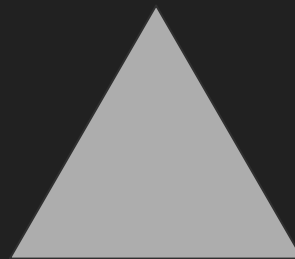
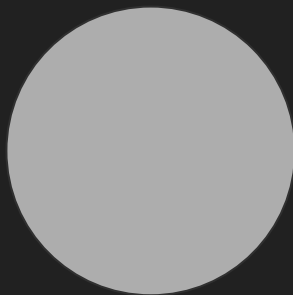


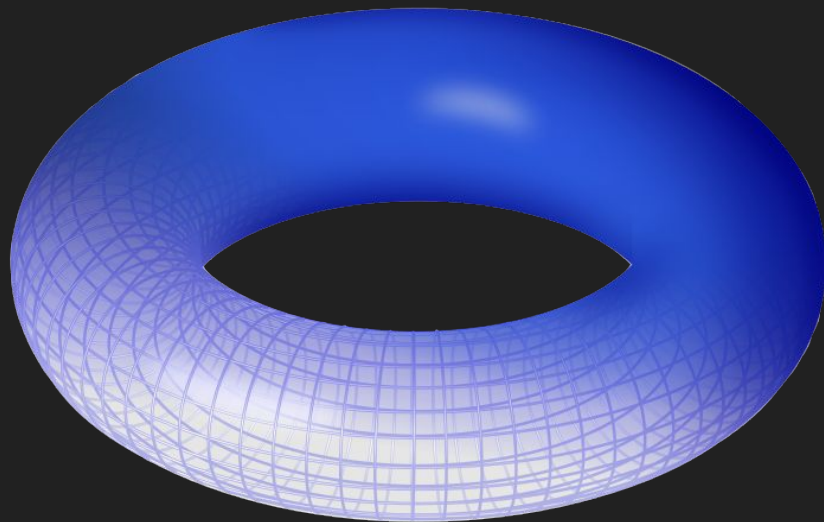
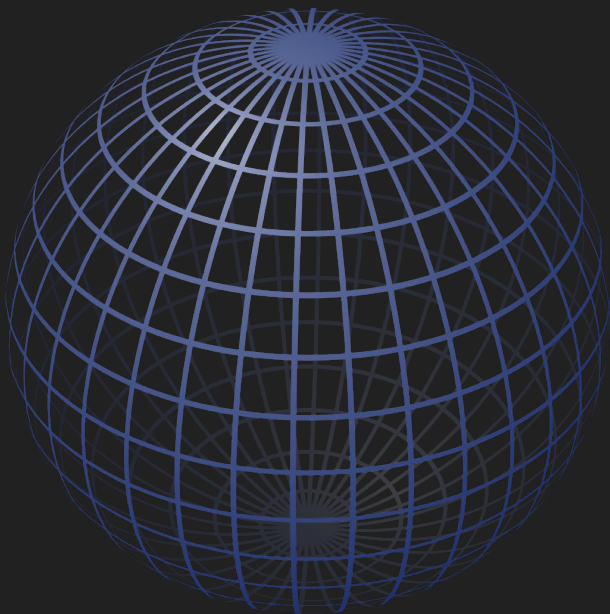
Topological Data Analysis to understand Convolutional Neural Networks

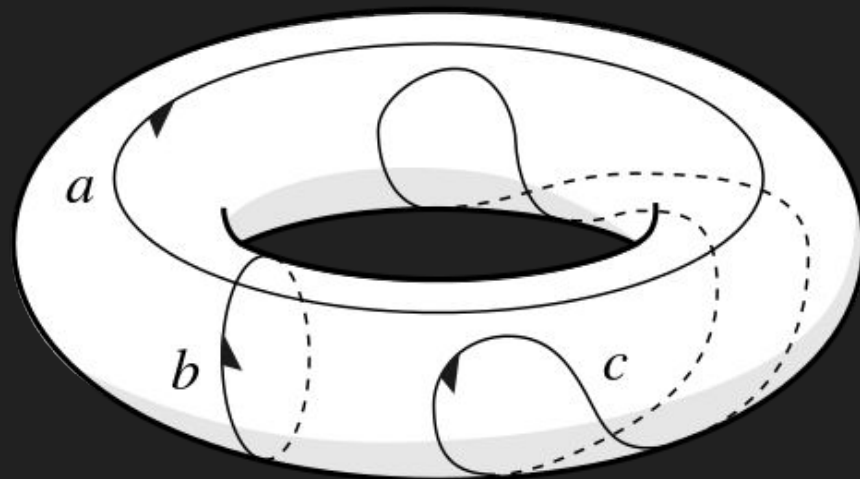
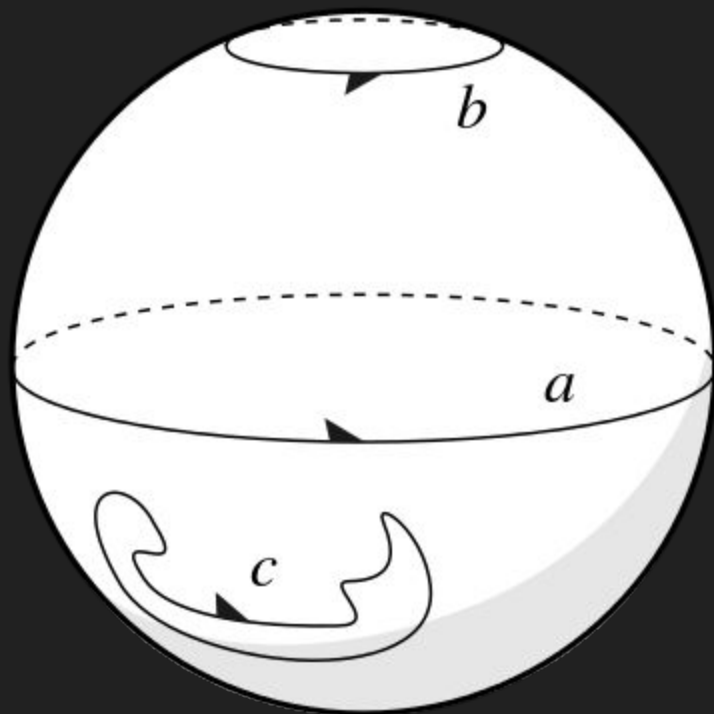
Aleksei Prokopev, SeoulAI, 2018

Shape



Topology



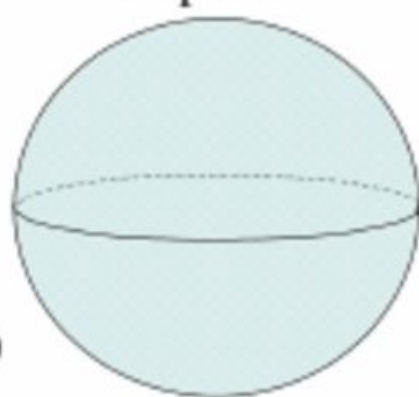


A solid 2-dimensional blob



$$\beta_0 = 1$$
$$\beta_{i>0} = 0$$

A sphere



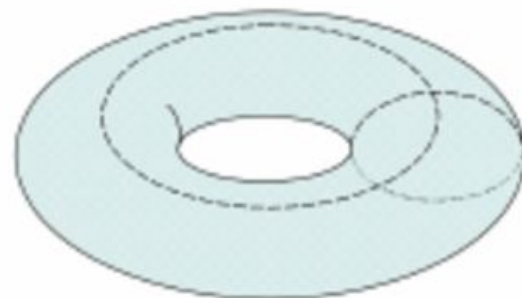
$$\beta_0 = 1$$
$$\beta_1 = 0$$
$$\beta_2 = 1$$
$$\beta_{i>2} = 0$$

A 2D blob with three holes



$$\beta_0 = 1$$
$$\beta_1 = 3$$
$$\beta_{i>1} = 0$$

A torus

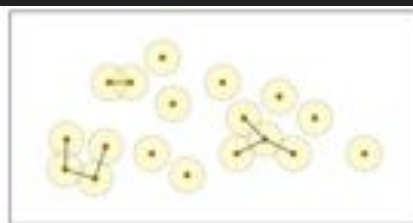


$$\beta_0 = 1$$
$$\beta_1 = 2$$
$$\beta_2 = 1$$
$$\beta_{i>2} = 0$$

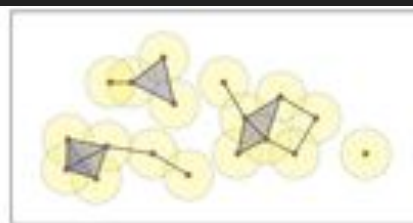
Topological Data Analysis



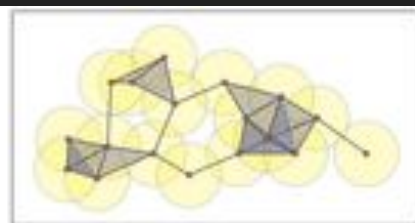
$\varepsilon = 1.5$



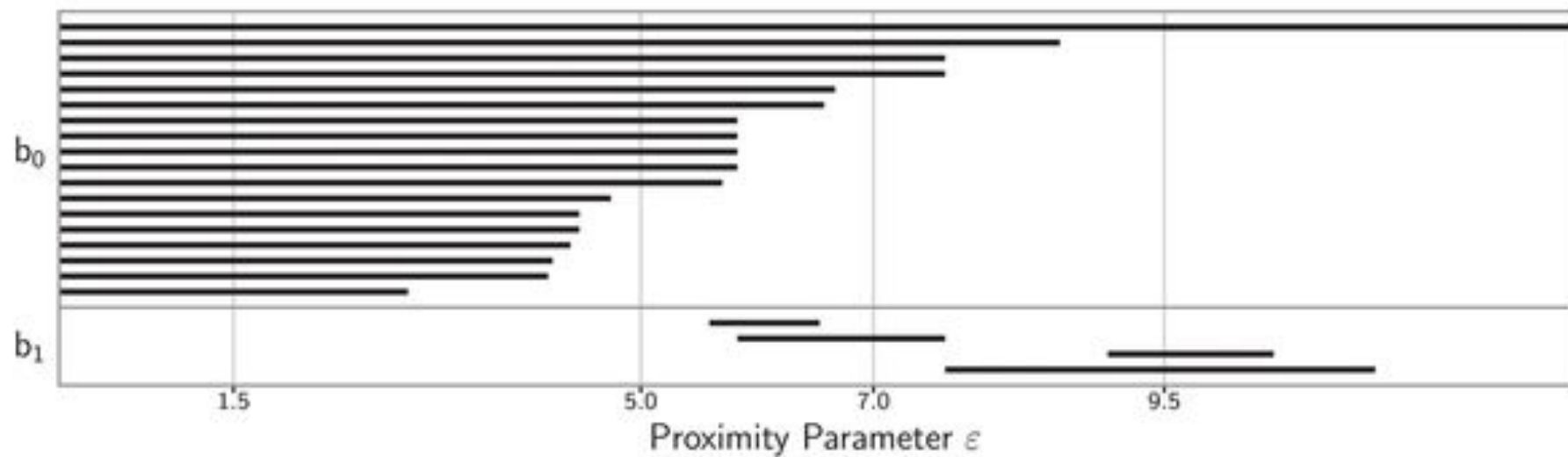
$\varepsilon = 5.0$



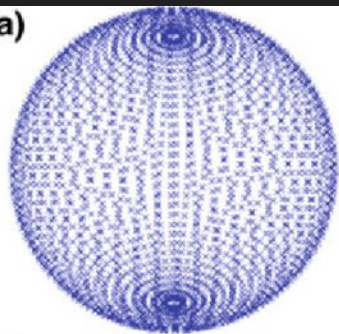
$\varepsilon = 7.0$



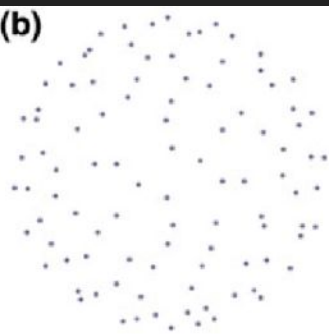
$\varepsilon = 9.5$



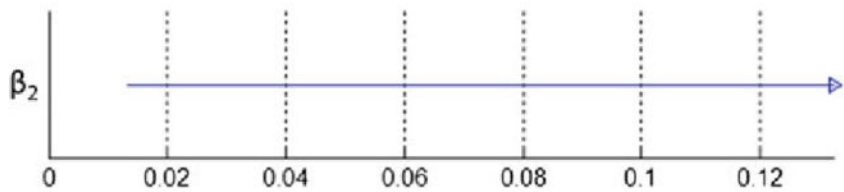
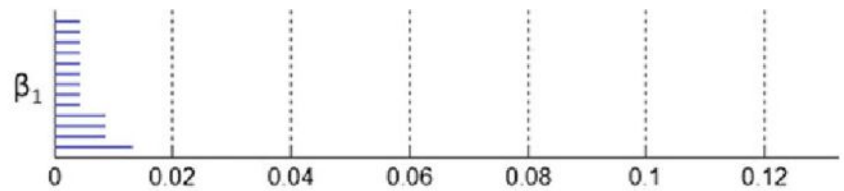
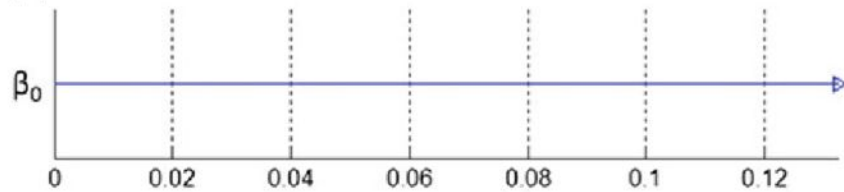
(a)

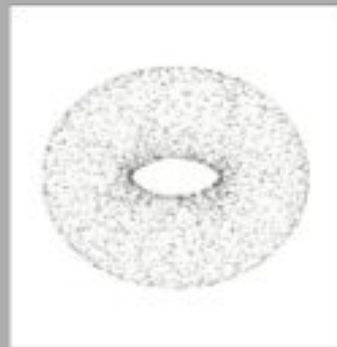
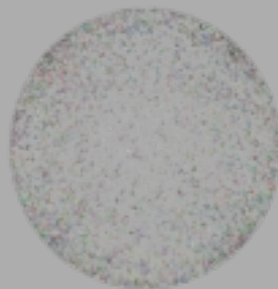


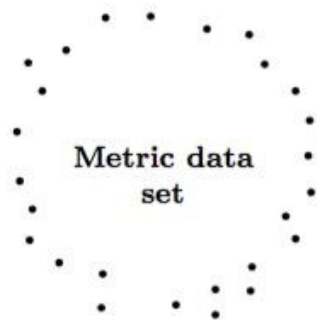
(b)



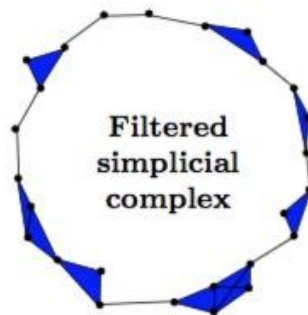
(c)



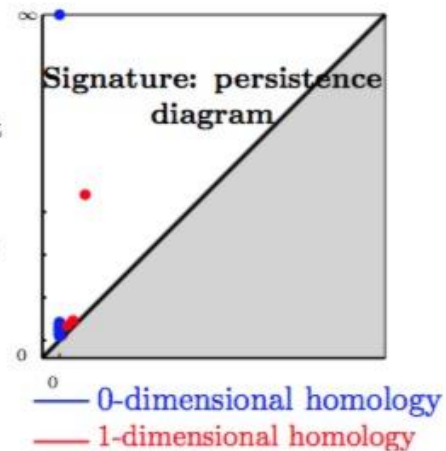





Build geometric
filtered complex on
top of data



Compute persistent
homology of the
complex.



