Topological Analysis of Decision Boundaries

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Introduction

- Machine learning classifiers partition their input space into regions corresponding to different class labels $1 \ldots n$
- The boundaries between these regions, *decision boundaries*, are important for generalization
- Let's use topological data analysis to study how decision boundaries evolve during training to detect overfitting

Illustration of decision boundaries in 2D here.

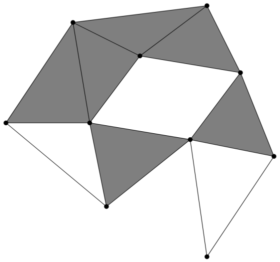
Theoretical background: Overfitting

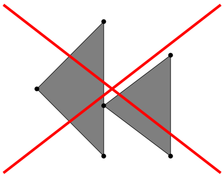
- Model fits training data too closely, fails to generalize to unseen data
- Performance improves on training data, but degrades on validation data
- Maybe this is reflected in the topology of decision boundaries?

Illustration of overfitting here; plot of training acc improving, validation acc dropping.

Theoretical background: Persistent homology

- Simplicial complex: a collection of simplices glued together “nicely”





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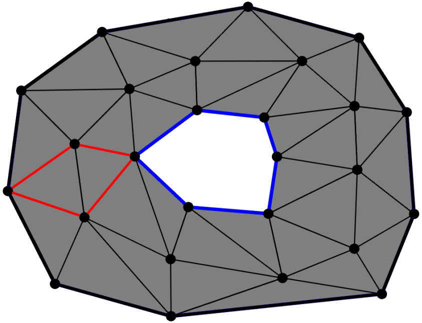
  - $p = 1$: unfilled cycles



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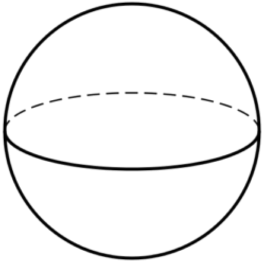

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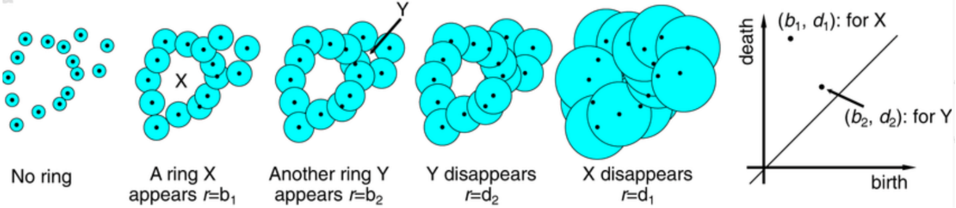
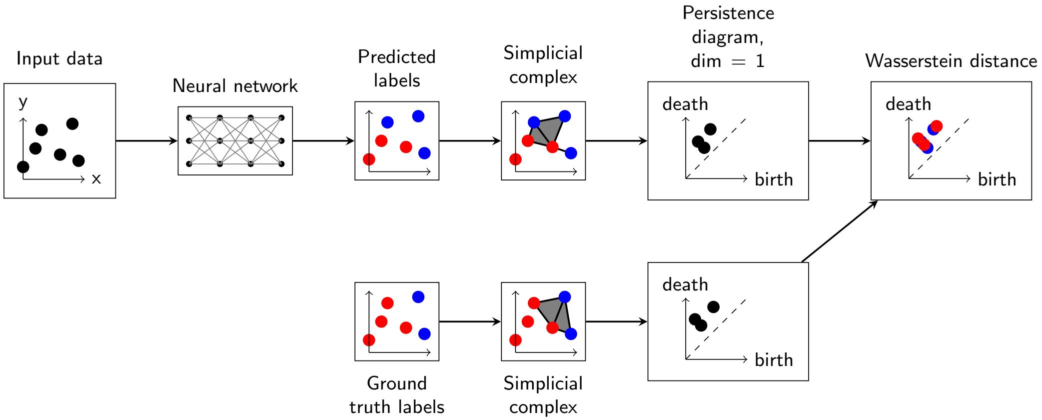
- *Persistent* homology: homology groups of a simplicial complex as it evolves
- Example: growing balls



