Topological Inputs for Designing NNs

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Outline

- Space of local patches in natural images
- Space of weight vectors in neural networks
- Topological convolutional neural network (TCNN)

Space of Local Patches in Natural Images

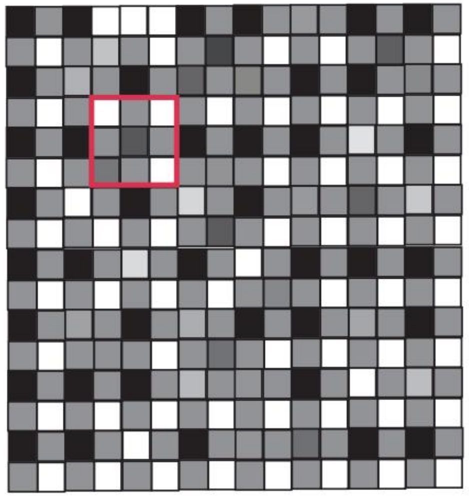
Local Behavior of Natural Images

- Collect 3×3 high contrast patches from a collection of images (Regarded as 9-vectors).
- Normalize mean intensity by subtracting mean from each pixel value to obtain patches with mean intensity = 0. (mean-center)
- Divide by the norm and put the data on a 7-dimensional sphere. (Normalization)

dimensionality reduction

Approaches:

- Density Filtration
- Denoising
- Persistent Homology



3×3 patches in images

Density Filtration

Threshholding $\mathcal{M}$

Define $\mathcal{M}[T] \subseteq \mathcal{M}$ by

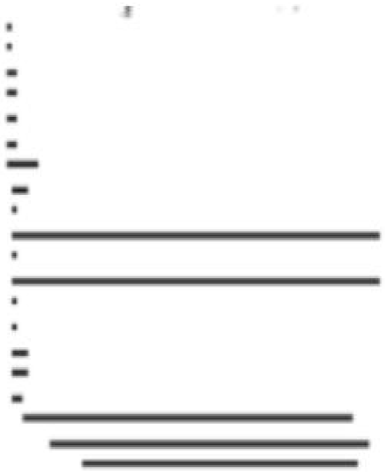
$$\mathcal{M}[T] = \{x | x \text{ is in } T\text{-th percentile of densest points}\}$$

Core Set of M

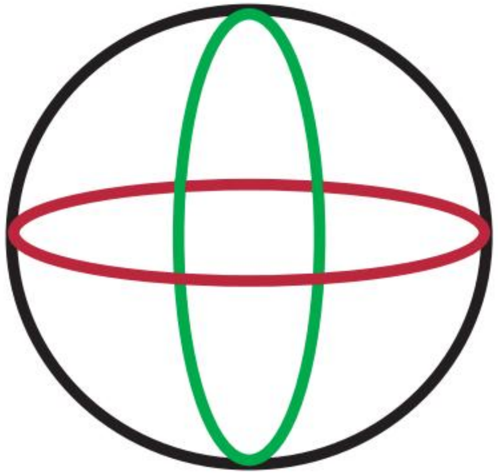
What is the persistent homology of these $\mathcal{M}[T]$'s?