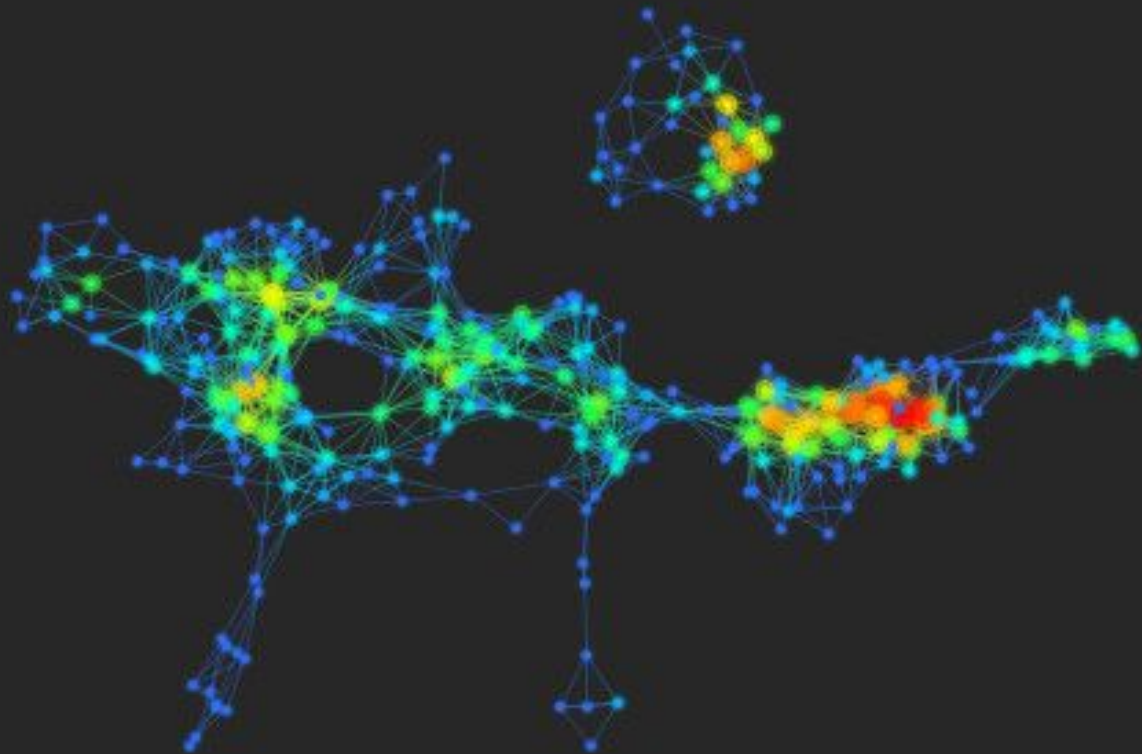


Refine your data into
knowledge with Topological
Data Analysis



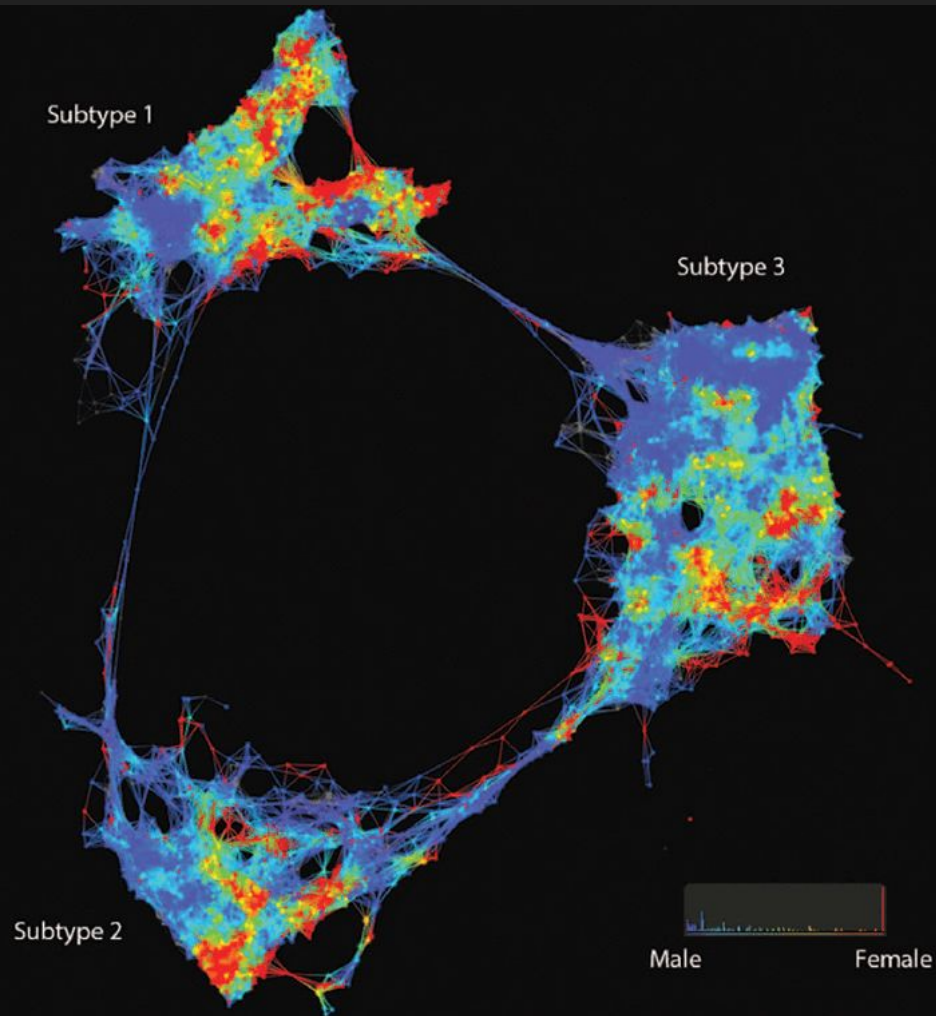
AYASDI

Examples



AYASDI

B



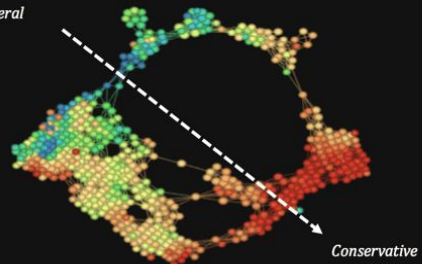
Nodes are groups of similar data points

Edges connect similar nodes

Colors let you see values of interest

Position of a node on the screen doesn't matter

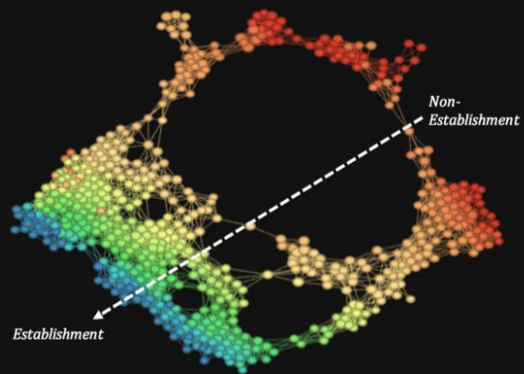
Liberal



Conservative

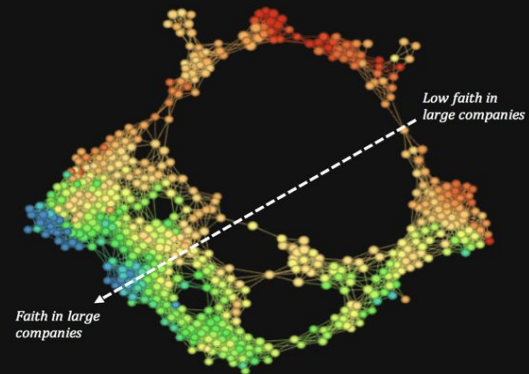
Non-Establishment

Establishment



Low faith in large companies

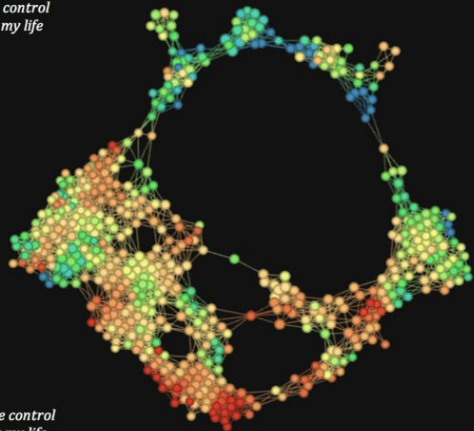
Faith in large companies



Lack control over my life

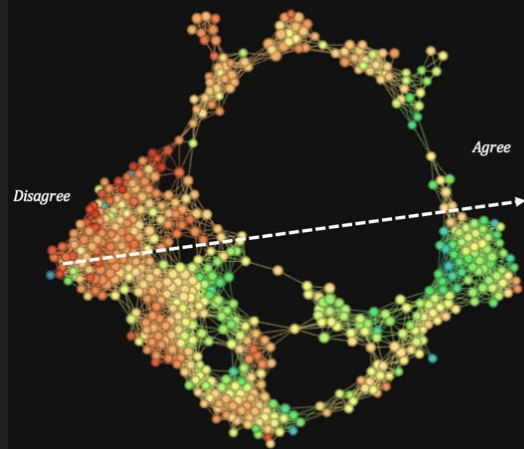


Have control over my life



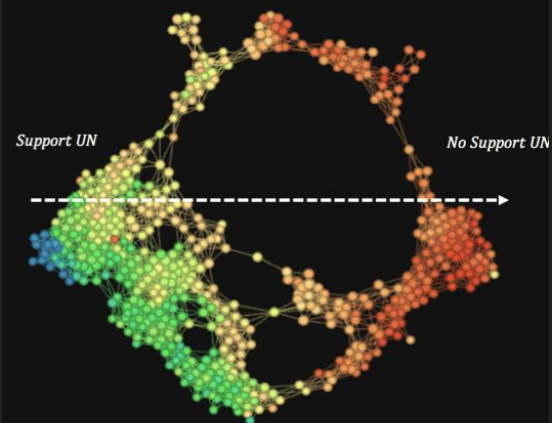
Agree

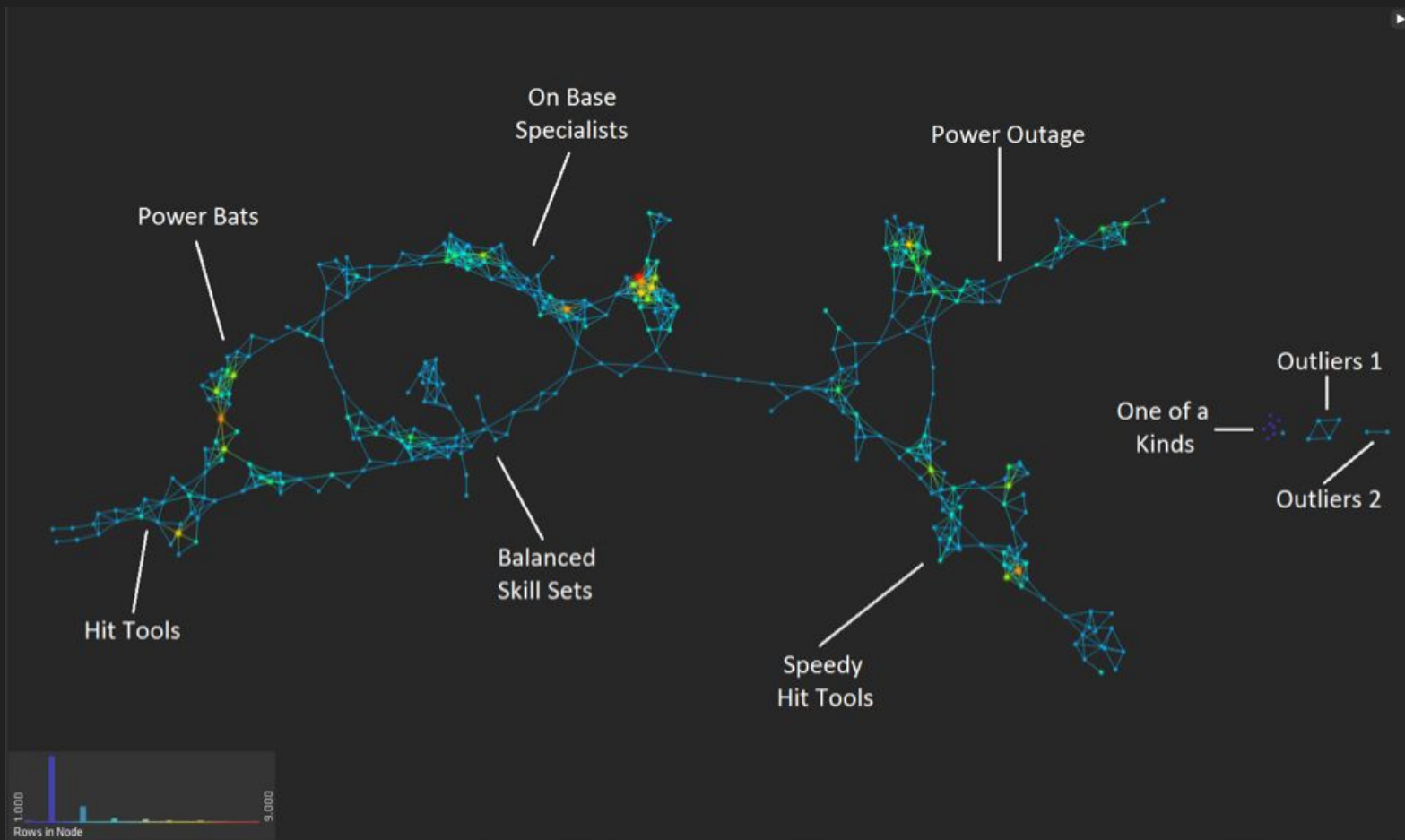
Disagree

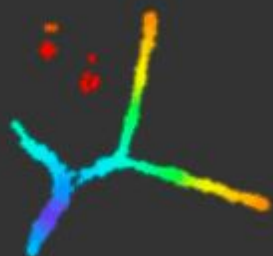


Support UN

No Support UN







Breast invasive carcinoma

Kidney renal clear cell carcinoma

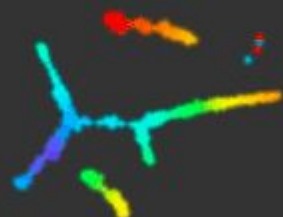


Cervical squamous cell carcinoma
and endocervical adenocarcinoma



Bladder Urothelial Carcinoma

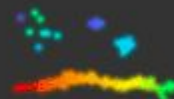
Lung squamous cell carcinoma



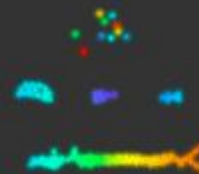
Ovarian serous cystadenocarcinoma



Uterine Corpus
Endometrioid Carcinoma



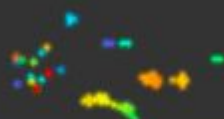
Colon adenocarcinoma



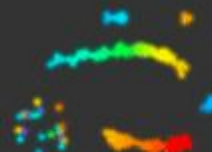
Glioblastoma multiforme



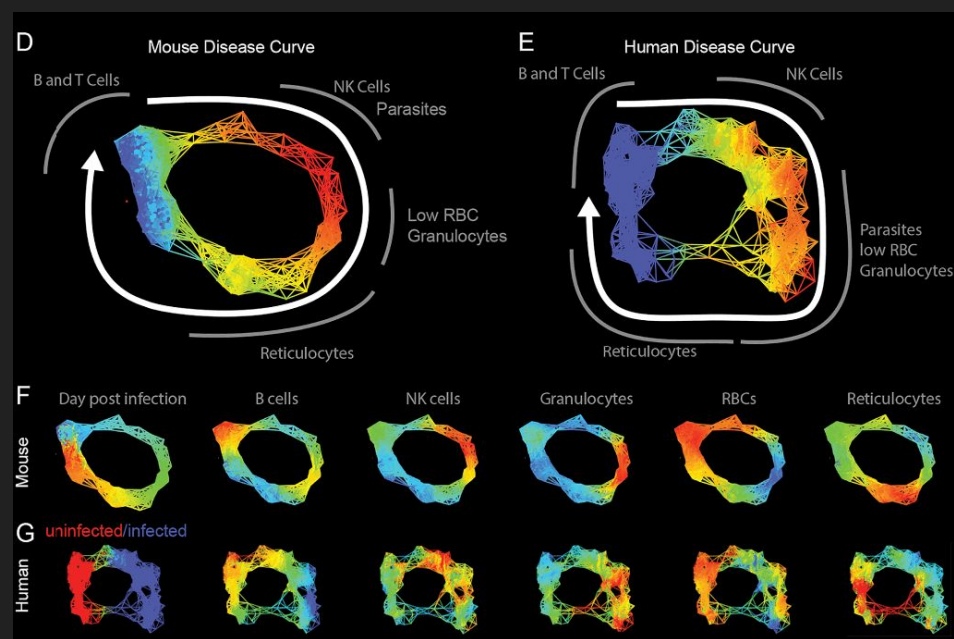
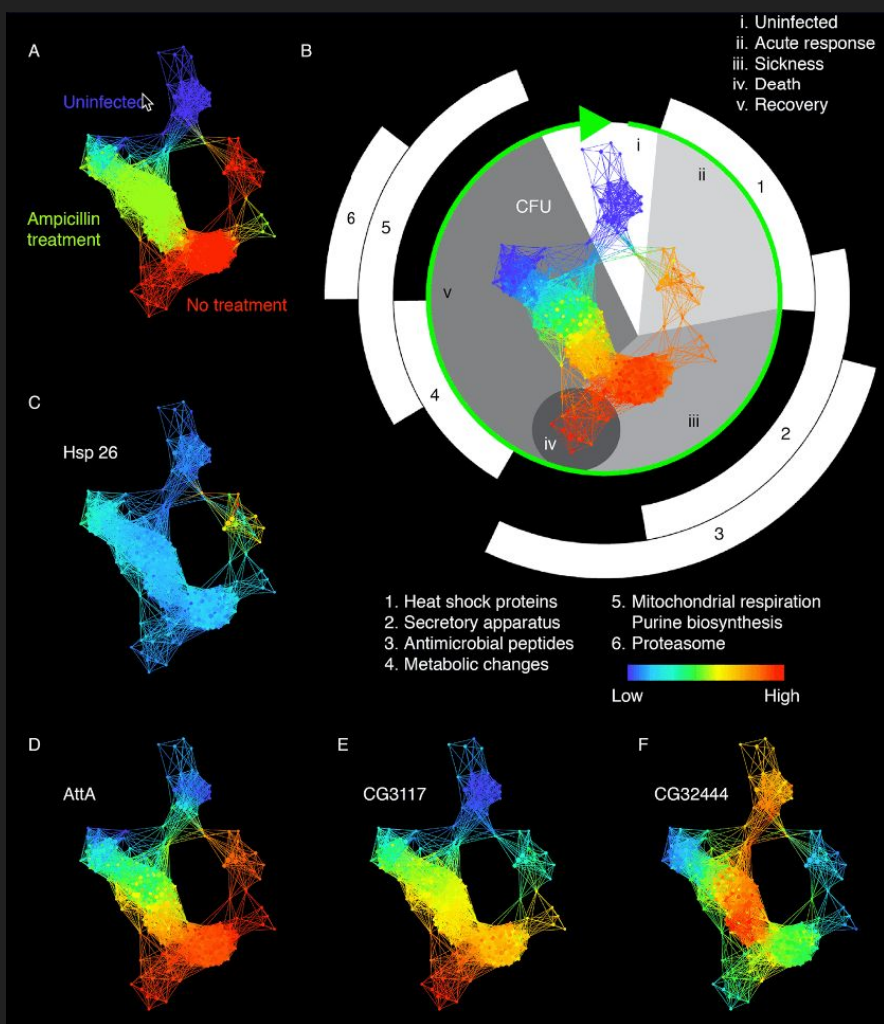
Prostate adenocarcinoma



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)



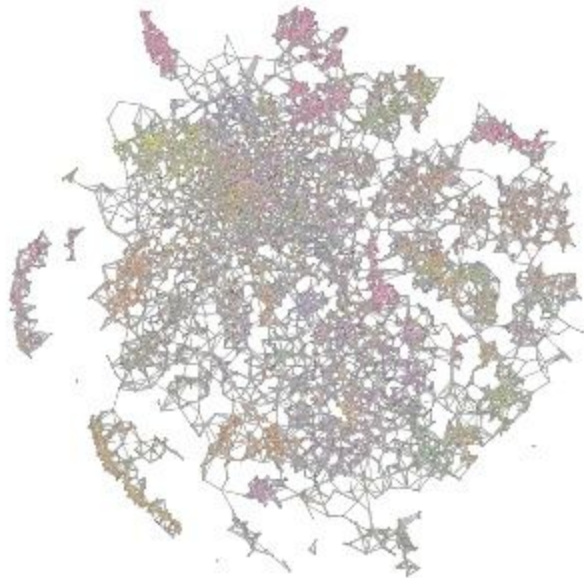
LLE
(366 sec)



