

Discovering the underlying topological space of extracted features

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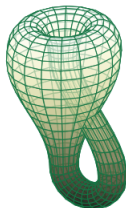
The Big Problem

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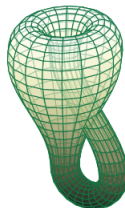
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Source:

www.gnuplotting.org/klein-bottle/

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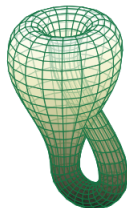
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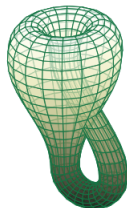
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- Question 1: What if our data isn't from a manifold? Could the features be parametrized by a manifold?

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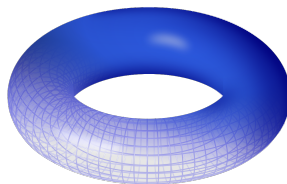
- Data is maybe from a manifold?
- Manifold learning makes this assumption
- Question 1: What if our data isn't from a manifold? Could the features be parametrized by a manifold?
- Question 2: Neural networks often become a black box. What is happening inside?

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www.gnuplotting.org/klein-bottle/

Why do we care?

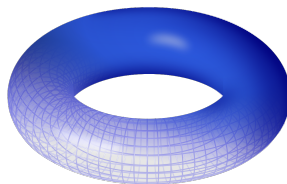
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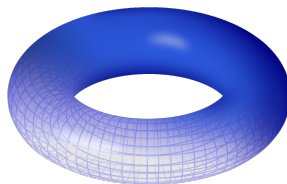
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Why do we care?

- Manifolds have nice mathematical structure (locally Euclidean, lots of structure, etc)
- Can assign coordinates on the manifold rather than in \mathbb{R}^n
- This might help with prediction!

Topology and Machine Learning

- Persistent homology: used to deduce topological structure from data points. Comes from Topological Data Analysis (TDA)
- Convolutional Neural Network (CNN): Great for feature extraction from images

Quick Topology Intro

Concerned with properties that don't change under continuous deformations

- Like stretching, shrinking, and bending
- But NOT cutting, gluing, etc.

Example: Circle = Square = Triangle



Source:
<https://www.shapeways.com/blog/archives/a-3d-printed-topology-joke.html>

Quick Topology Intro

Homology is a sequence of groups (an algebraic structure) that keeps track of "holes" and their higher dimensional analogues. So if X is a topological space, then:

- $H_0(X)$ counts the number of connected pieces
- $H_1(X)$ counts the number of loops
- $H_2(X)$ counts the number of "voids" (like the inside of a beach ball)

Persistent homology of rotations of everyday objects

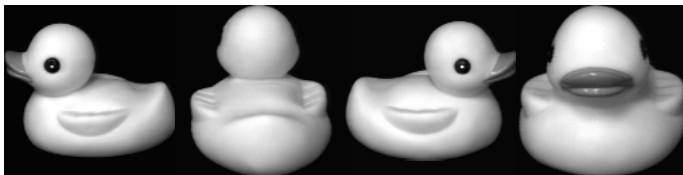
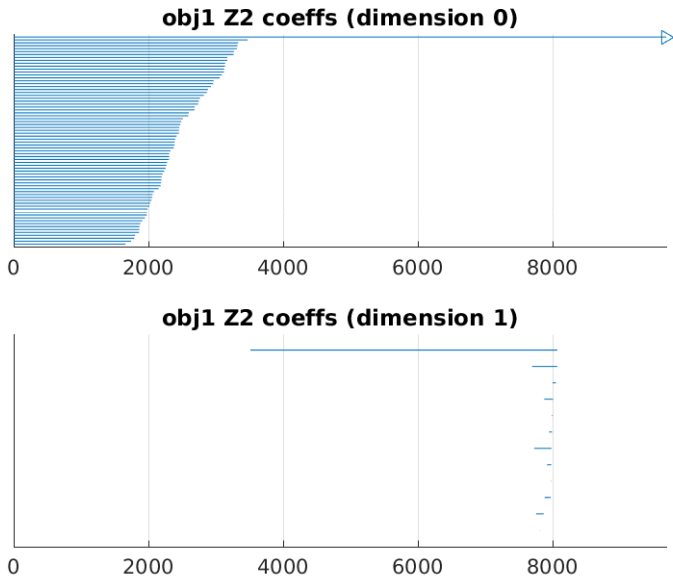