Three Circle Model

5×10^4 points, $T = 25$



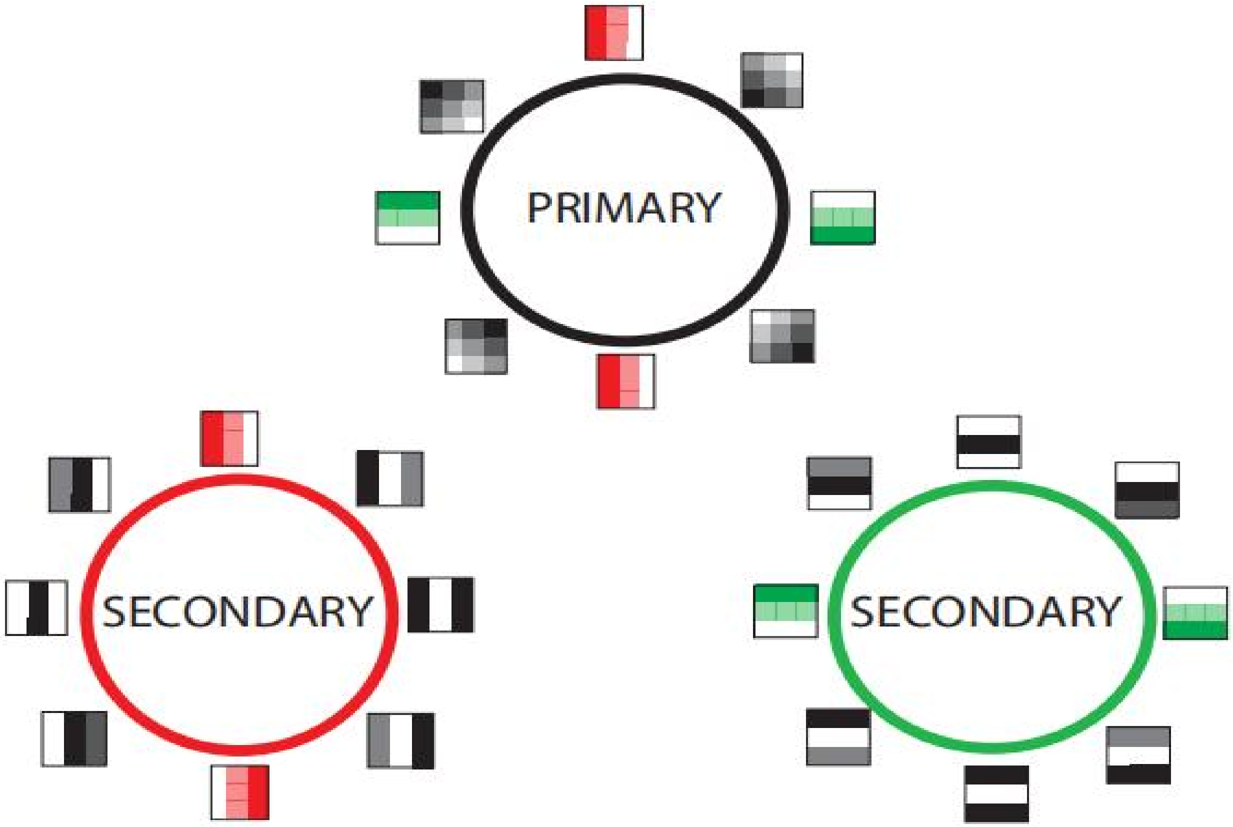
One-dimensional barcode, suggests $\beta_1 = 5$



THREE CIRCLE MODEL

Red and green circles do not touch, each touches black circle

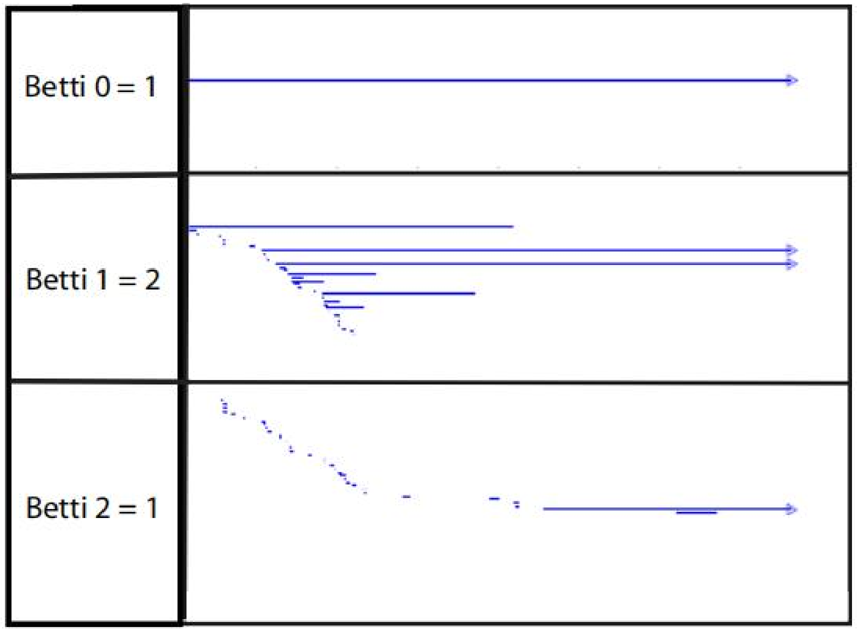
Three Circle Model



Is there a 2-dim surface containing these three circle?