Case study: Netflix competition

Result comparison: TDA with other techniques

Topological Data Analysis



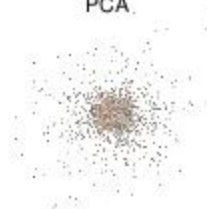
LLE



LTSA



PCA



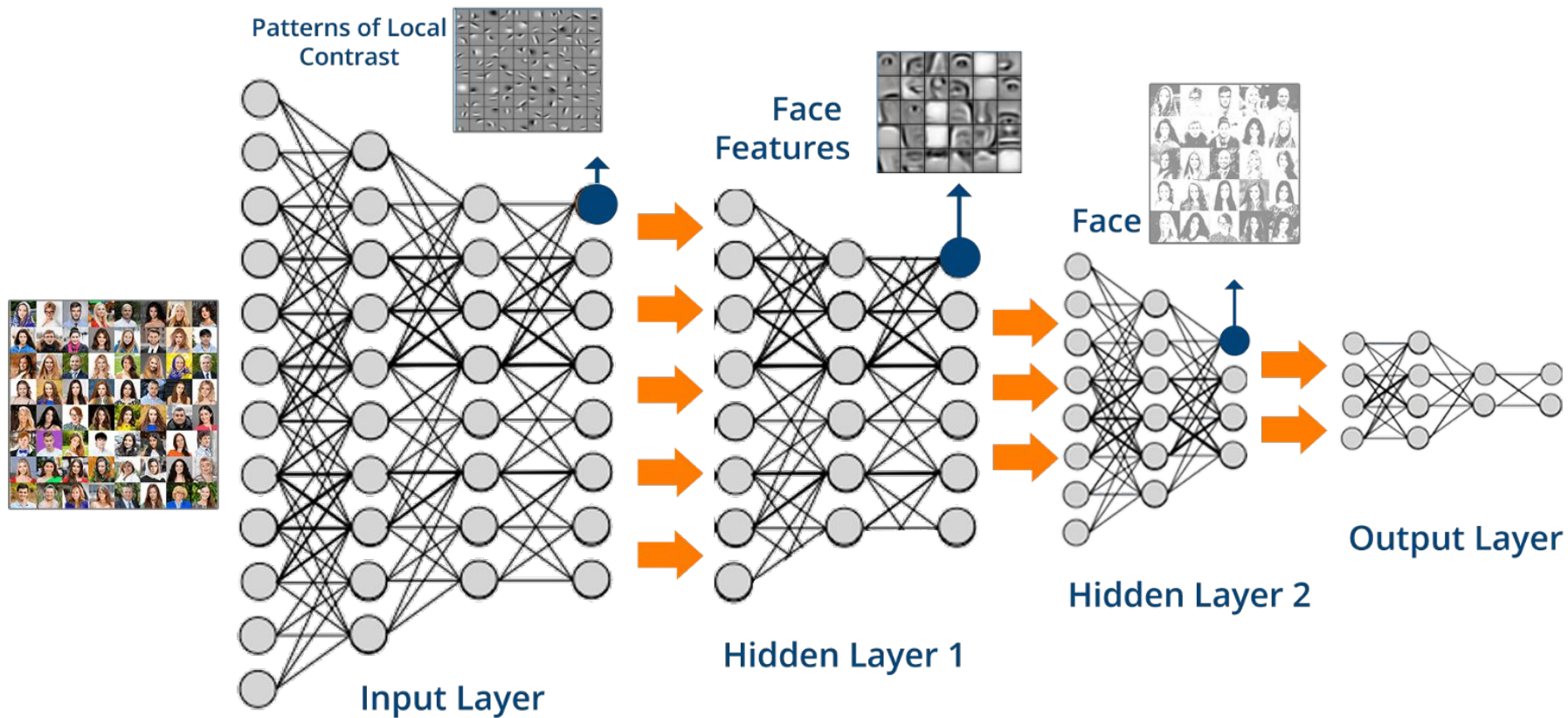
Hessian LLE



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

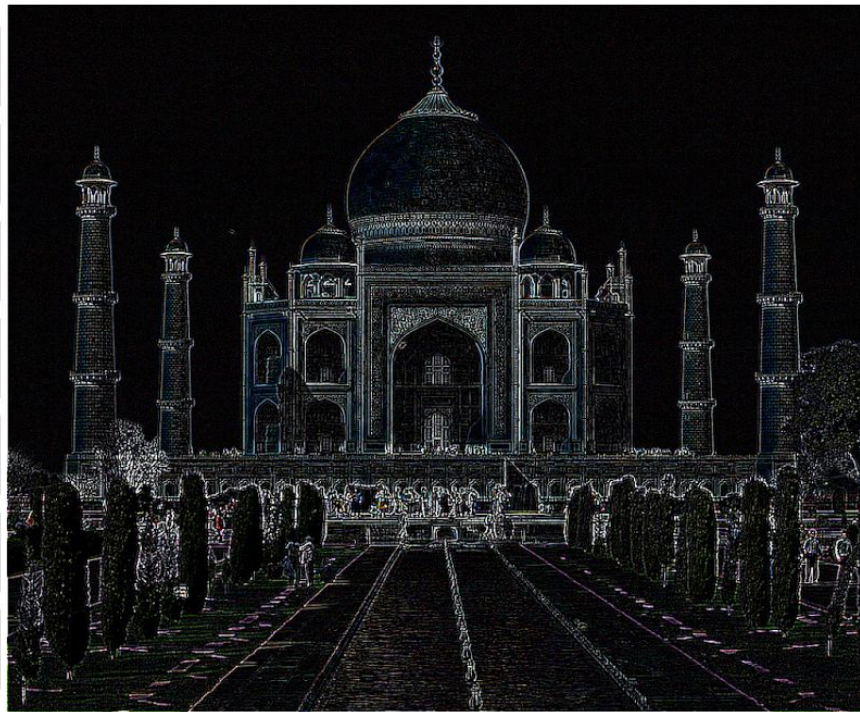






	0	1	0	
	0	0	0	
	0	0	0	



		42		

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>
$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$\frac{1}{16} \begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix}$	$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 5 & -1 \\ 0 & -1 & 0 \end{bmatrix}$	$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$
			

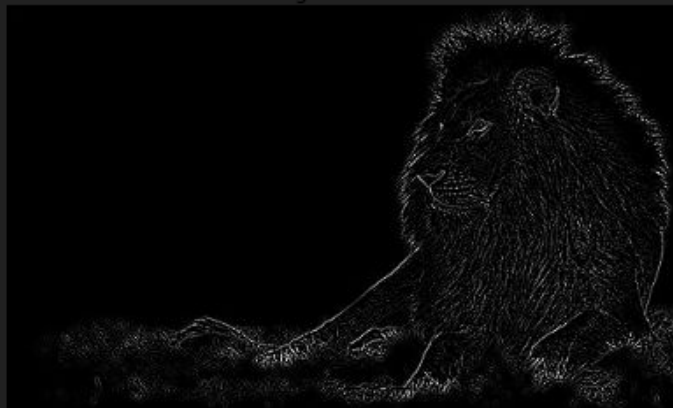
Original Image



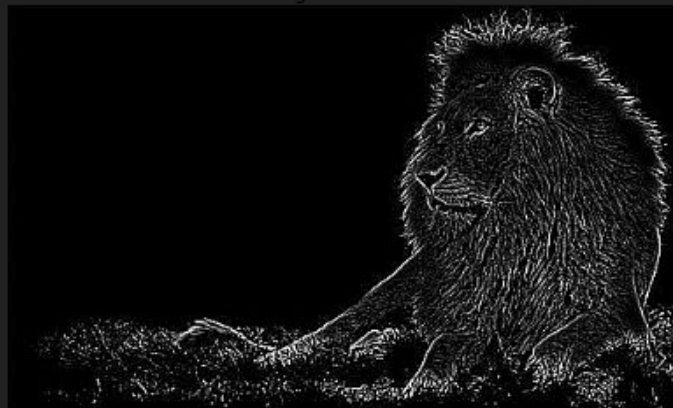
Edge Kernel 1



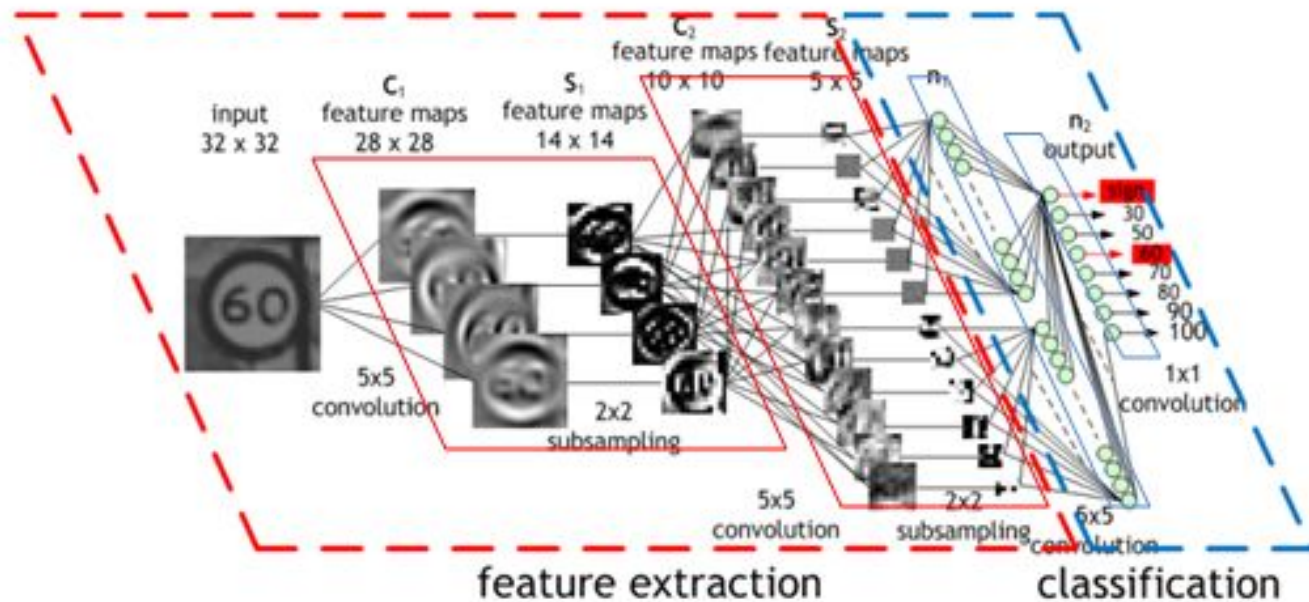
Edge Kernel 2



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	0.37	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	0.21	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

3.7

4.5

2.1

1.3

City
Beach

Input Volume (+pad 1) (7x7x3)

 $x[:, :, 0]$

0	0	0	0	0	0	0
0	0	0	1	0	2	0
0	1	0	2	0	1	0

0	1	0	2	2	0	0
0	2	0	0	2	0	0
0	2	1	2	2	0	0
0	0	0	0	0	0	0

 $x[:, :, 1]$

0	0	0	0	0	0	0
0	2	1	2	1	1	0
0	2	1	2	0	1	0

0	0	2	1	0	1	0
0	1	2	2	2	2	0
0	0	1	2	0	1	0
0	0	0	0	0	0	0

 $x[:, :, 2]$

0	0	0	0	0	0	0
0	2	1	1	2	0	0
0	1	0	0	1	0	0

0	0	1	0	0	0	0
0	1	0	2	1	0	0
0	2	2	1	1	1	0
0	0	0	0	0	0	0

Filter W0 (3x3x3)

 $w0[:, :, 0]$

-1	0	1
0	0	1
1	-1	1

 $w0[:, :, 1]$

-1	0	1
1	-1	1
0	1	0

 $w0[:, :, 2]$

-1	1	1
1	1	0
0	-1	0

Bias b0 (1x1x1)

 $b0[:, :, 0]$

1

Filter W1 (3x3x3)

 $w1[:, :, 0]$

0	1	-1
0	-1	0
0	-1	1

 $w1[:, :, 1]$

-1	0	0
1	-1	0
1	-1	0

 $w1[:, :, 2]$

-1	1	-1
0	-1	-1
1	0	0

Bias b1 (1x1x1)

 $b1[:, :, 0]$

0

Output Volume (3x3x2)

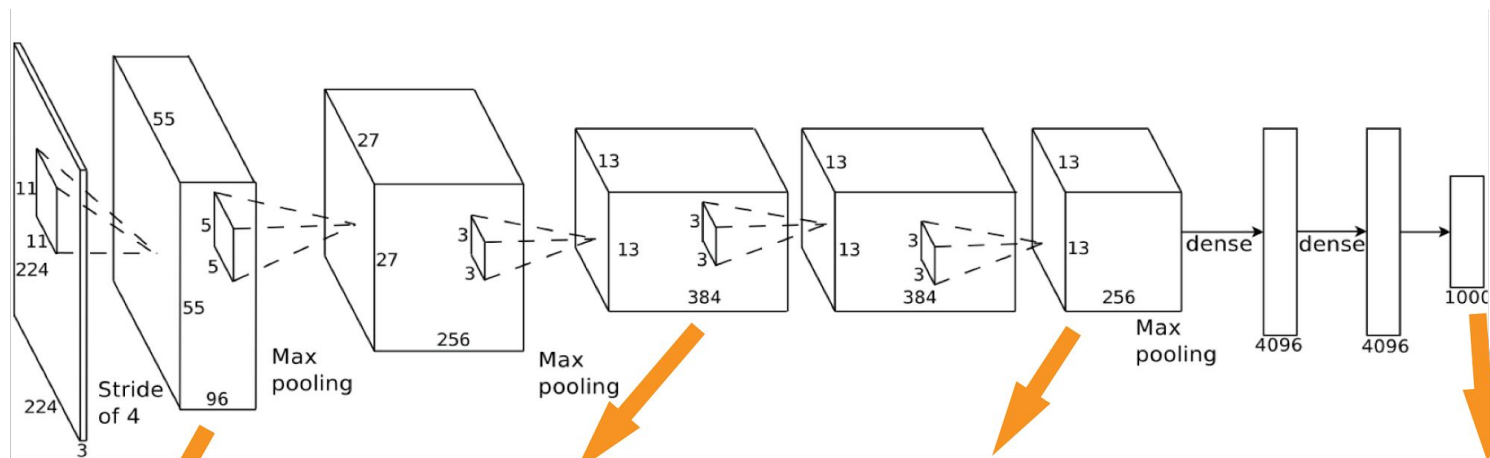
 $o[:, :, 0]$

2	3	3
3	7	3
8	10	-3

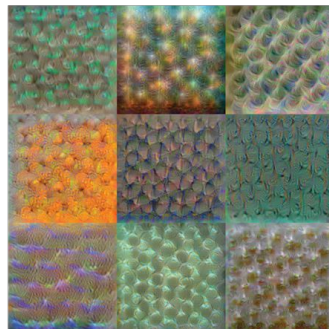
 $o[:, :, 1]$

-8	-8	-3
-3	1	0
-3	-8	-5

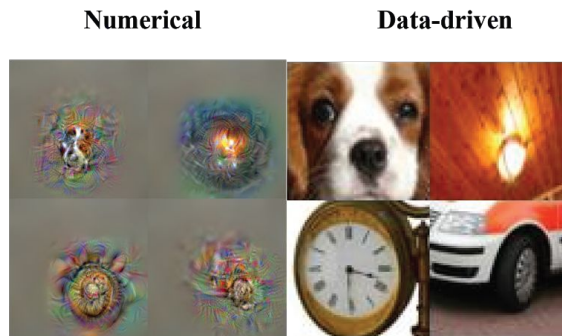
toggle movement



Conv 1: Edge+Blob



Conv 3: Texture

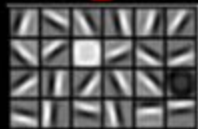


Conv 5: Object Parts

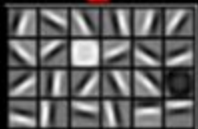


Fc8: Object Classes

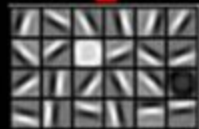
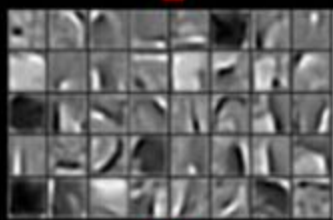
Faces



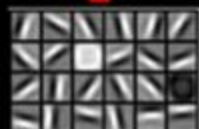
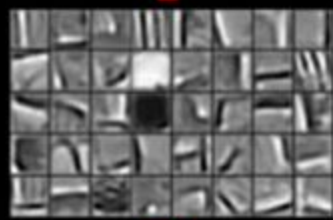
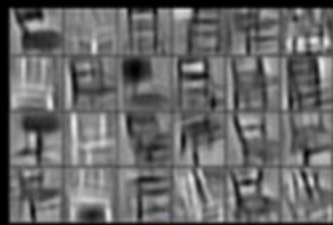
Cars