Figure: Rotation of rubber duck

Inspiration

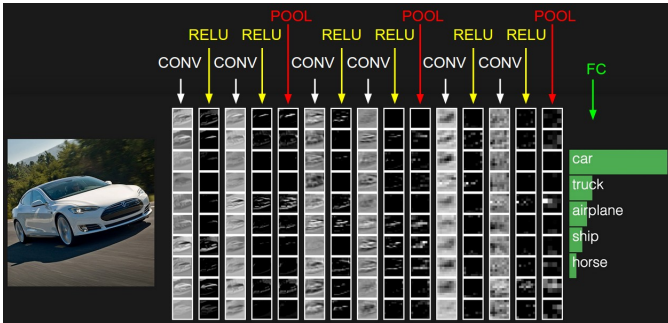


Our Data

Needed thousands of photos to train a neural network - so we used the CASIA-Webface dataset. It is a public dataset consisting of of 494,414 images [2].



Convolutional neural network

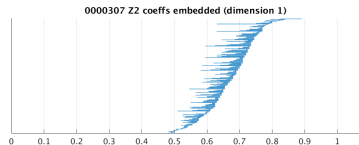
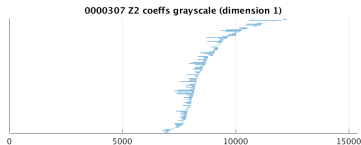
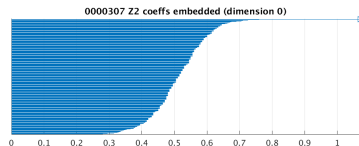
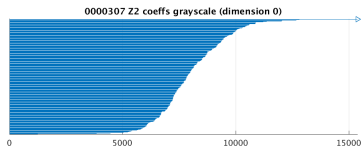


Architecture

layer	size-in	size-out	kernel	param
conv1	$220 \times 220 \times 3$	$110 \times 110 \times 64$	$7 \times 7 \times 3, 2$	9K
pool1	$110 \times 110 \times 64$	$55 \times 55 \times 64$	$3 \times 3 \times 64, 2$	0
rnorm1	$55 \times 55 \times 64$	$55 \times 55 \times 64$		0
conv2a	$55 \times 55 \times 64$	$55 \times 55 \times 64$	$1 \times 1 \times 64, 1$	4K
conv2	$55 \times 55 \times 64$	$55 \times 55 \times 192$	$3 \times 3 \times 64, 1$	111K
rnorm2	$55 \times 55 \times 192$	$55 \times 55 \times 192$		0
pool2	$55 \times 55 \times 192$	$28 \times 28 \times 192$	$3 \times 3 \times 192, 2$	0
conv3a	$28 \times 28 \times 192$	$28 \times 28 \times 192$	$1 \times 1 \times 192, 1$	37K
conv3	$28 \times 28 \times 192$	$28 \times 28 \times 384$	$3 \times 3 \times 192, 1$	664K
pool3	$28 \times 28 \times 384$	$14 \times 14 \times 384$	$3 \times 3 \times 384, 2$	0
conv4a	$14 \times 14 \times 384$	$14 \times 14 \times 384$	$1 \times 1 \times 384, 1$	148K
conv4	$14 \times 14 \times 384$	$14 \times 14 \times 256$	$3 \times 3 \times 384, 1$	885K
conv5a	$14 \times 14 \times 256$	$14 \times 14 \times 256$	$1 \times 1 \times 256, 1$	66K
conv5	$14 \times 14 \times 256$	$14 \times 14 \times 256$	$3 \times 3 \times 256, 1$	590K
conv6a	$14 \times 14 \times 256$	$14 \times 14 \times 256$	$1 \times 1 \times 256, 1$	66K
conv6	$14 \times 14 \times 256$	$14 \times 14 \times 256$	$3 \times 3 \times 256, 1$	590K
pool4	$14 \times 14 \times 256$	$7 \times 7 \times 256$	$3 \times 3 \times 256, 2$	0
concat	$7 \times 7 \times 256$	$7 \times 7 \times 256$		0
fc1	$7 \times 7 \times 256$	$1 \times 32 \times 128$	maxout p=2	103M
fc2	$1 \times 32 \times 128$	$1 \times 32 \times 128$	maxout p=2	34M
fc7128	$1 \times 32 \times 128$	$1 \times 1 \times 128$		524K
L2	$1 \times 1 \times 128$	$1 \times 1 \times 128$		0
total				140M