Klein Bottle

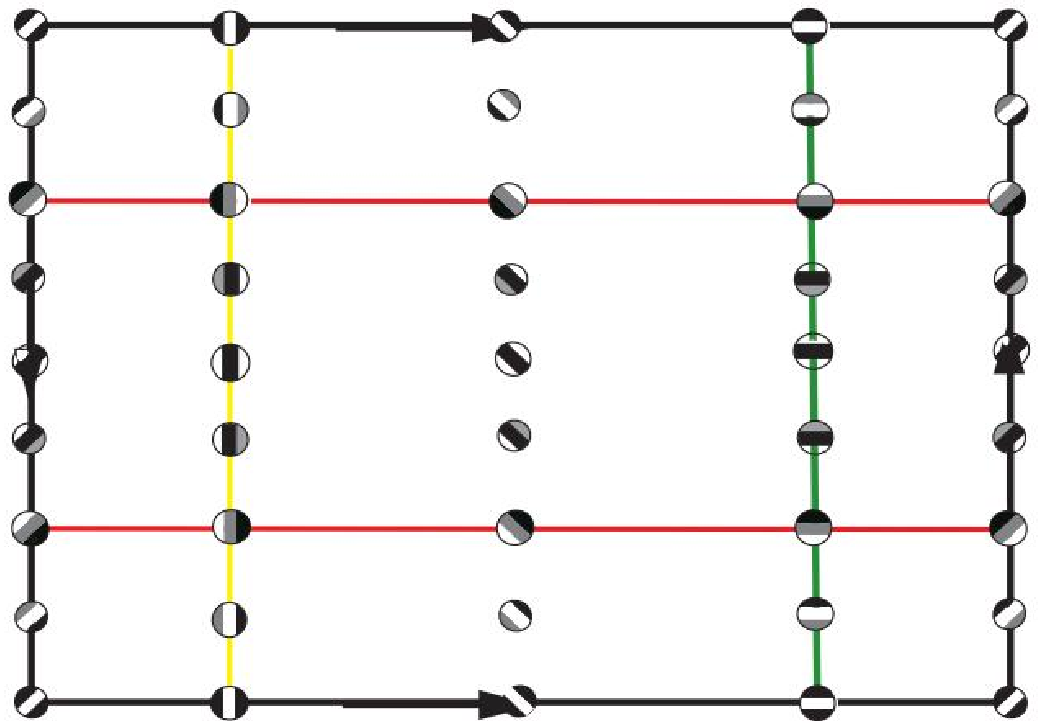
4.5×10^6 points, $T = 10$



Barcode

Klein Bottle

Embed Three Circles into Klein Bottle



Conclusion

There is a large portion of the space of patches which is topologically equivalent to a well-known two-manifold, the Klein bottle.

Motivations for the Next Part

- Filters of CNNs have the same size of local patches. Can we try to put similar analysis on the space of weight vectors?
- We know that neurons in the primary visual cortex and the weight vectors and the filters in CNNs are reflecting responses or functions on the space of patches.
- There is a conjecture that weight vectors or filters are also distributed in similar structures and can be regarded as a function on patches via inner product constructions to better extract features.

Space of Weight Vectors in Neural Networks

Space of Weight Vectors

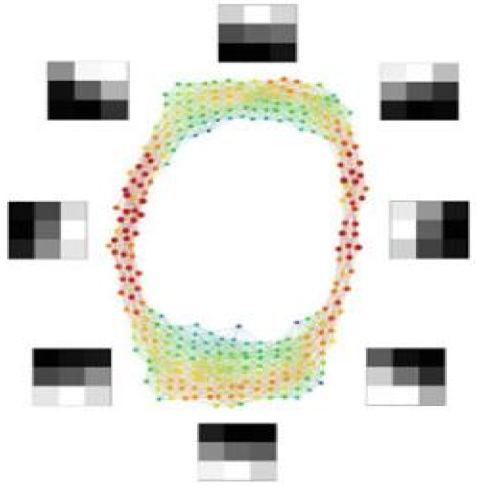
- Fix an architecture and train CNNs for several times.
- Obtain a space of weight vectors (after mean-centering and normalization) and apply TDA on it.