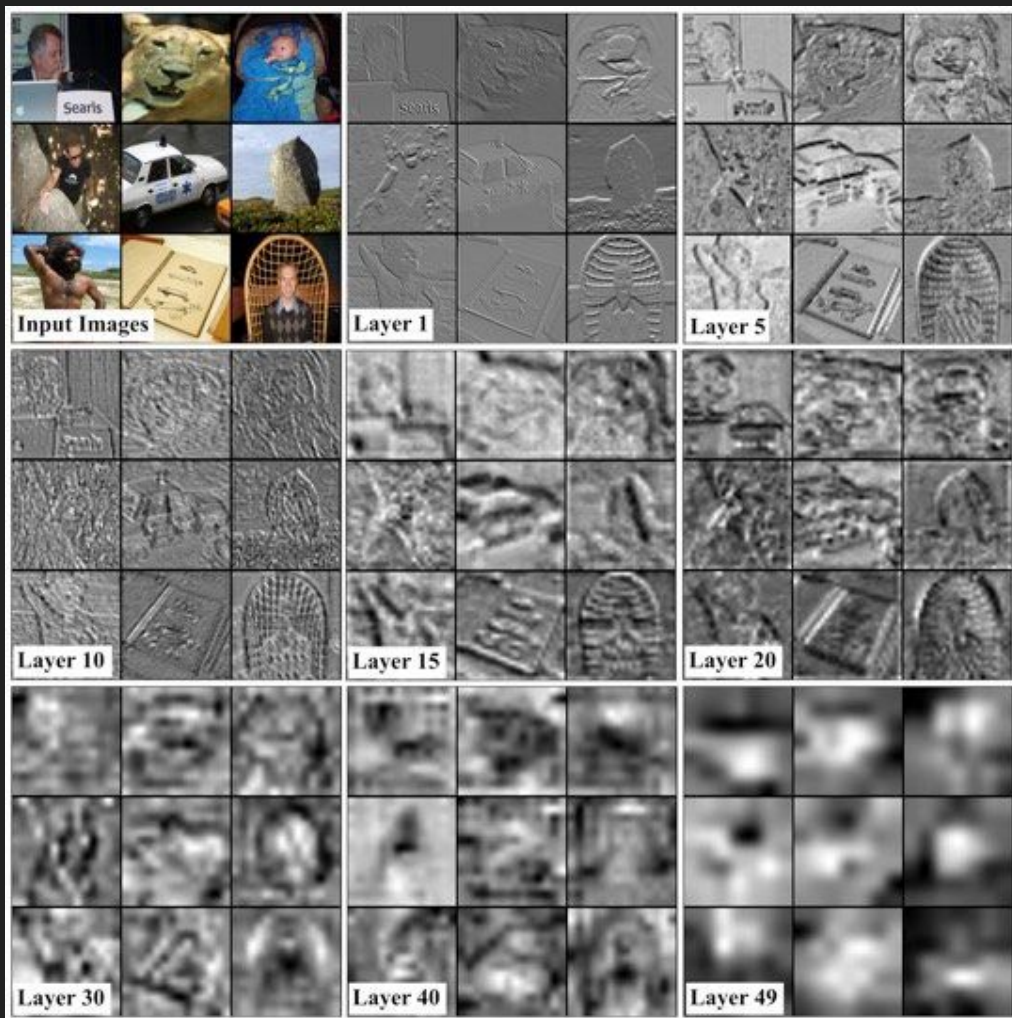
Elephants

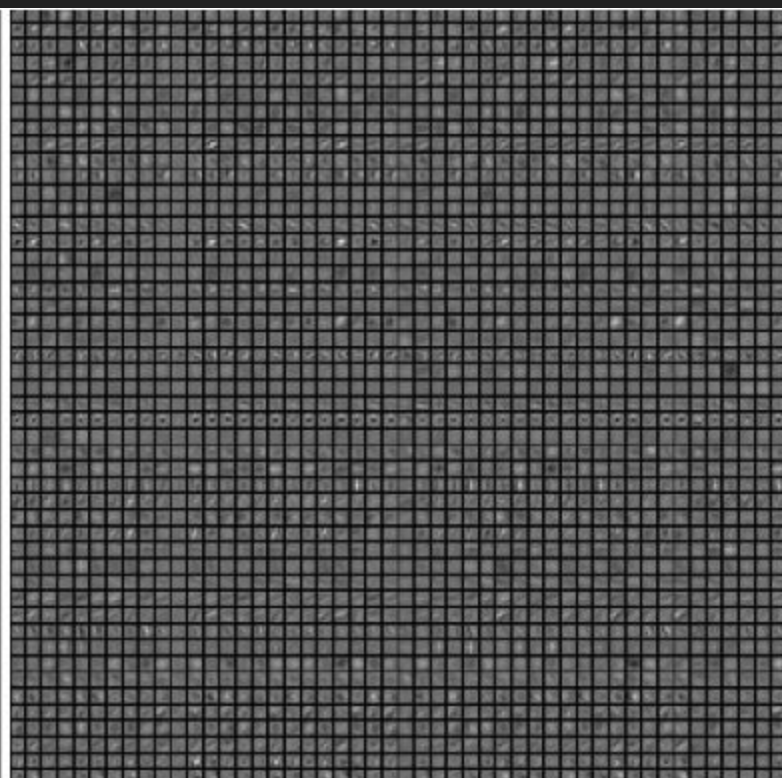
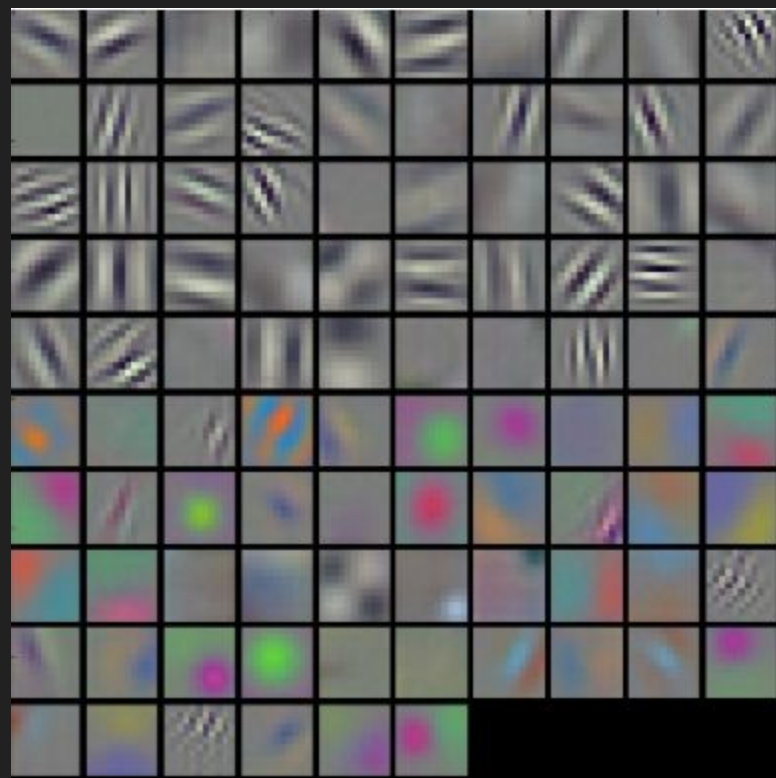


Chairs

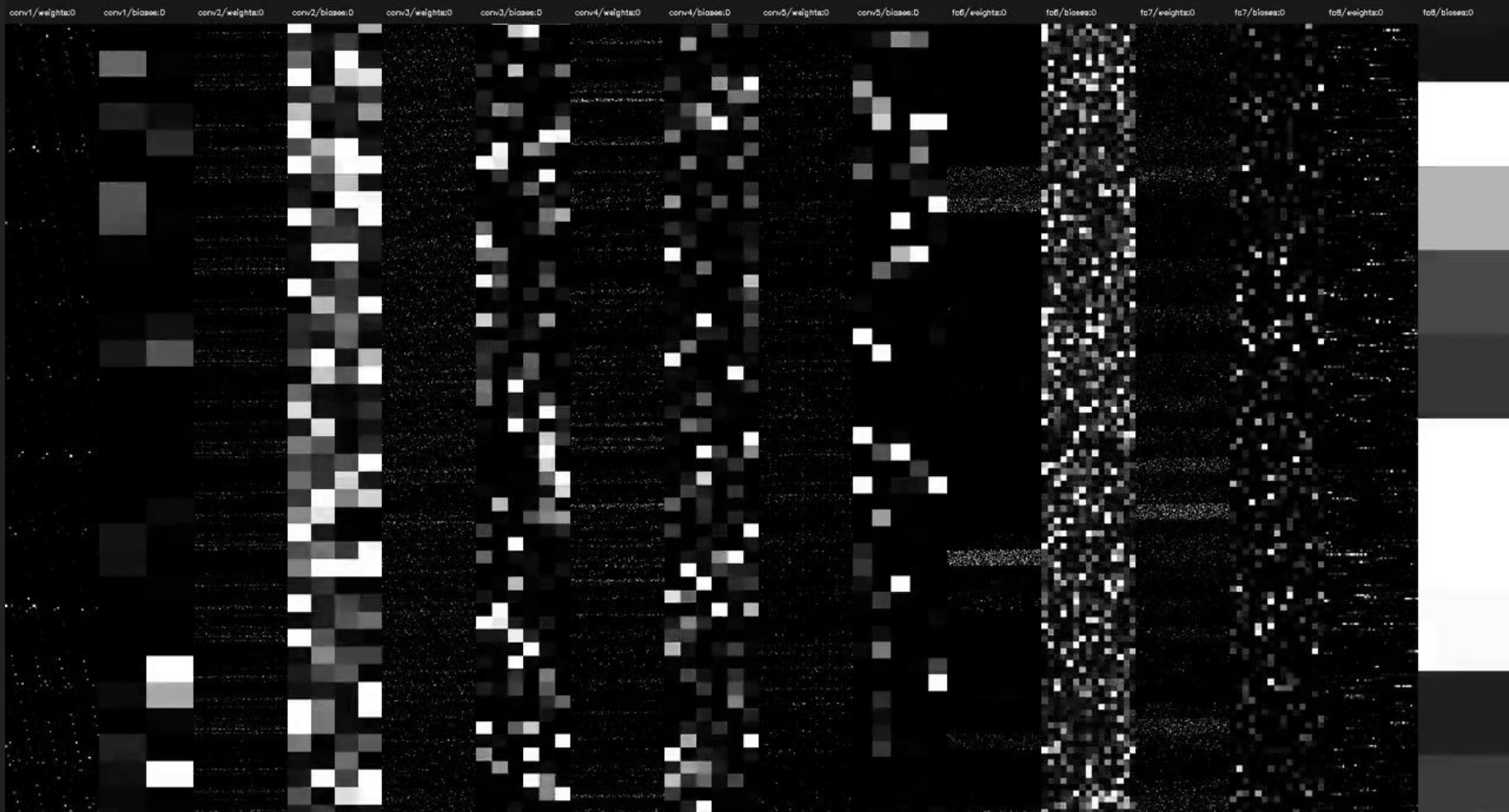


Problems







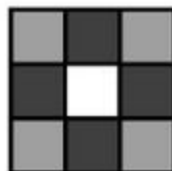
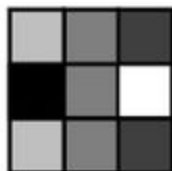
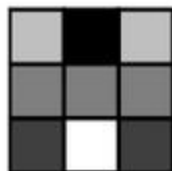
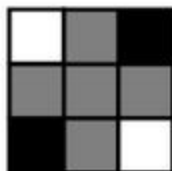
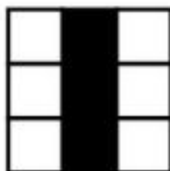
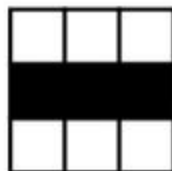
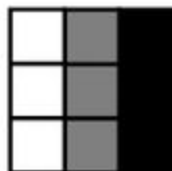
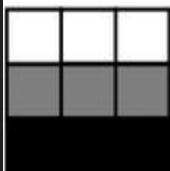


TDA for CNN

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
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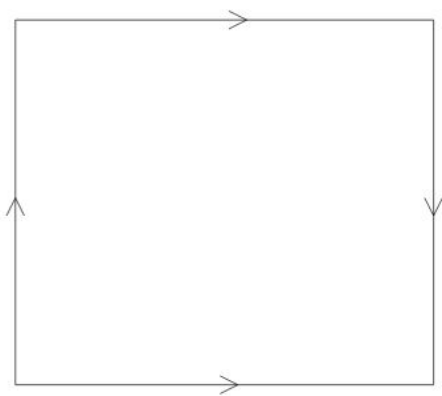


Fig. 4 Klein bottle representation as a rectangle with opposite edges identified

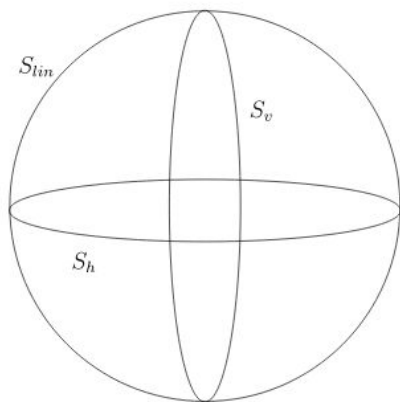


Fig. 5 The 'three circle' space

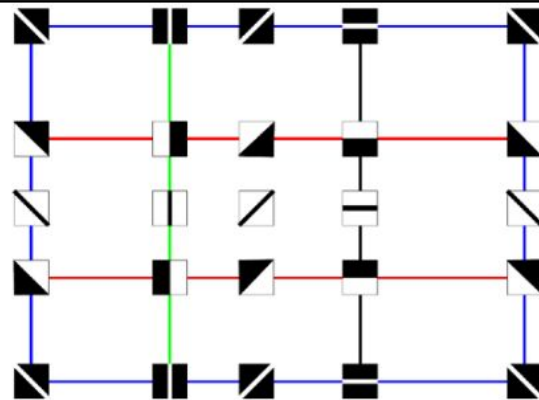


Fig. 6 3 by 3 patches parametrized by the Klein bottle

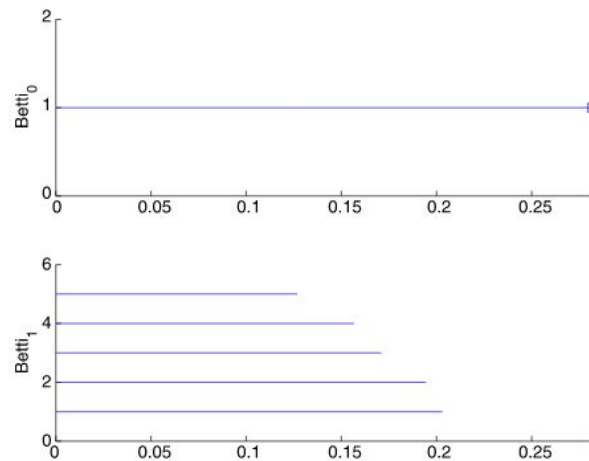
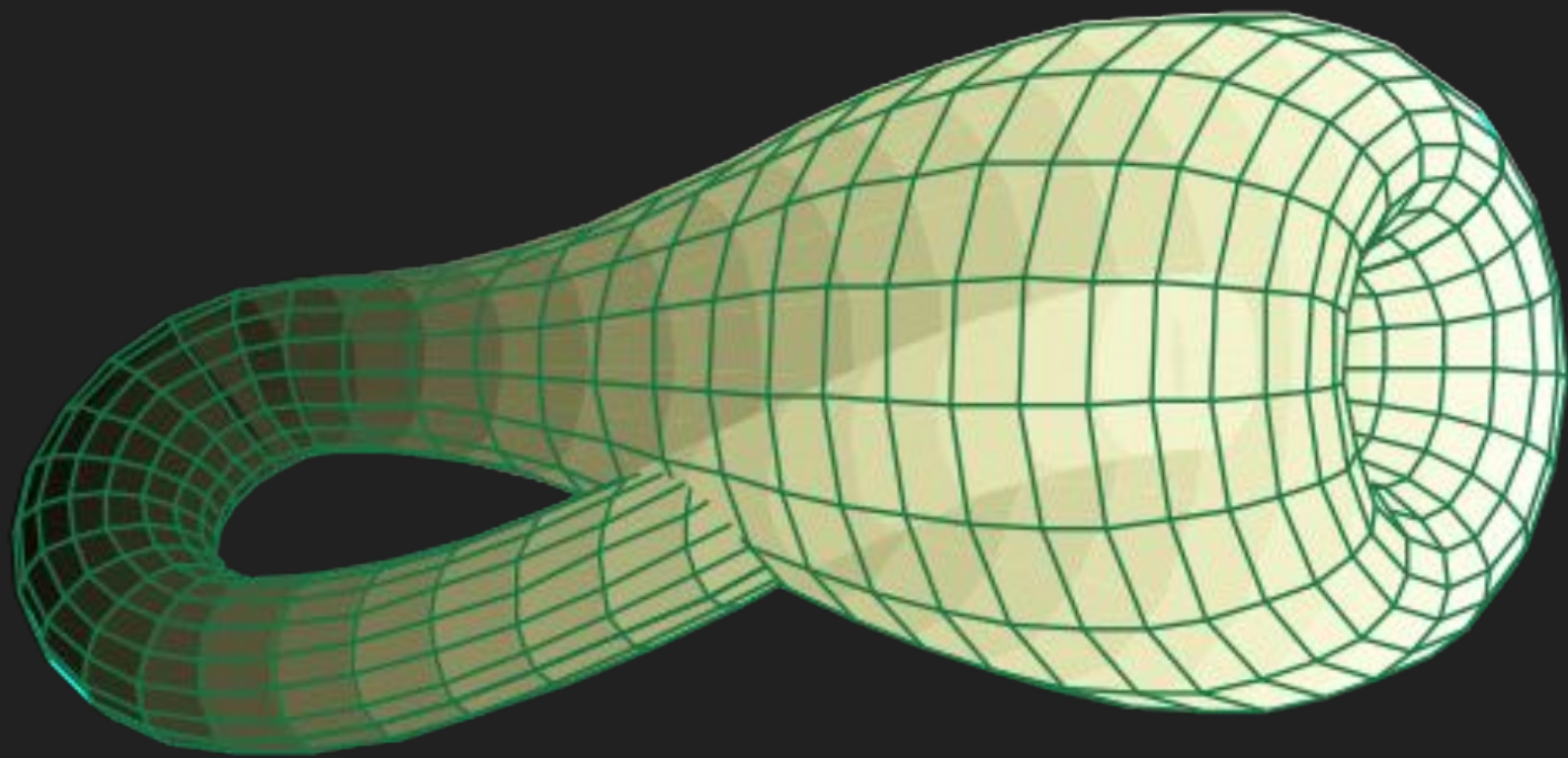
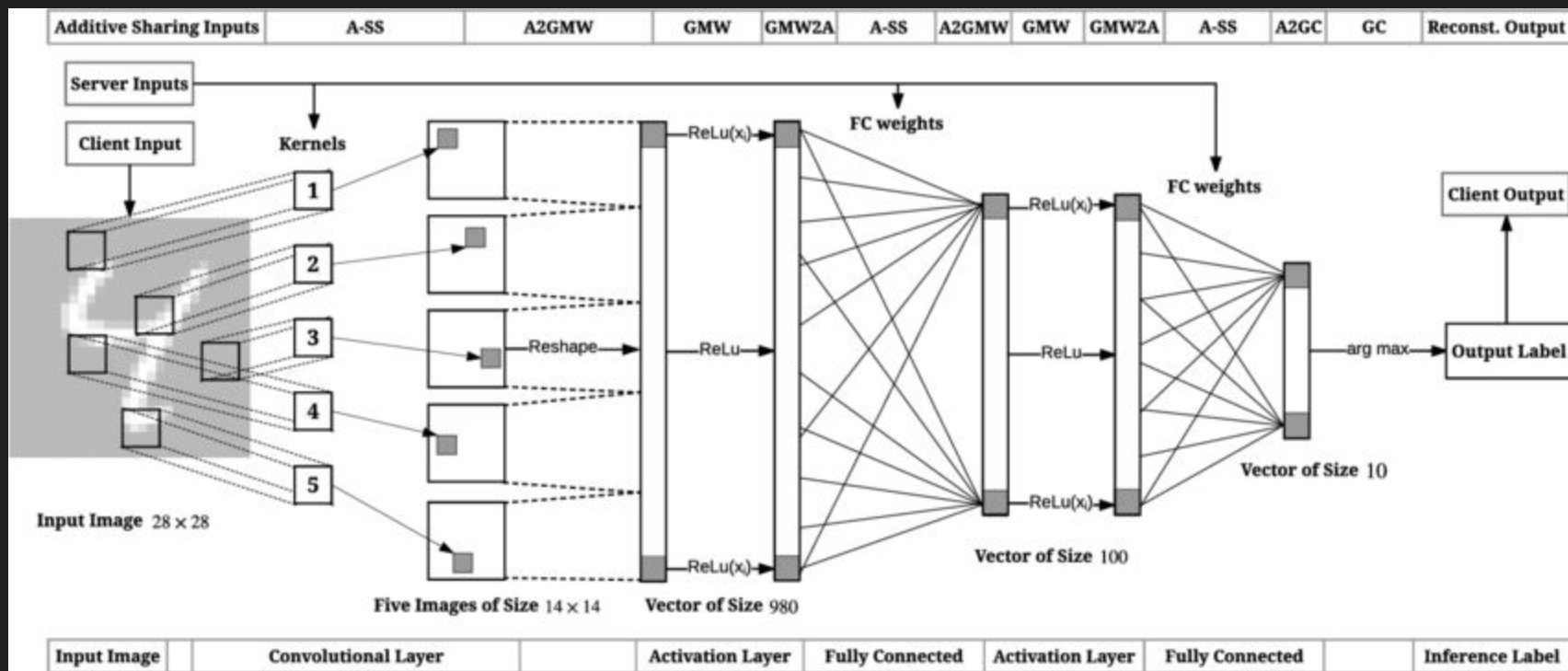
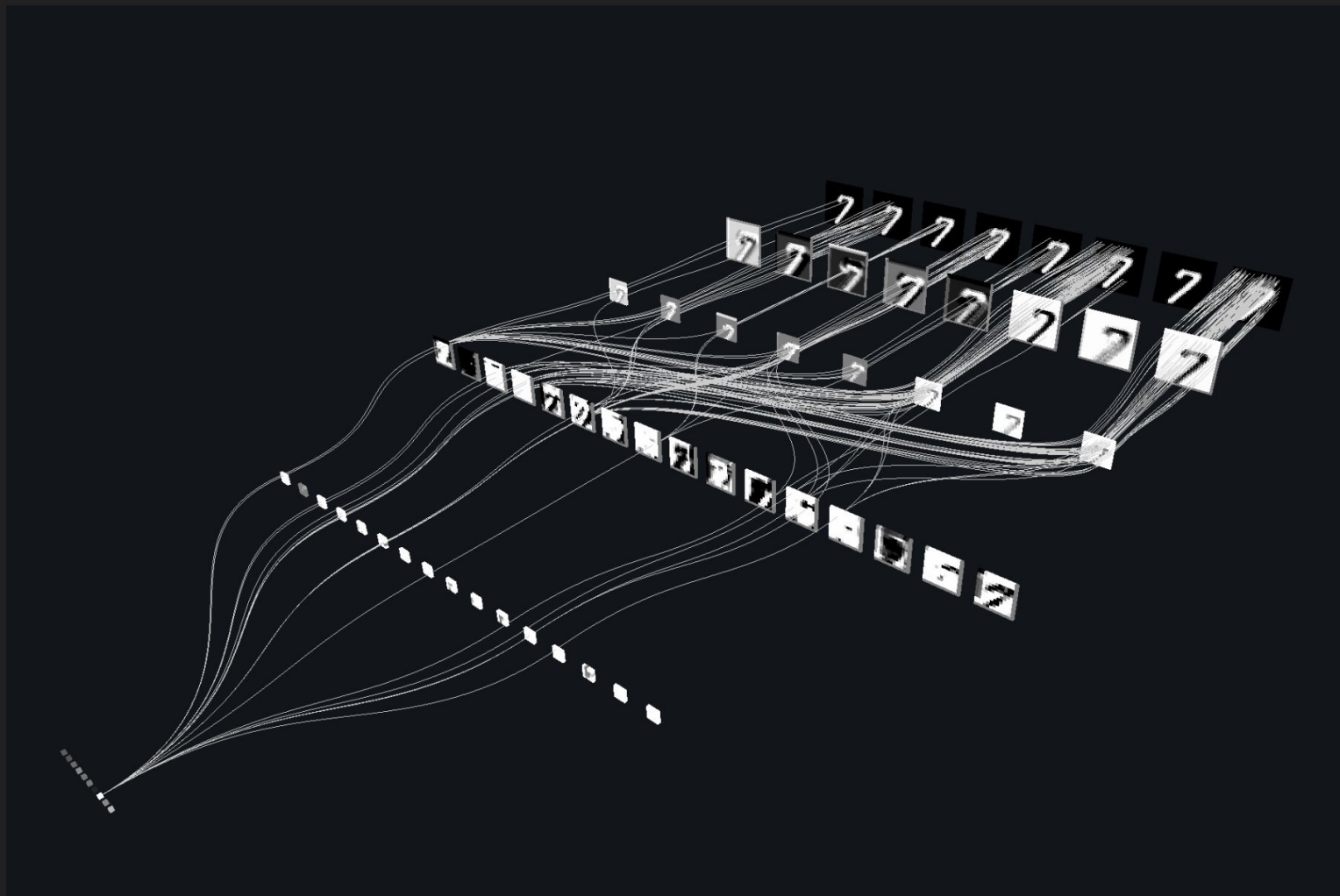