Shape of Data

Helena Bonham Carter - 254 images - Original features on left (pixels),
128 features on right (embedding from CNN)



New loss function

- We are basically interested in function f which embeds our data X in d -dimensional Euclidean space.

$\mathcal{C}^i \leftarrow$ Data with same labels as i -th instance

$C^i \leftarrow$ centroid of \mathcal{C}^i in embedded space

[1] Previous, $L_{i,j,k} = \lambda d(f^i, f^j) + (1 - \lambda)[1 + d(f^i, f^j) - d(f^i, f^j)]_+$

Current, $L_{i,j,k} = d(f^i, f^j) + [1 + d(f^i, f^j) - d(f^i, f^k)]_+$
 $+ d(f^i, C^i) + d(f^j, C^i) + d(f^k, C^k)$
 $+ [1 - d(C^i, C^k)]_+$

such that, $C^i = \frac{1}{|\mathcal{C}^i|} \sum_{s \in \mathcal{C}^i} f^s$ centroid in embedded space

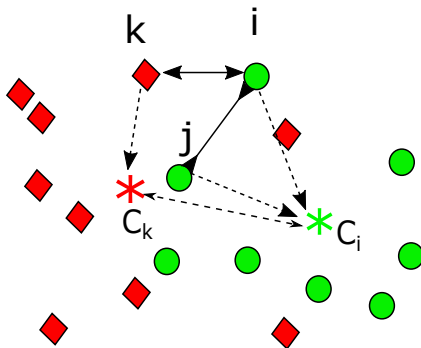
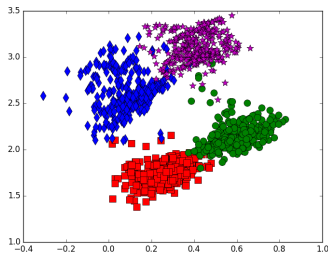
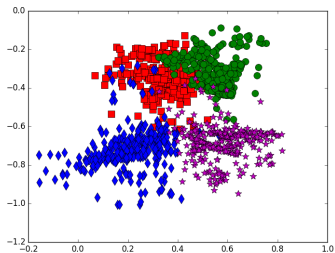
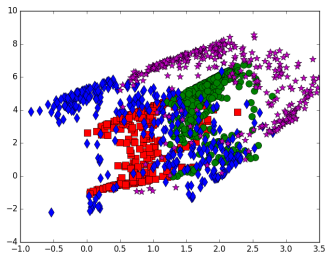
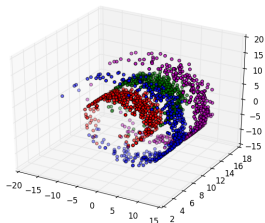


Figure: Graphical representation of loss function in the embedded space

Results on a toy data



Conclusions and Future Work

Conclusions thus far:

- From homology perspective, data appears to be connected with no loops
- Maybe other structure - like a dendrite? Clusters?

Future work:

- Apply more tools from TDA (mapper algorithm - check for dendrite structures)
- Other standard datasets (MNIST, natural images, spoken language) with appropriate NN architectures (CNN, RNN, etc)
- Scale space instead of pixel space for images

Bibliography



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