Pipeline


Input data
y
x
Neural network
Predicted labels
Simplicial complex
Persistence diagram, dim = 1
death
birth
Wasserstein distance
death
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Ground truth labels
Simplicial complex
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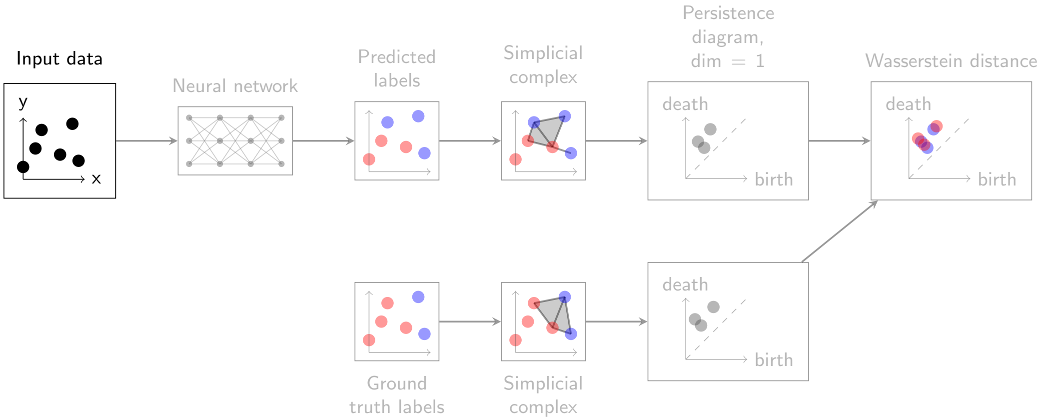

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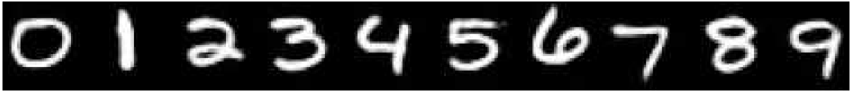
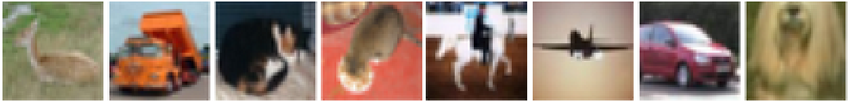
Input data

- MNIST: 28x28 grayscale images of handwritten digits, dim = 784



- FashionMNIST: 28x28 grayscale images of fashion articles, dim = 784

- CIFAR-10: 32x32 color images of 10 classes, dim = 3072



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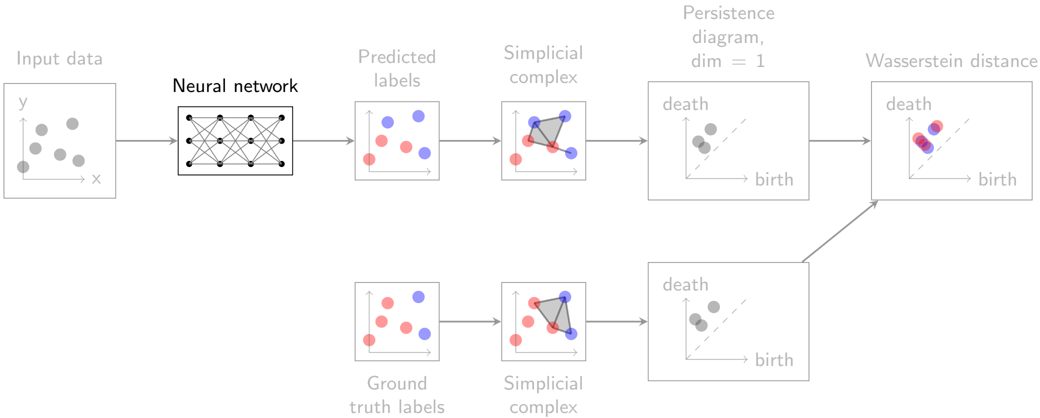