Fig. 7 PLEX results for $X(15, 30)$

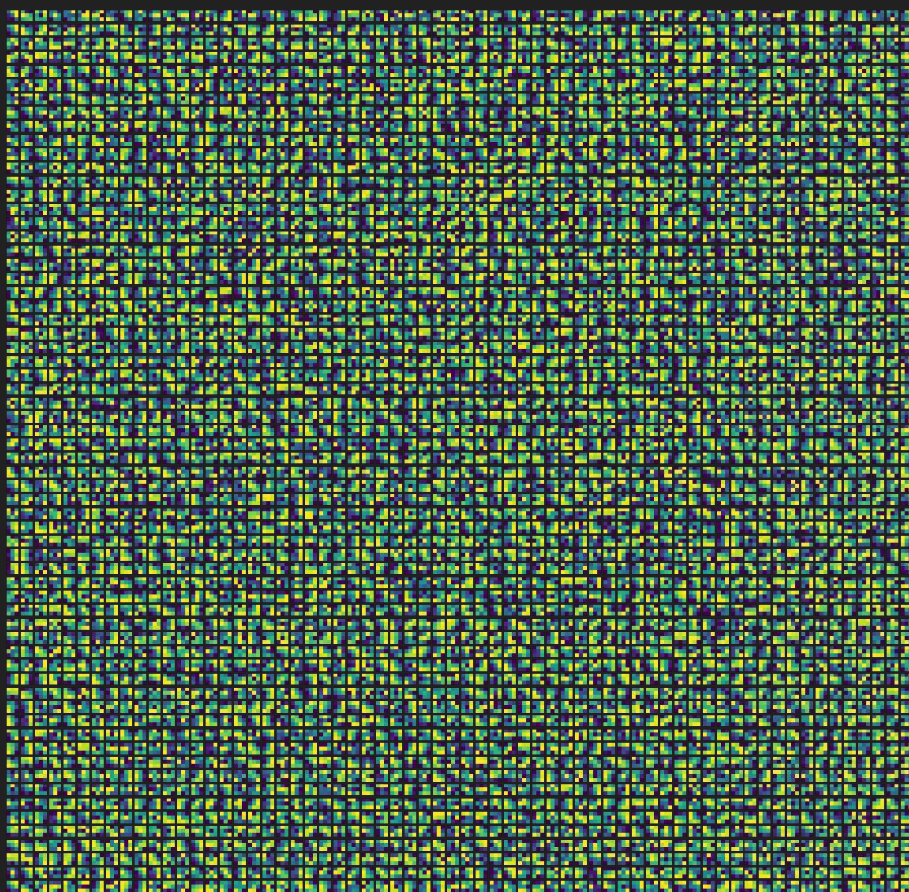


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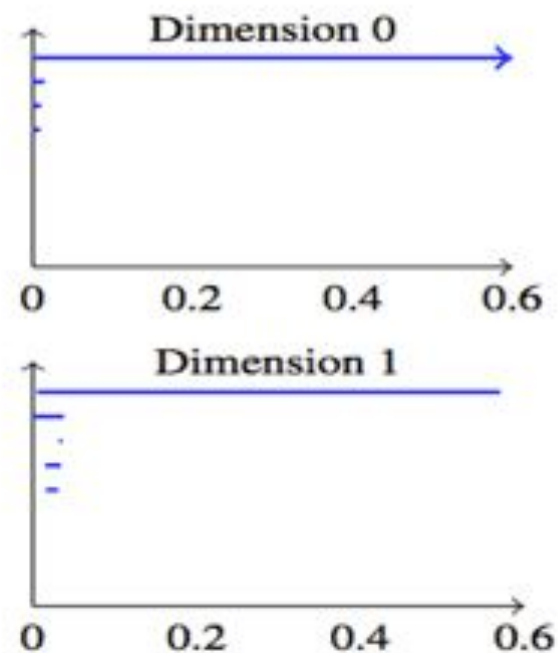
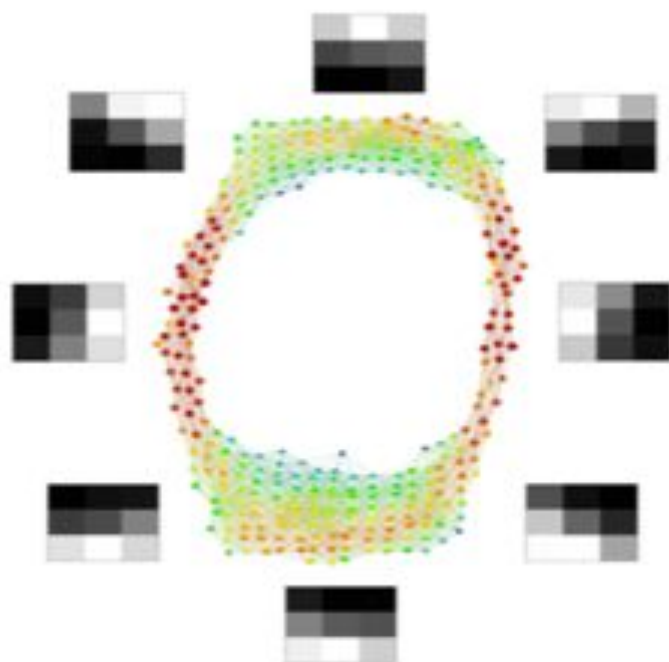
Using Topological Data Analysis to Understand the Behavior of Convolutional Neural Networks

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

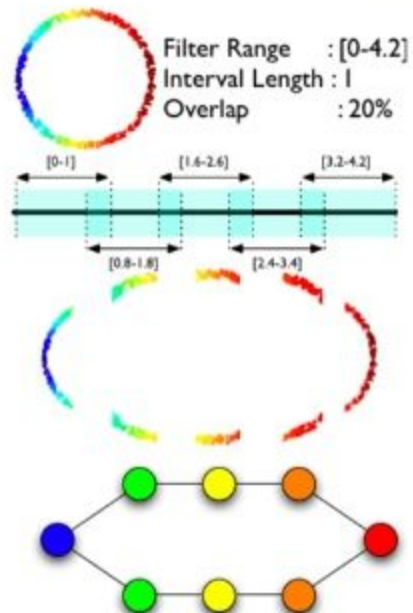
B Coloring by filter value



C Binning by filter value



D Clustering and network construction





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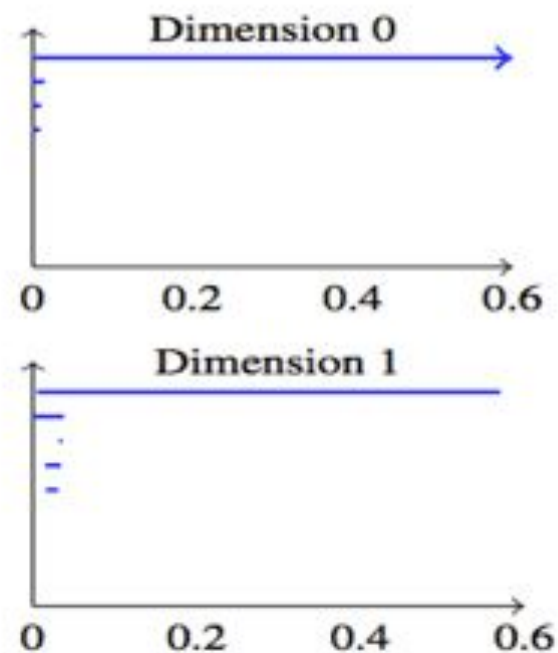
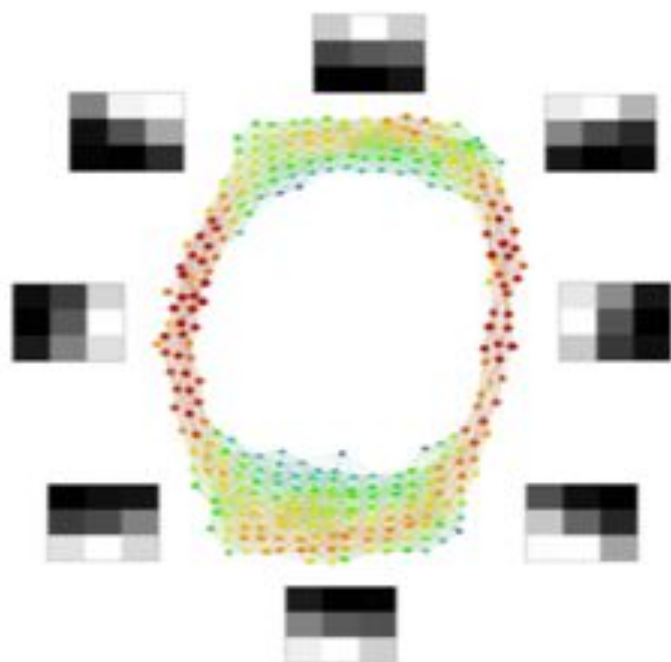
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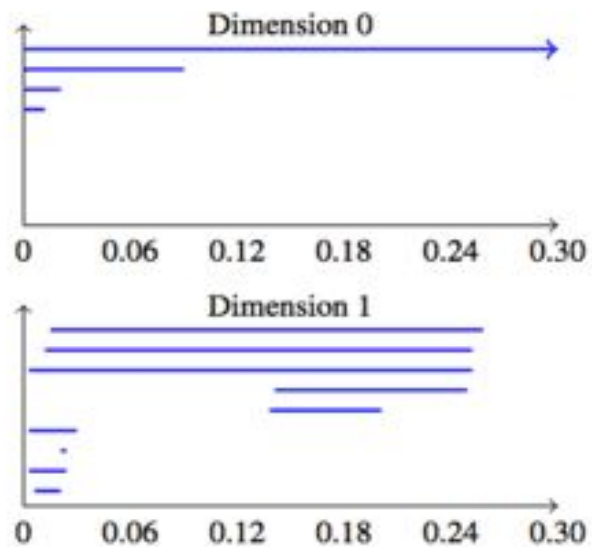
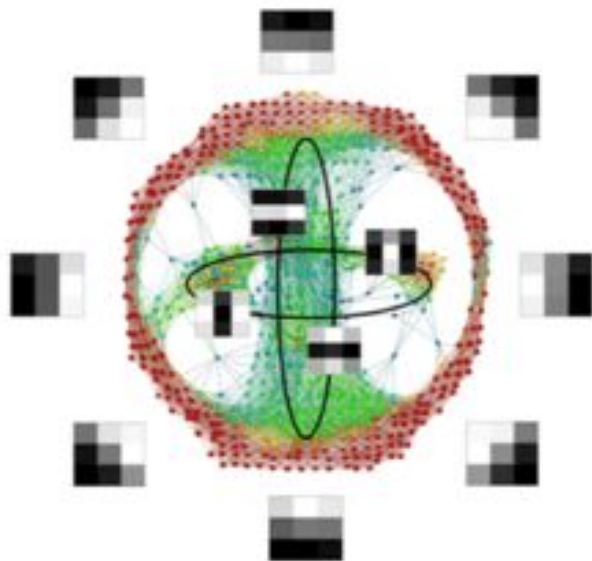