Approaches:

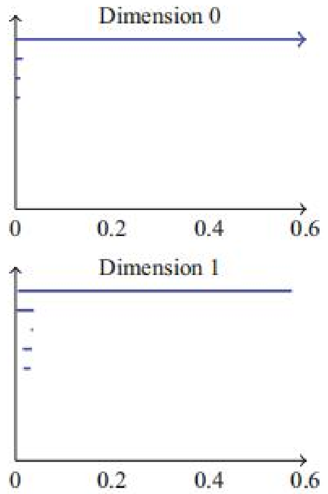
- Mapper
- Density Filtration
- Persistent Homology

Practice: MNIST

- Train 100 CNNs of type M(64,32,64) for 40,000 batch iterations with a batch size of 128 to a test accuracy of about 99.0%.
- These 100 trained CNNs give us 64 × 100 = 6400 9-dimensional points (first layer spatial filters) which we mean-center and normalize.
- Then analyze the dataset by TDA approaches.

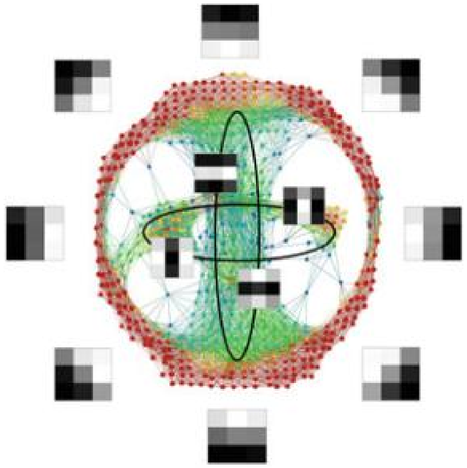


First Layer

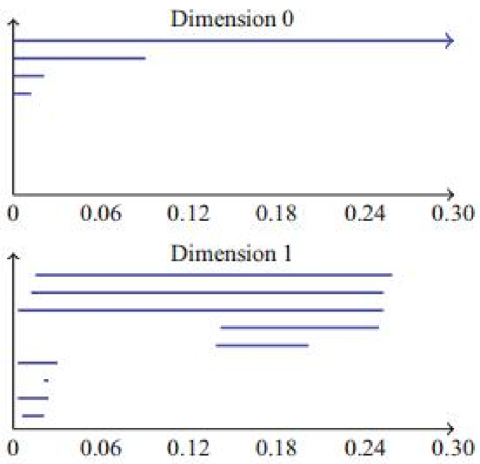


Barcode

Practice: CIFAR-10

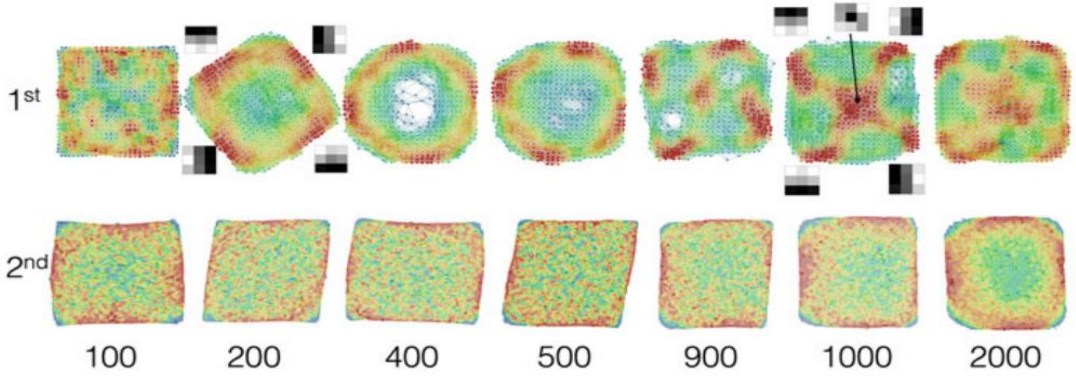


First Layer



Barcode

Learning Process:



Batch Iterations

Significance

☆ An effective tool to obtain understanding of the functioning of CNNs

- It showed that the spaces of spatial filters learn simple global structures. (Not only for the first layer, but occurs at least up to layers at depth 13.)
- Also demonstrated the change of the simple structures over the course of training.

