by very smart people
- Intellectually satisfying and intuitive
- Terra incognita

# Questions to ask

- How topology changes over layers?
- How topology changes over training?
- Do different nets have the same underlying structures?
- What do these structures mean?
- ...

# Further research

- CNNs:
  - Do they have the same structure?
  - What happens when overfit?
  - How topology of learned weights depends on topology of training data
  - ...
- RNNs:
  - What do the cycles mean?

Thank you !

# Aleksei Prokopev

[aleksei@akaintelligence.com](mailto:aleksei@akaintelligence.com)

+82 10 3742 3945