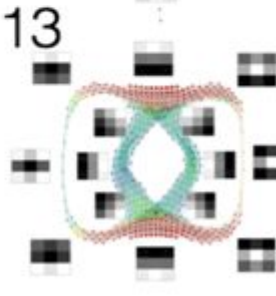
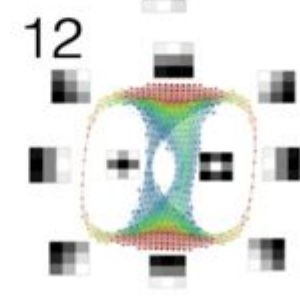
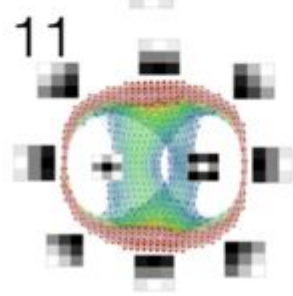
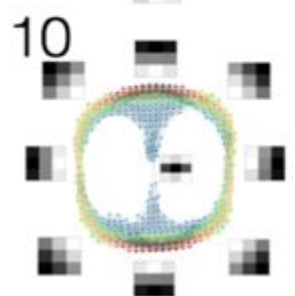
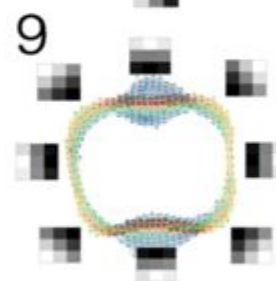
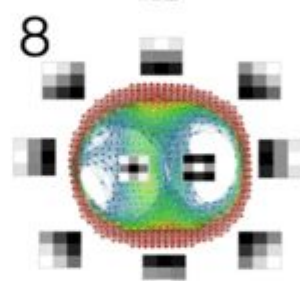
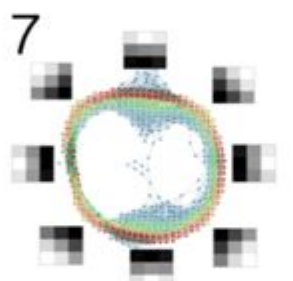
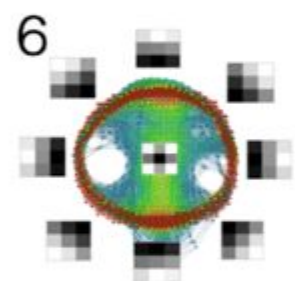
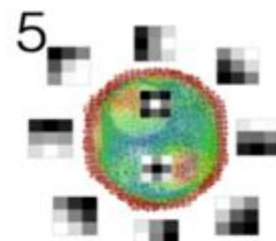
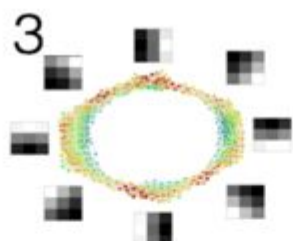
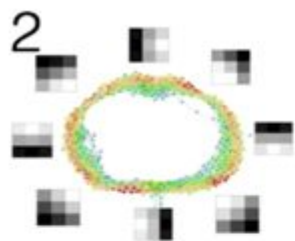
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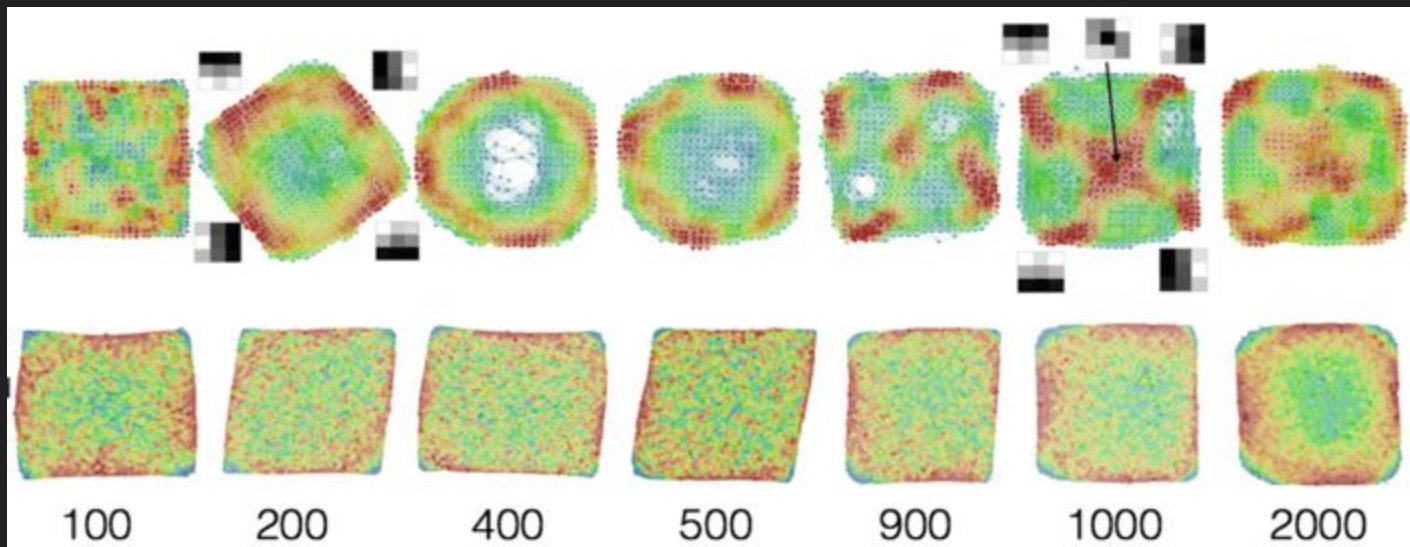
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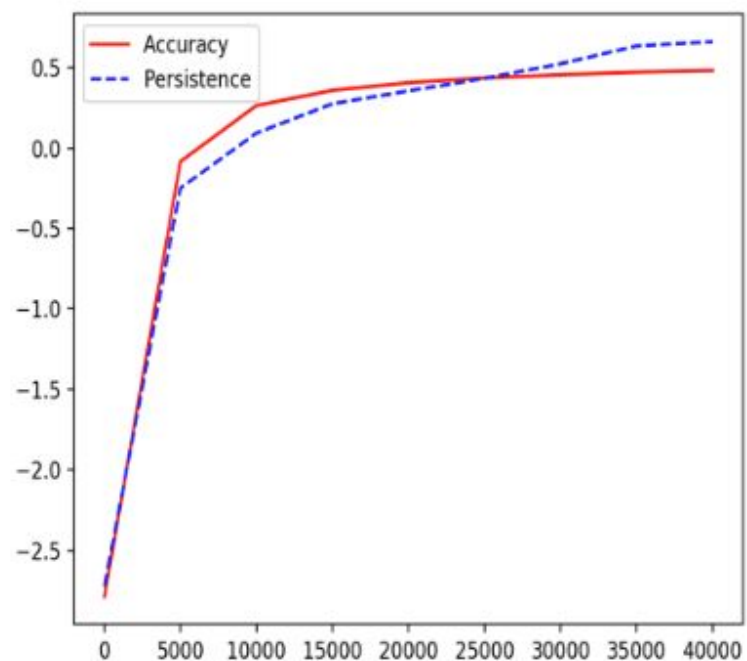
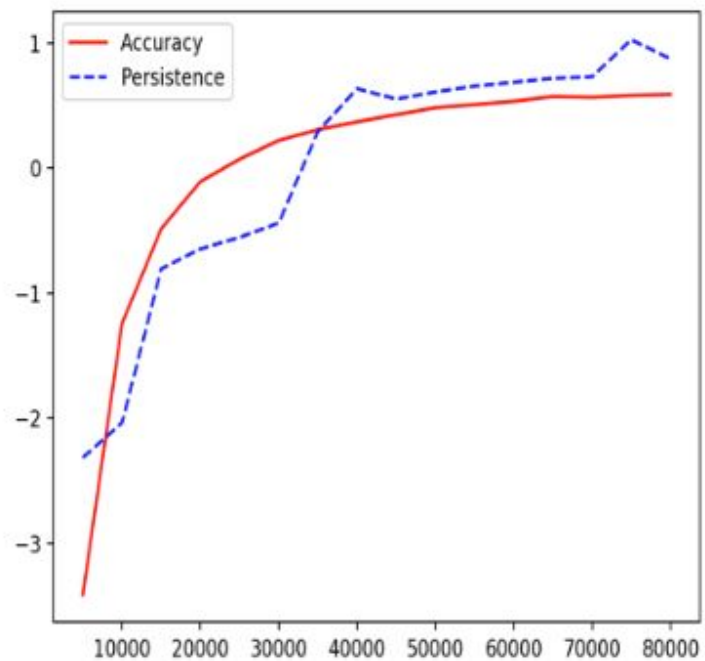
Going Deeper: Understanding How Convolutional Neural Networks Learn Using TDA

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



325

50

-35-

45

30

-20-

300

575



?

Weapon of choice



ਗੁਫੀ 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](#)

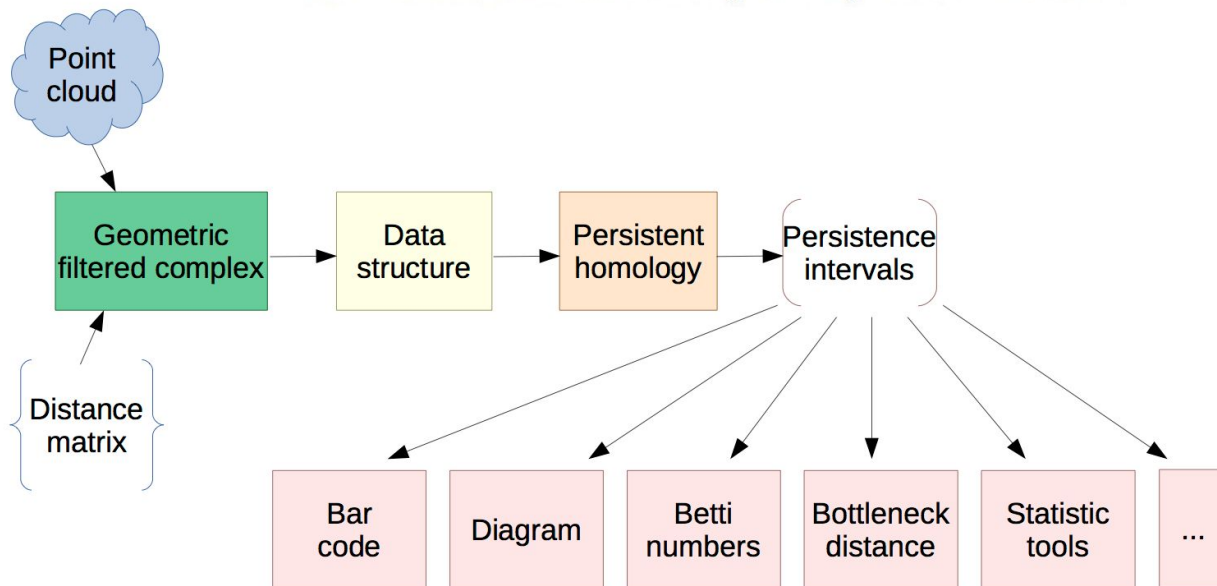
New release - [GUDHI version 2.1.0](#)

New release - [GUDHI version 2.0.1](#)

[More](#) ›

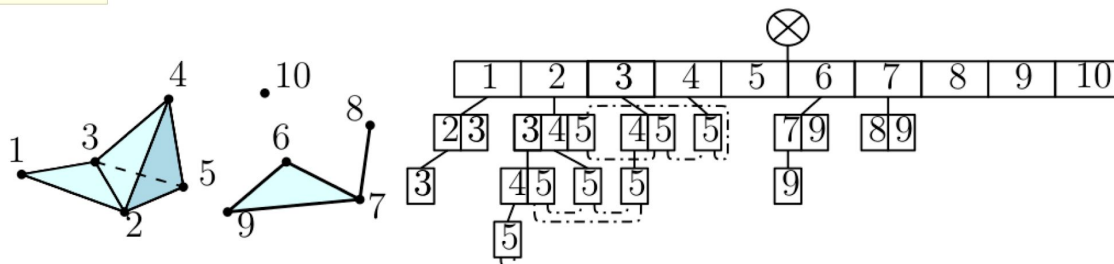
गुढी GUDHI

Geometric Understanding in Higher Dimensions



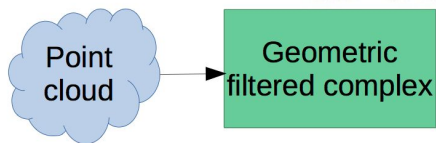
Data
structure

Filtered simplicial complexes – Simplex tree

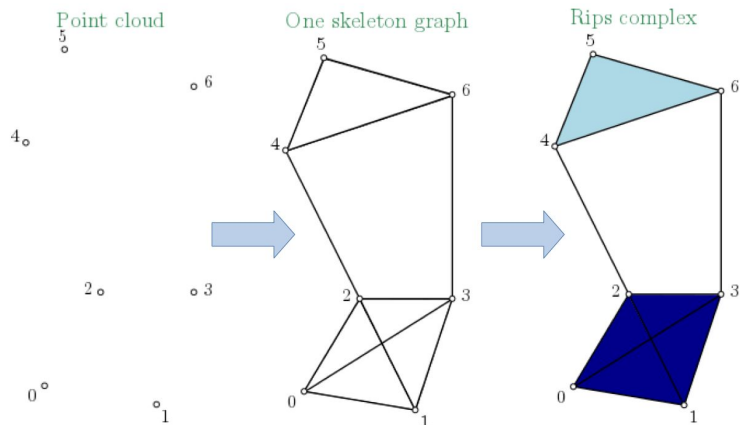


- Memory and time-efficient data structure to store simplicial complexes.
- Every simplex is a word stored in the tree.
- The nodes corresponding to simplices of the same dimension having the same maximal vertex are stored in a cyclic list.
- It is a base of all algorithms to compute persistence of weighted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

by Clément Maria



Geometric filtered complex – Rips from a point cloud



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.

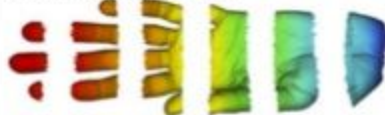
The authors of Python mapper are [Daniel Müllner](#) and [Aravindakshan Babu](#). (PyPI apparently suppresses everything but the first name in the “author” field, hence only one author is displayed below.)

MAPPER IV

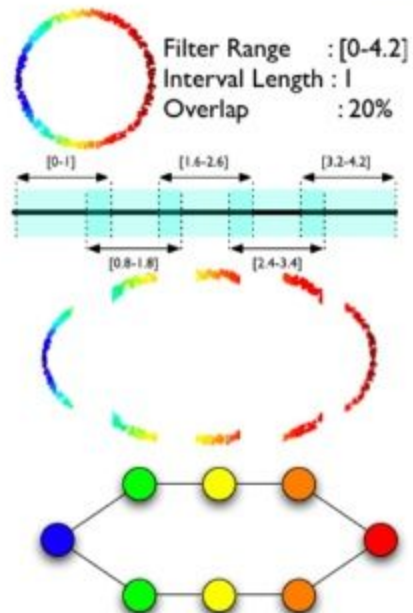
B Coloring by filter value

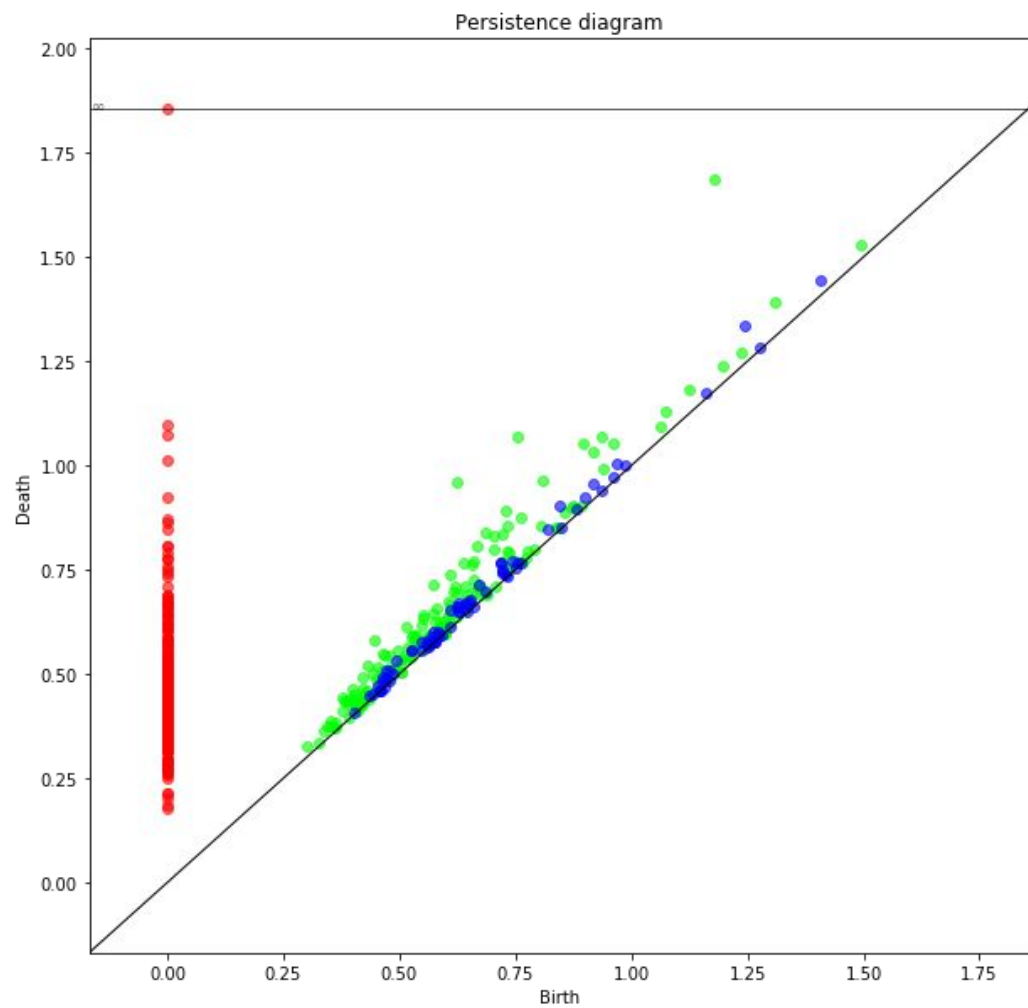


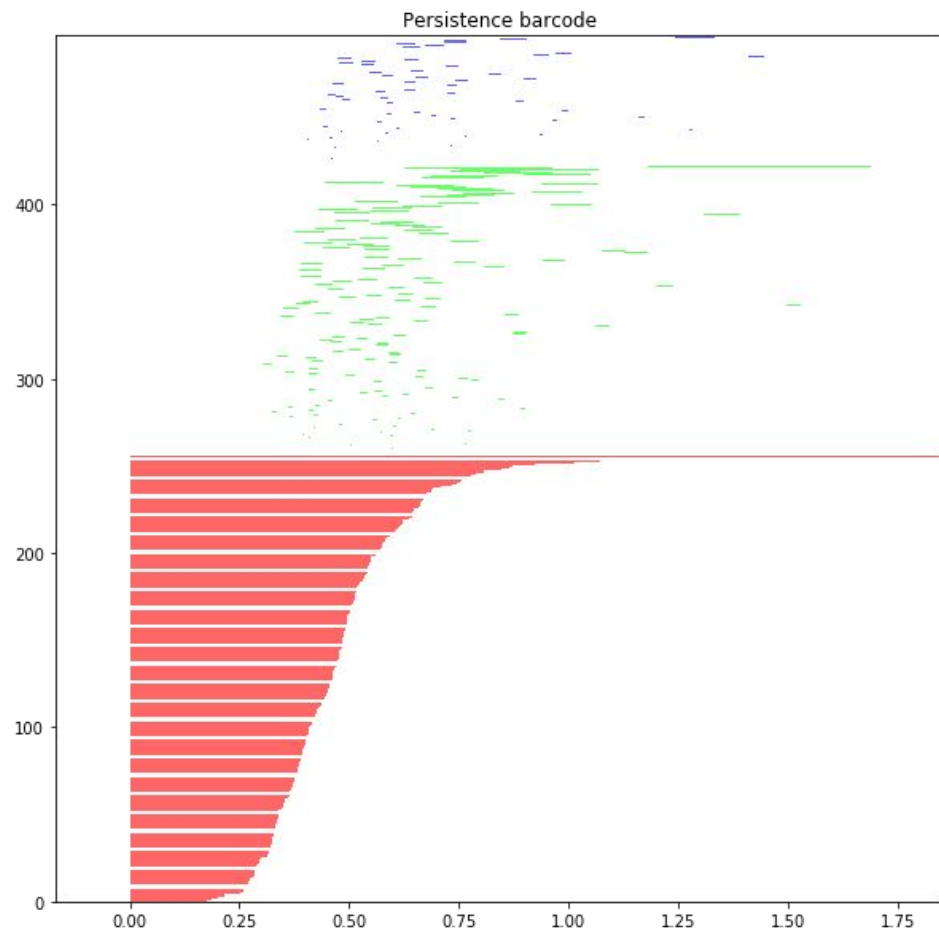
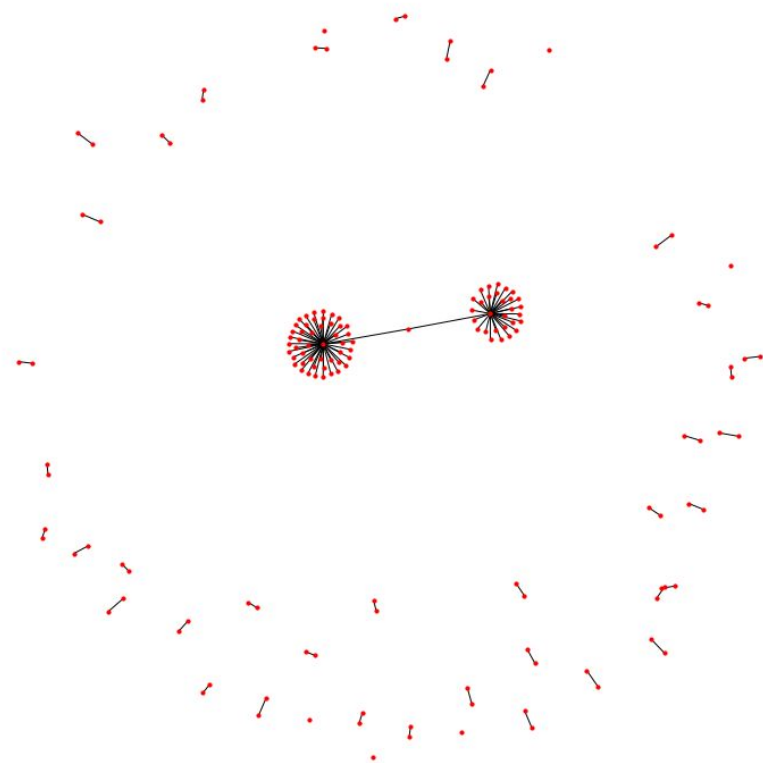
C Binning by filter value