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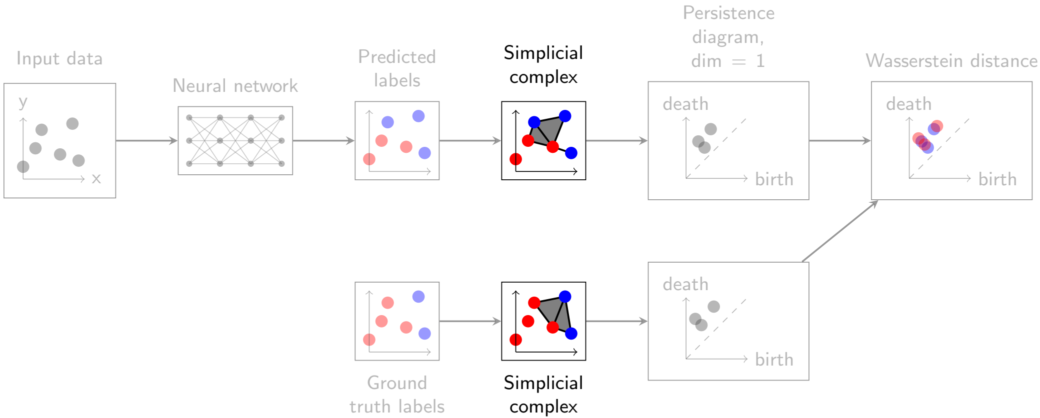
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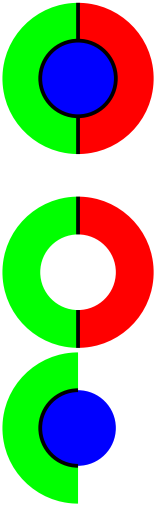
Binarization

Previous work only considered binary classification by splitting a dataset with n classes into $\binom{n}{2}$ binary datasets. This changes the homology groups:

- Original has $H_1 \not\cong 0$
- All binary decompositions have $H_1 \cong 0$

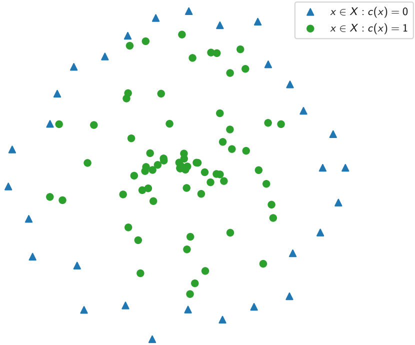
It is better to avoid binarization.



Labeled Vietoris-Rips complex

- Set of points X
- Labels $c : X \to \mathbb{Z}_k$
- Parameter ε

Constructed in three steps:



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Constructed in three steps:

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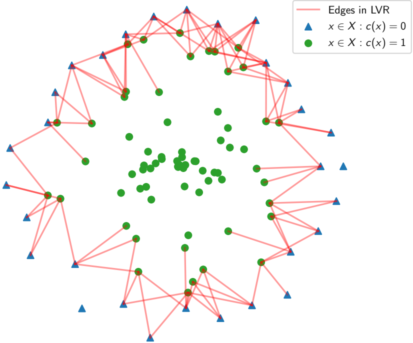
   - $\|x_i - x_j\| \leq \varepsilon$ (points are close enough)
   - $c(x_i) \neq c(x_j)$ (different classes)



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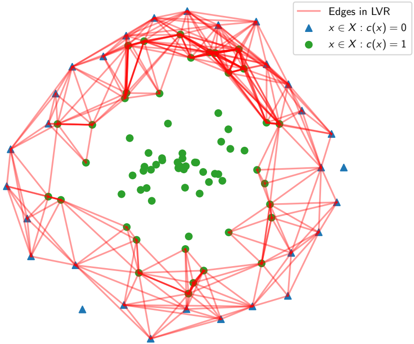

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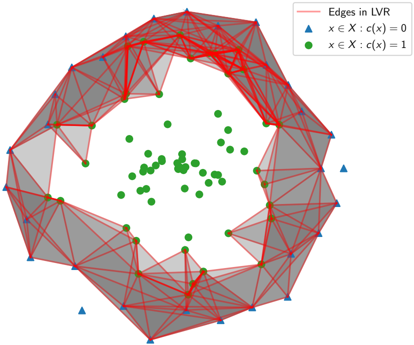