Significance

☆ Better Generalization

Train a network of type M(64, 32, 64) on MNIST under three different circumstances:

(i) Fix the first convolutional layer to a perfect discretization of the primary circle.

(ii) Fix the first convolutional layer to a random gaussian.

(iii) Train the network as in regular circumstances with nothing fixed.

Then test on 26,032 images of SVHN:

Test accuracies of the three circumstances above:

(i) 28 % (ii) 12 % (iii) 11 %.

Significance

☆ Faster Speed

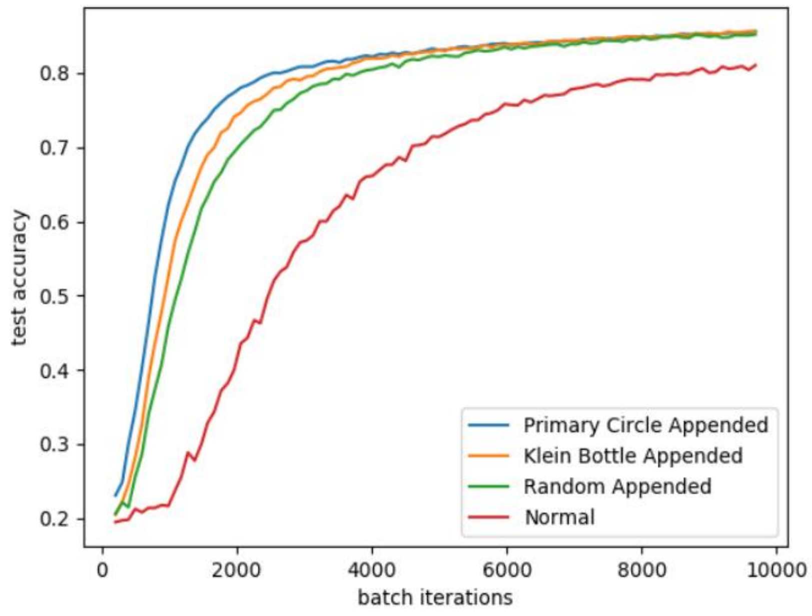
Preprocess each input image with a set of fixed 3×3 weights whose inner product with each 3×3 patch of the input image was appended to the central pixel value of the patch.

Three different sets of proprocessing weights:

(1) 64 weights from the idealized primary circle

(2) 64 weights from the idealized extension to the three-circle structure, i.e. the Klein bottle

(3) a random gaussian



Future Work

Topological information may serve as a measure of generality.

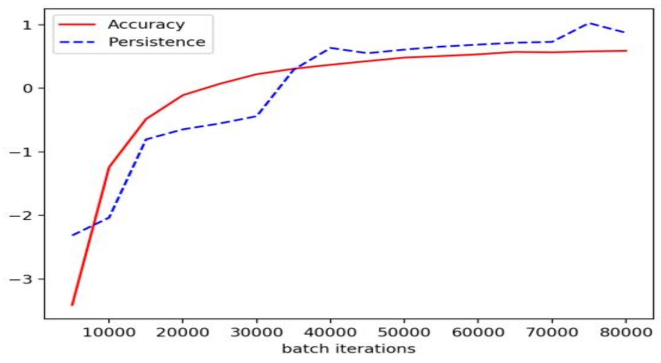


Figure 12: MNIST: Test accuracy and Persistence

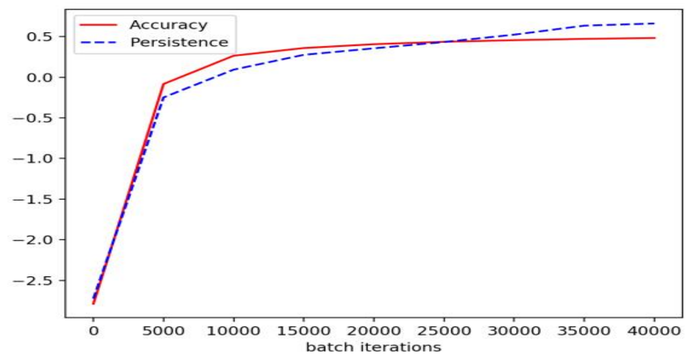


Figure 13: SVHN: Test accuracy and Persistence

- It shows a measure of the strength (or simplicity) of a topological feature and how it correlates with test accuracy on unseen test data.
- It indicates the connection between the existence of simple topological models of the learned weight spaces and the ability to generalize across data sets.