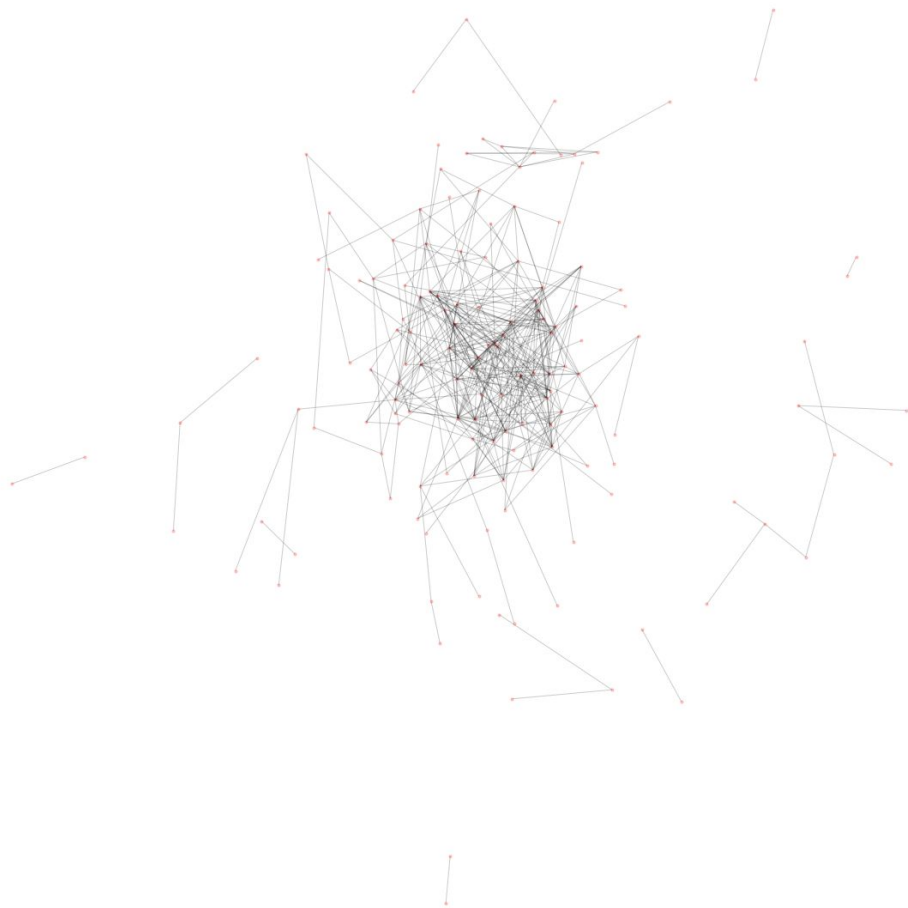


D Clustering and network construction

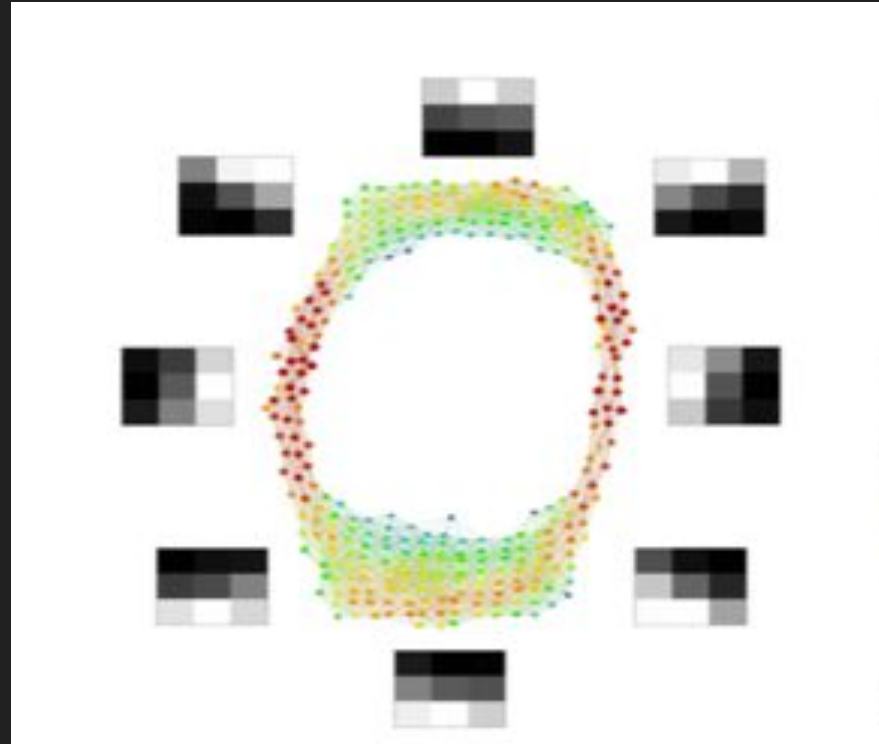








???



```
model.summary()
```

Layer (type)	Output Shape	Param #
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

=====
Total params: 14,714
Trainable params: 14,714
Non-trainable params: 0
=====

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

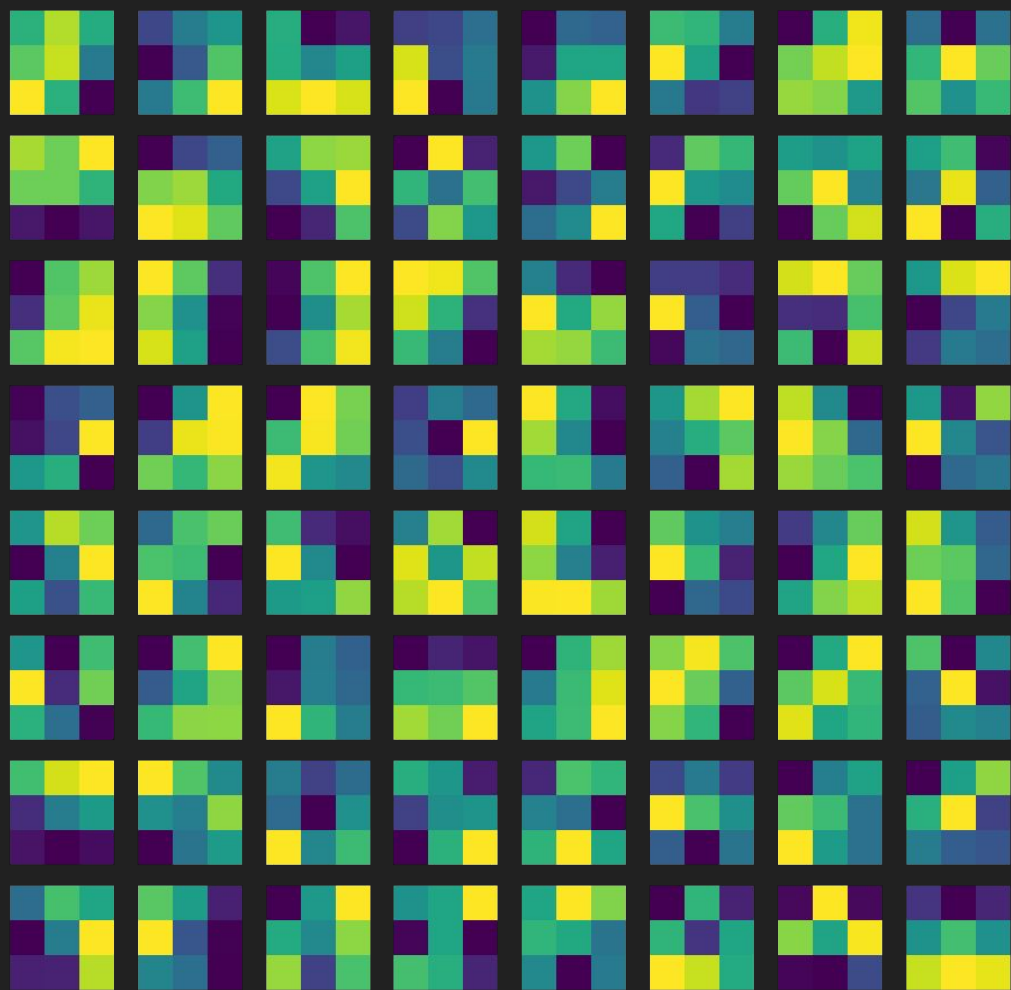
Epoch 6/8
60000/60000 [=====] - 3s 48us/step - loss: 0.0605 - acc: 0.9822 - val_loss: 0.0509 - val_acc : 0.9828

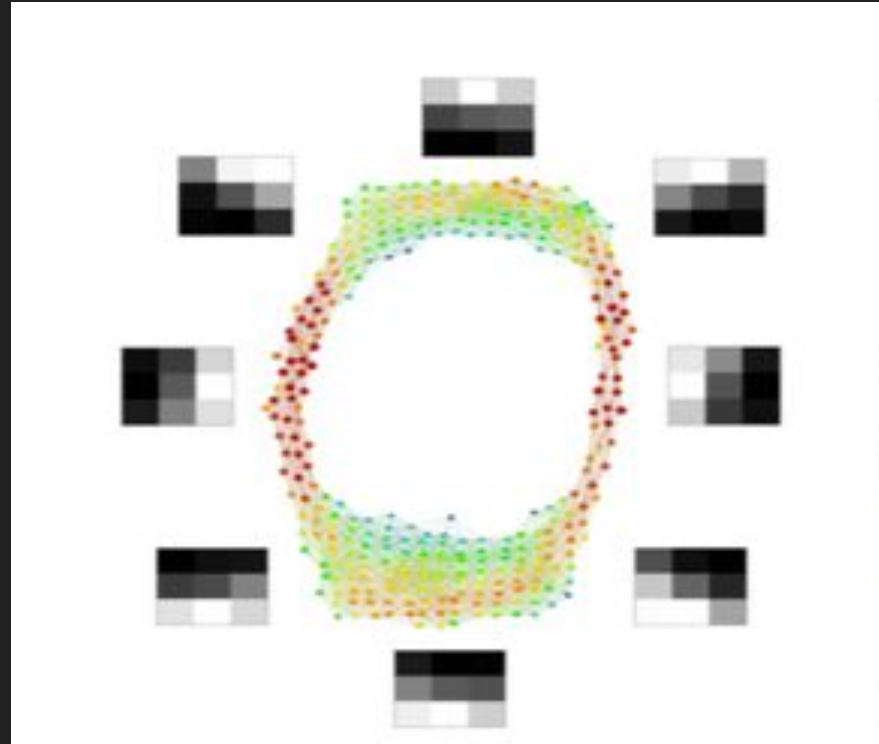
Epoch 7/8
60000/60000 [=====] - 3s 48us/step - loss: 0.0540 - acc: 0.9837 - val_loss: 0.0562 - val_acc : 0.9826

Epoch 8/8
60000/60000 [=====] - 3s 47us/step - loss: 0.0486 - acc: 0.9850 - val_loss: 0.0528 - val_acc : 0.9829

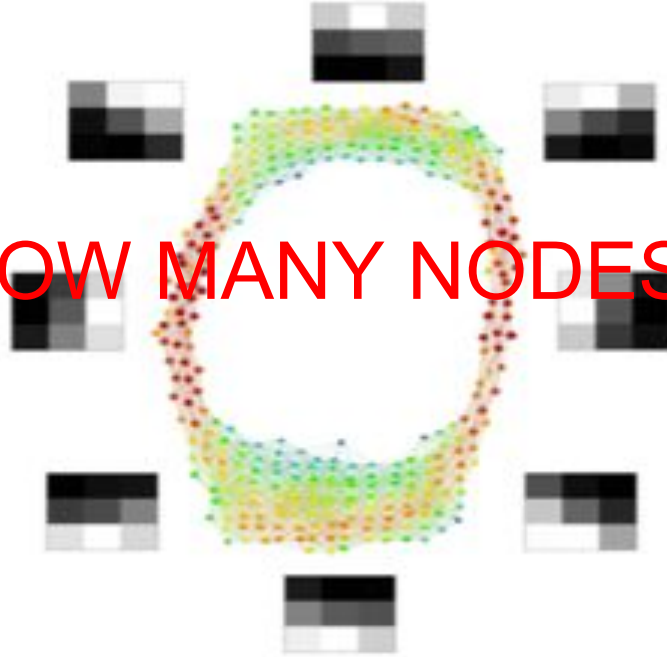
Test loss: 0.05276332234479487

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
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1. 引言