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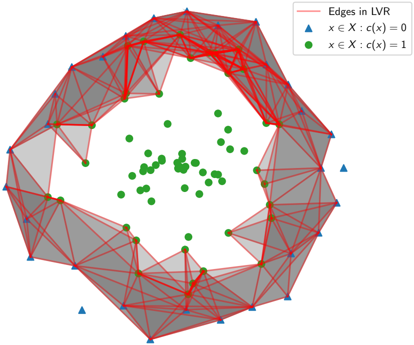
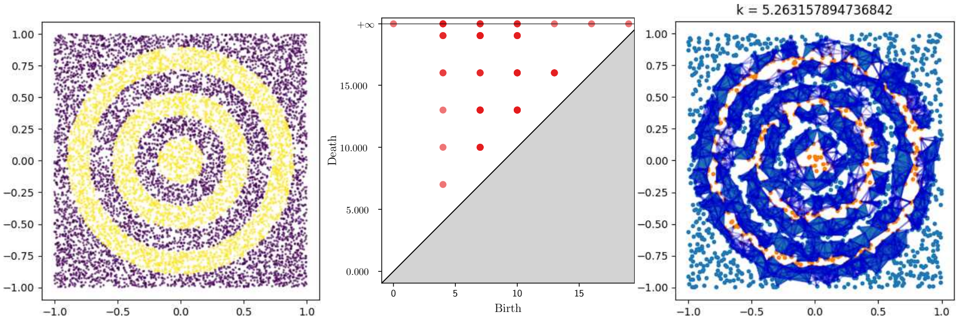
- Simplices cross the boundary
- Applicable to multiple classes



Synthetic 2D experiemnts

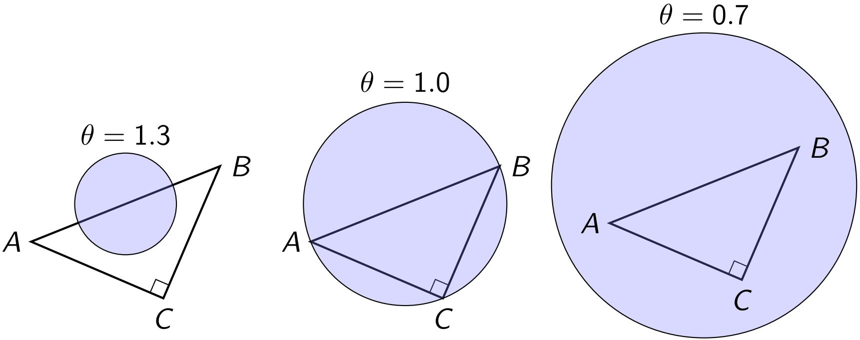
To see if the LVR complex recovers the homology of the decision boundary, we use synthetic 2D data with nested annuli.



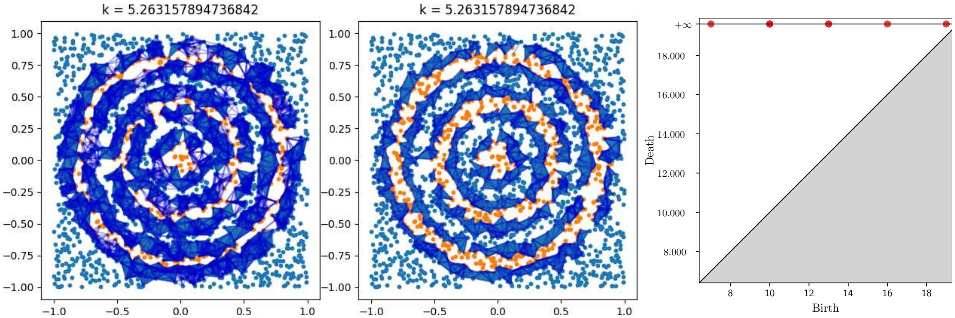
Edges cross the decision boundary multiple times $\implies$ spurious holes appear.

Circumcircle filtering

- Remove an edge AB if exists vertex $C : |AB|^2 > (|AC|^2 + |BC|^2)\theta$.
- θ is a parameter to relax the condition.