Topological Convolutional Neural Network (TCNN)

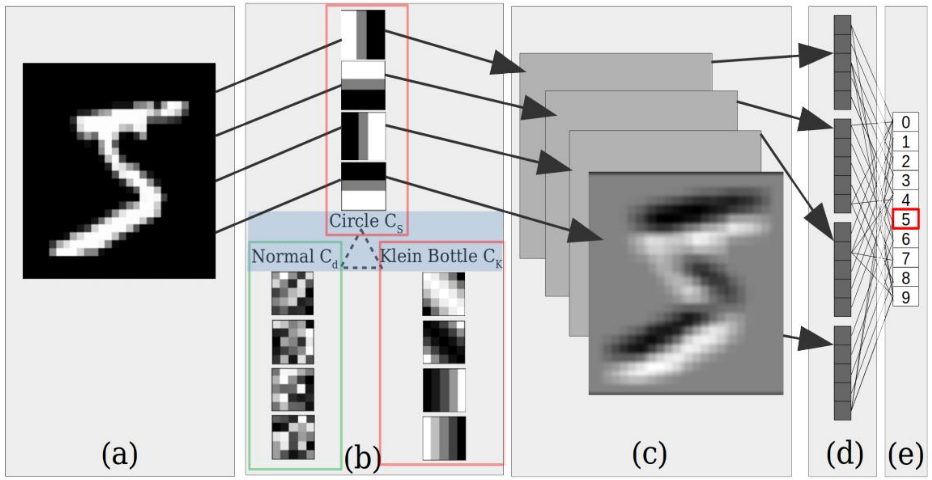
Key Properties of CNN

- Locality
- Homogeneity

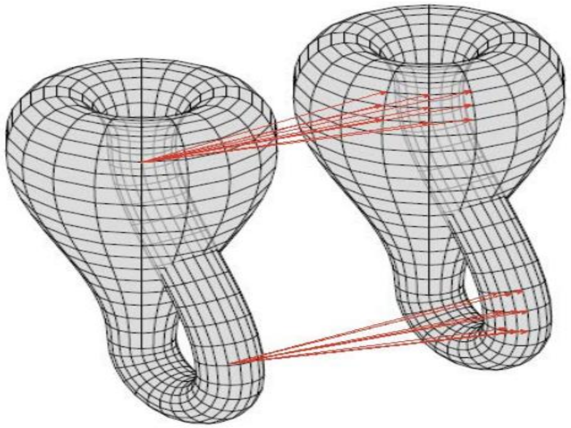
Kernel

Key Properties of TCNN (Improvements)

- Kernels are restricted on certain geometries. (Klein filters (KF) & Circle filters (CF))
- Filters between layers are locally connected based on relative geometrical positions, rather than being fully connected. (Klein one layer (KOL) & Circle one layer (COL))