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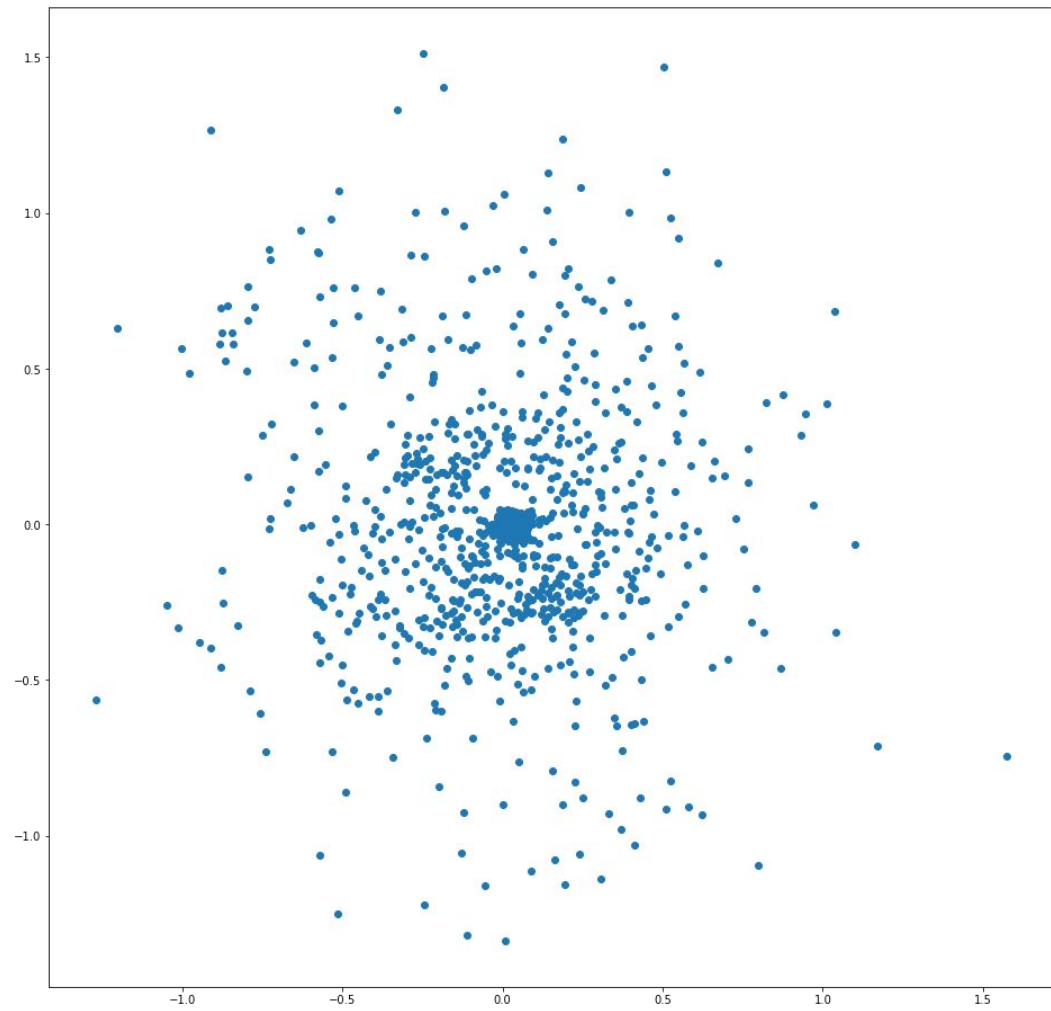
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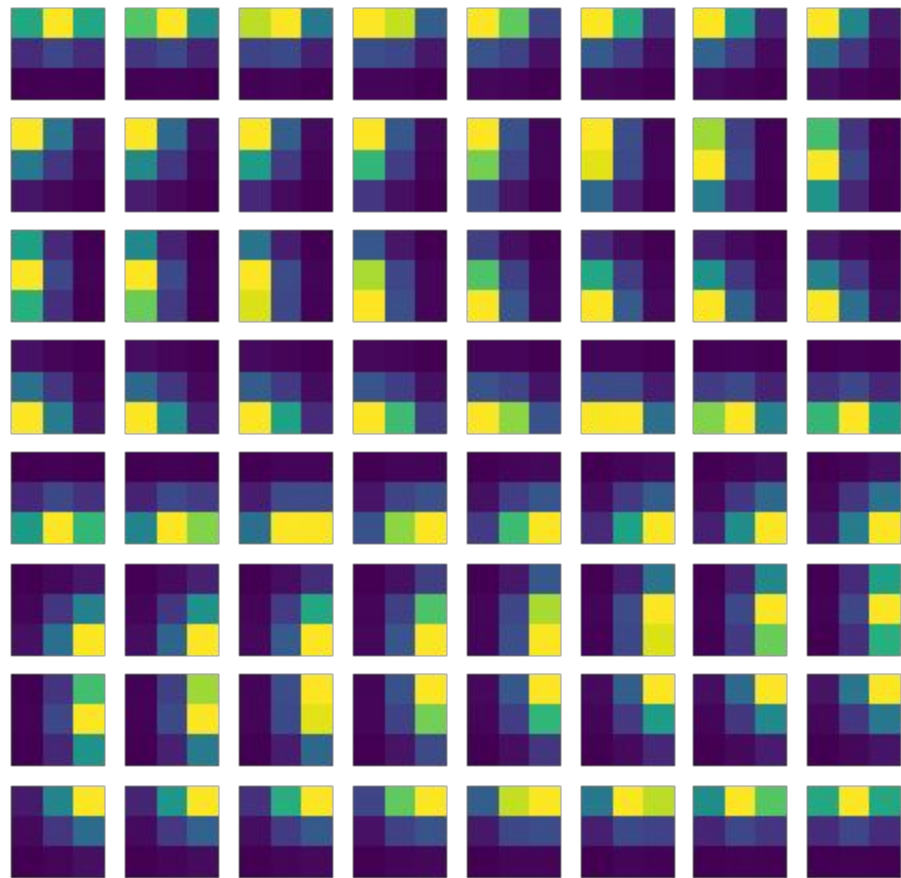
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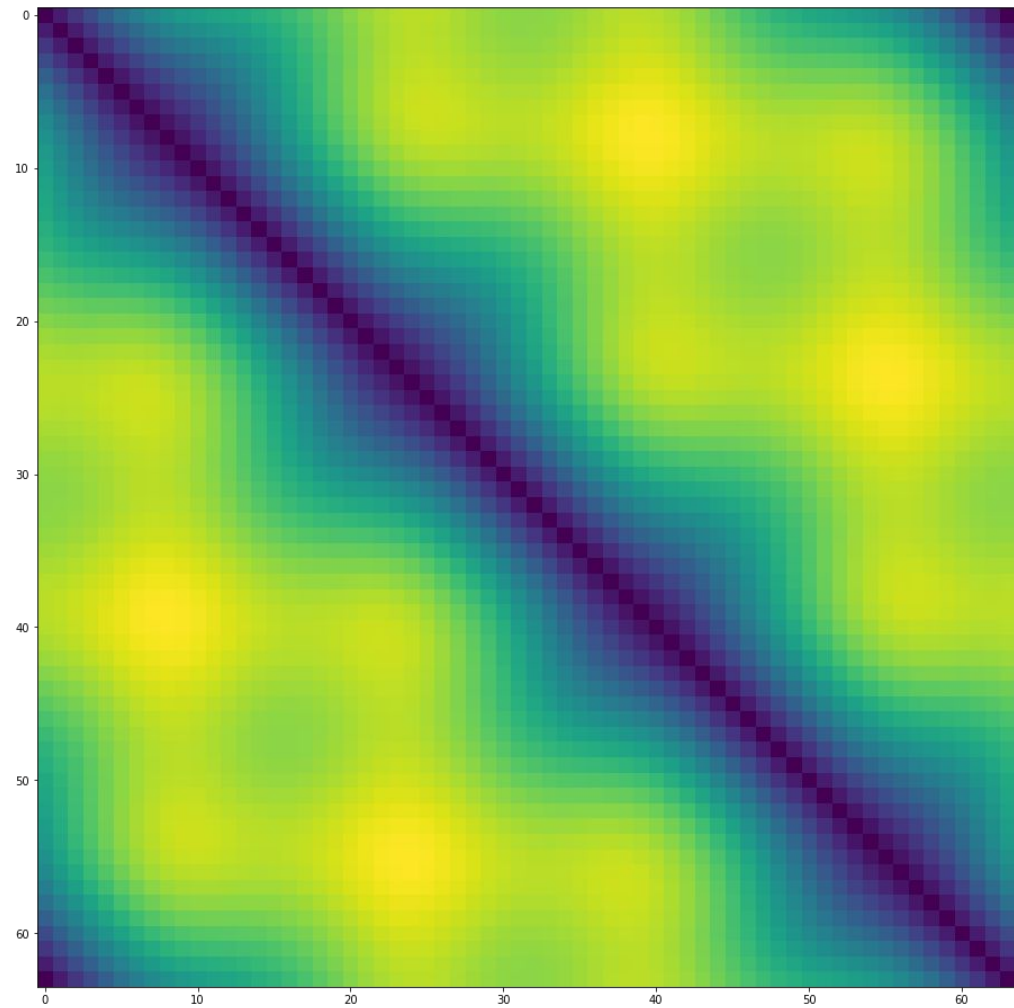
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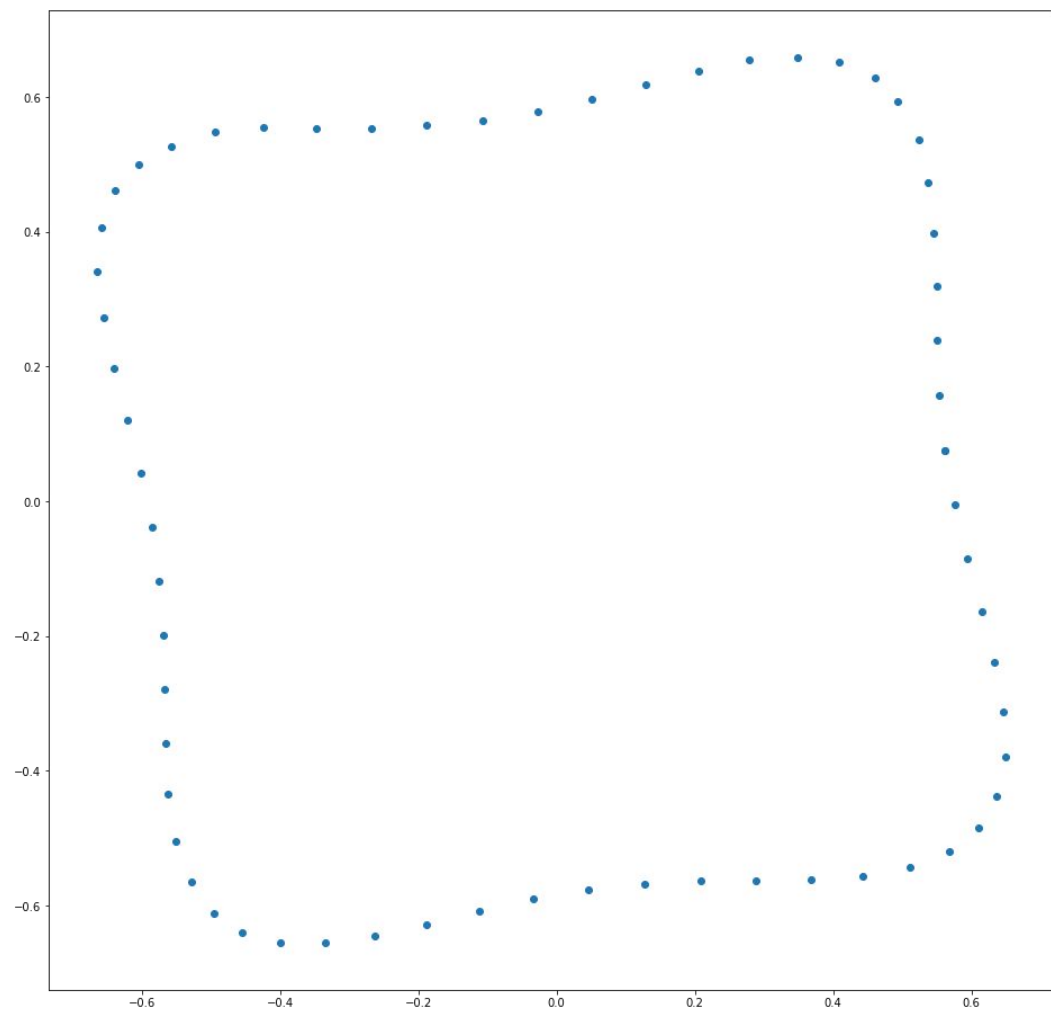
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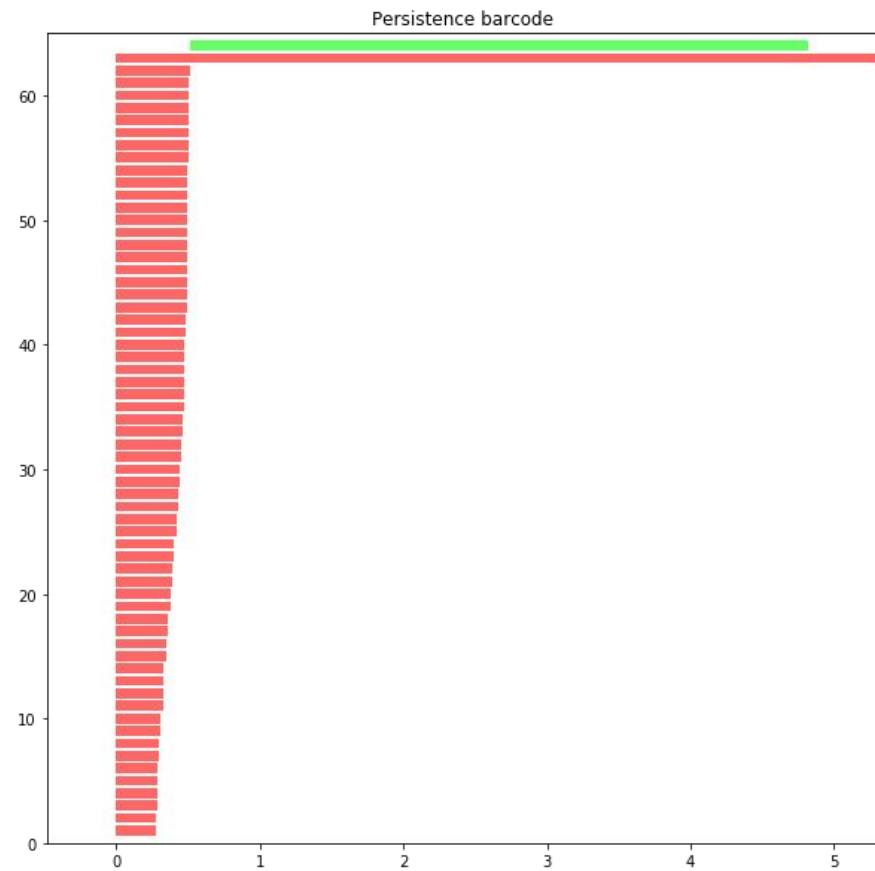
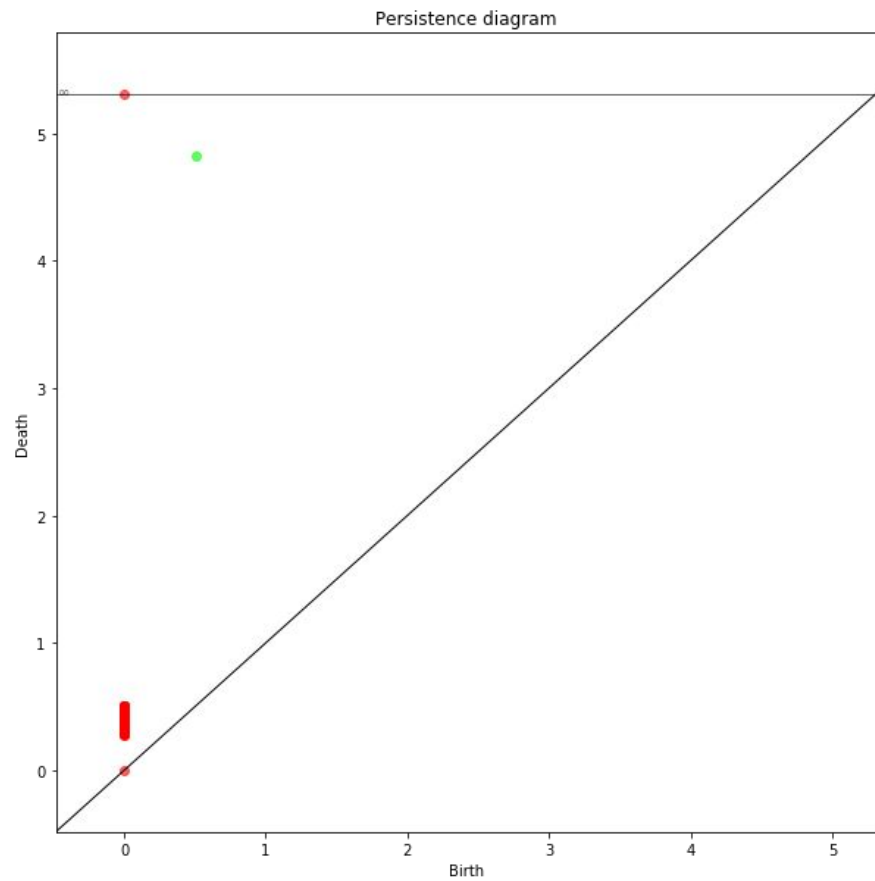


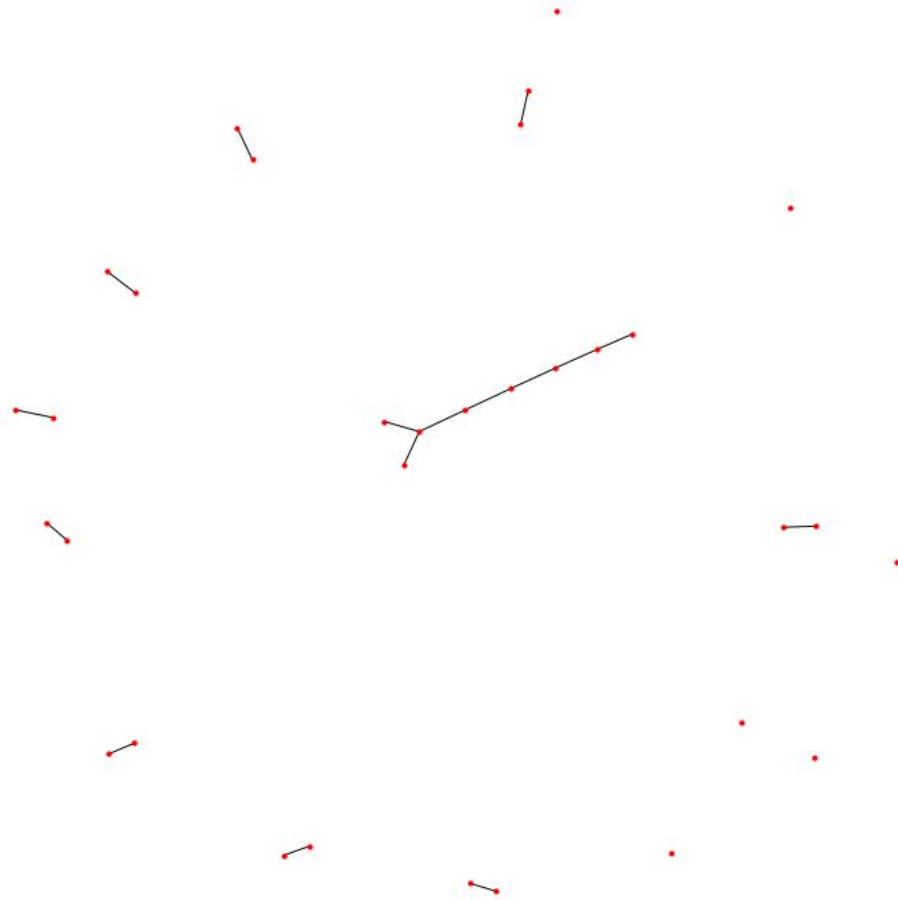
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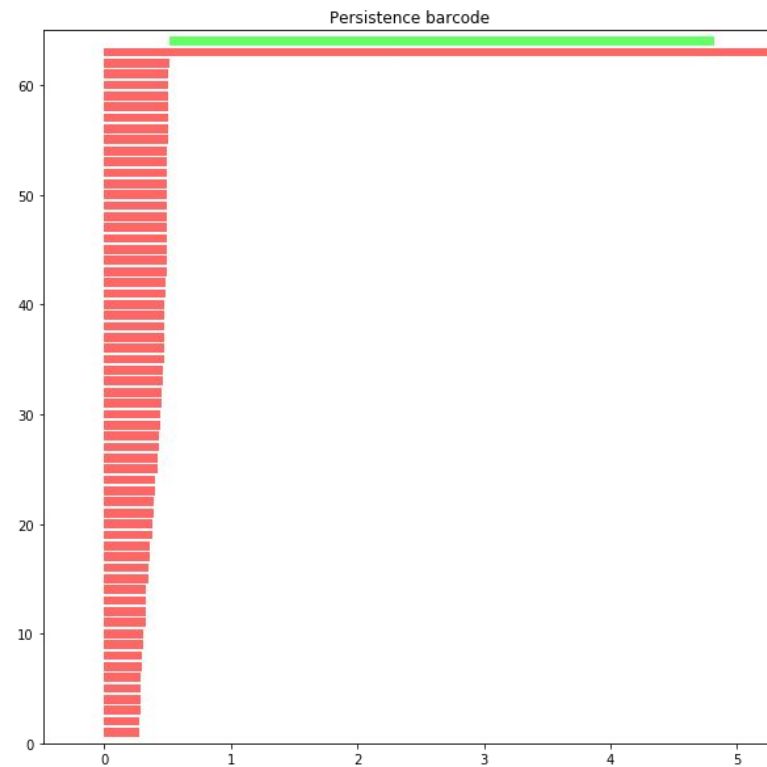
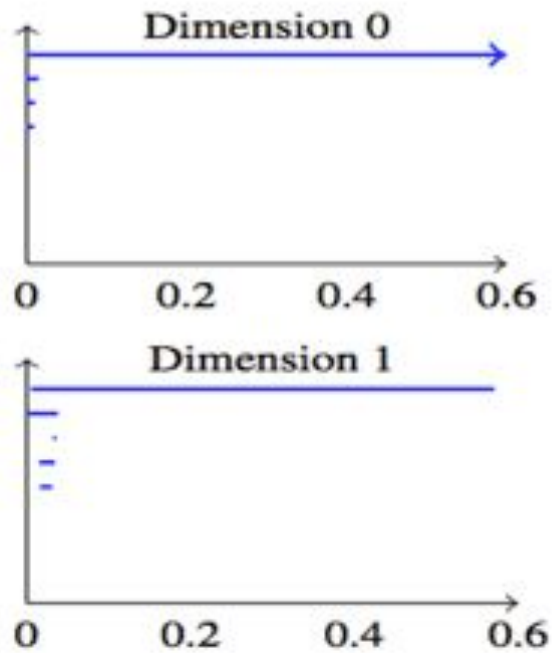












Conclusion

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 this 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 !

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