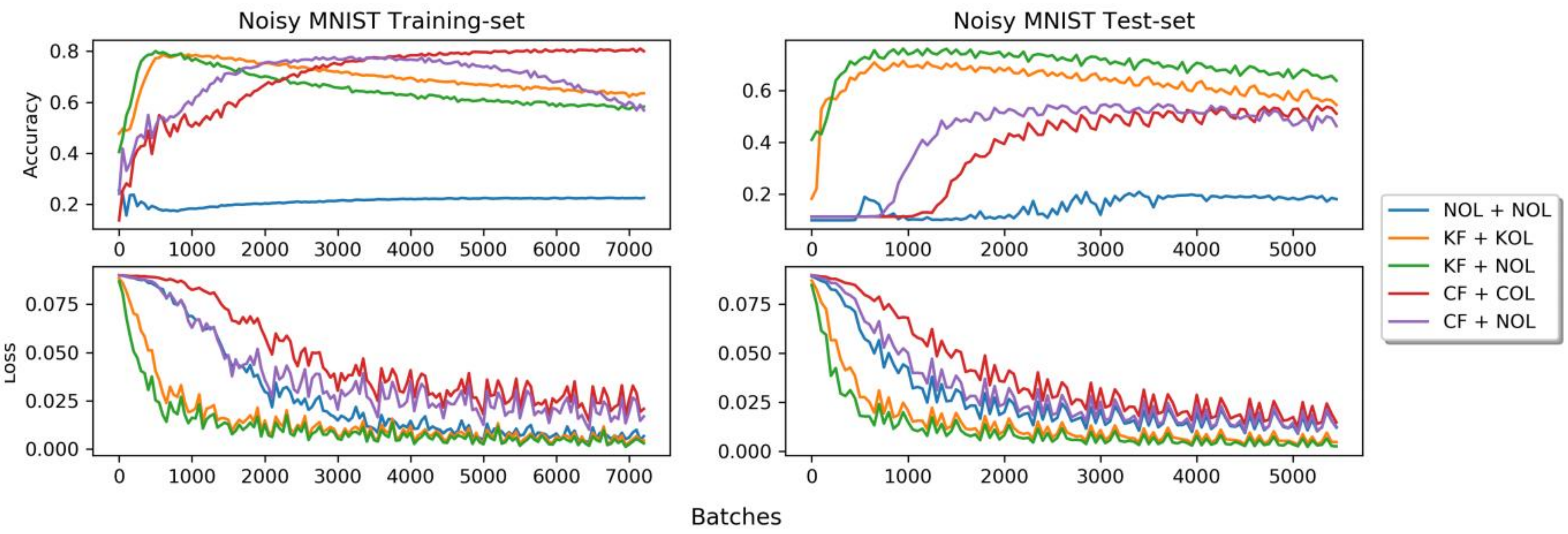
KF&CF



KOL

Evaluation

☆ Performance

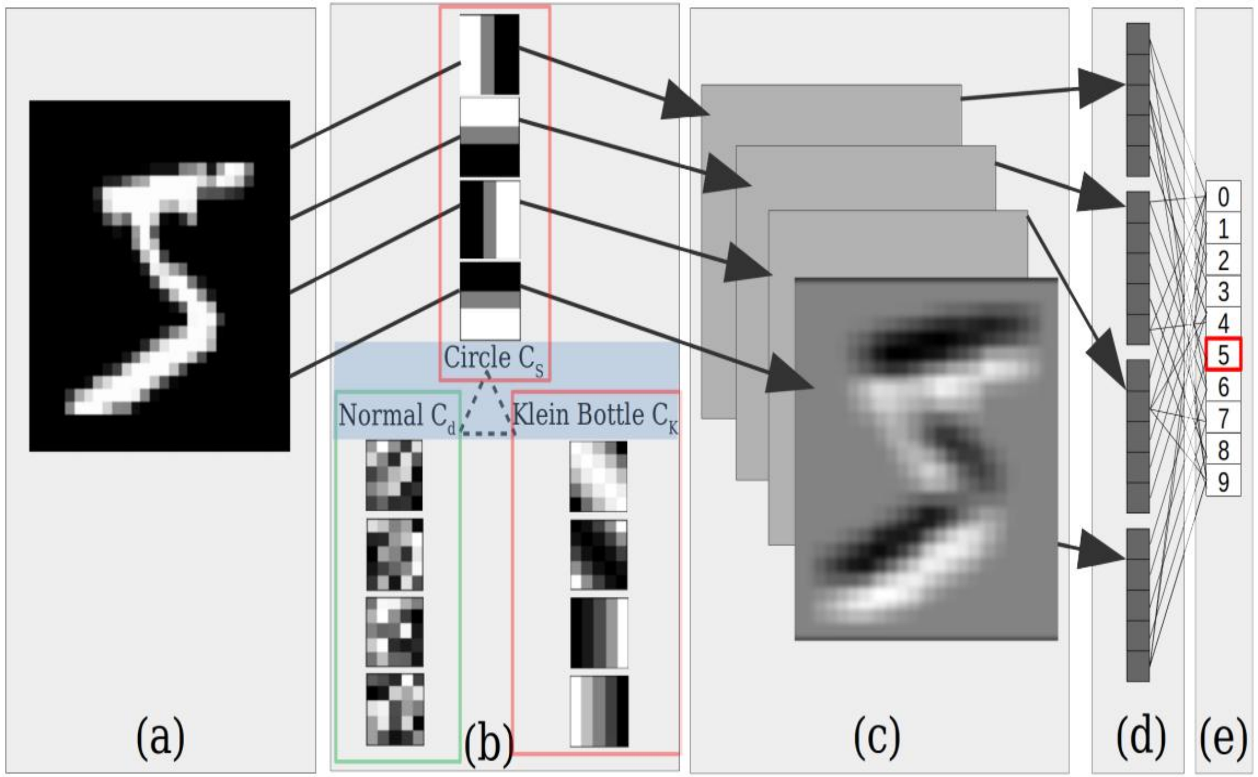


Evaluation

☆ Interpretability

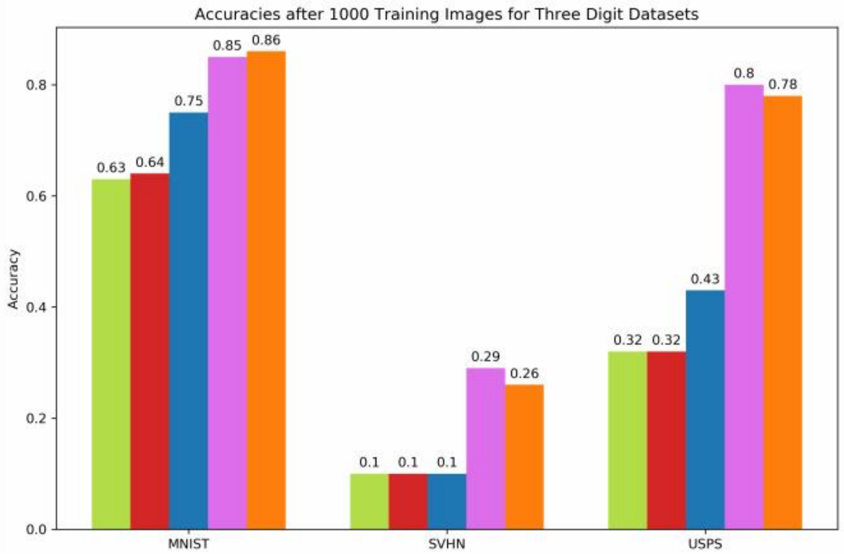
CF: the filters are edges at various angles, and the activations show where each such orientation of an edge appears in the image.

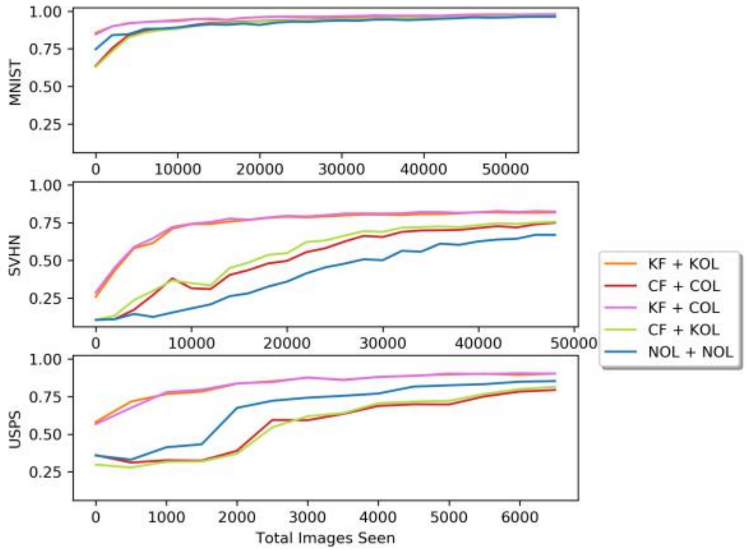
KF: filters containing interior lines are also included, and the activations reveal the presence of these interior lines in the image.



Evaluation

☆ Rate of learning





From a perspective of different networks, the networks with a KF layer achieve high accuracy earlier in training than those without, suggesting potential applications to smaller datasets for which less training can be done.

From a perspective of different datasets, the SVHN dataset, which is much richer than MNIST, and the USPS dataset, which has much lower resolution than MNIST, received larger benefits from theuse of a TCNN. This suggests that the benefit of the feature engineering in TCNNs is greatest when the local spatial priors are relatively weak or hidden.

Evaluation

☆ Generalizability