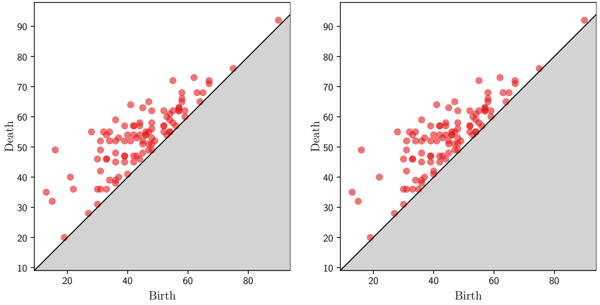
Circumcircle filtering impact



Circumcircle filtering impact on high-dimensional data

Dataset	Binary	Multiclass
MNIST	7	4
FashionMNIST	14	1
CIFAR10	7	0

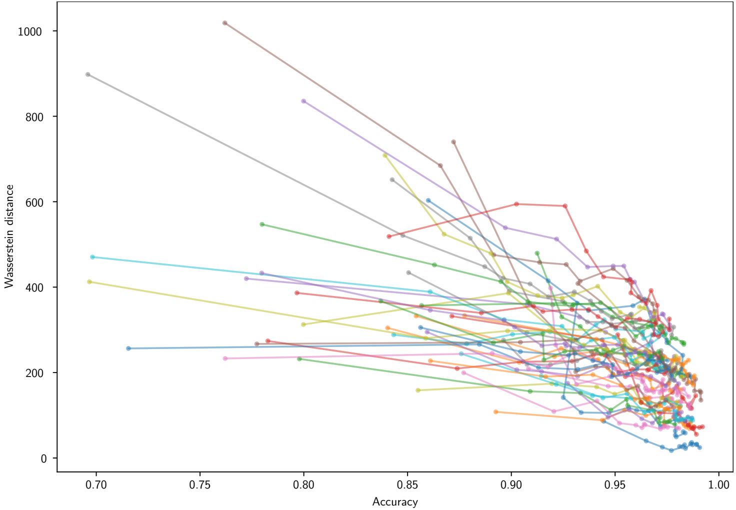
Maximum differences in Wasserstein distance between persistence diagrams with and without CC.



The two persistence diagrams that differ the most when CC is applied.

The difference is negligible $\implies$ CC is not used

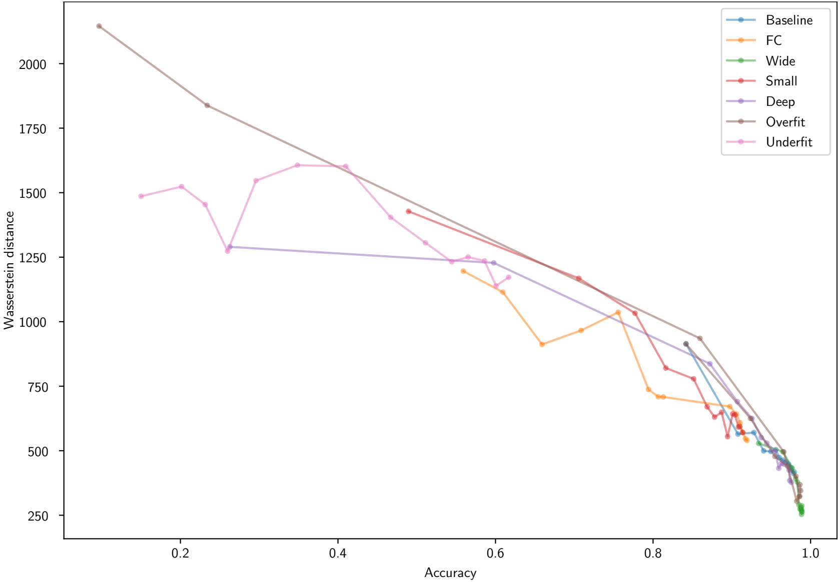
Results: binary classification



Relationship between Wasserstein distance and model accuracy across all binary classification pairs in MNIST. Connected points represent consecutive epochs for the same class pair.

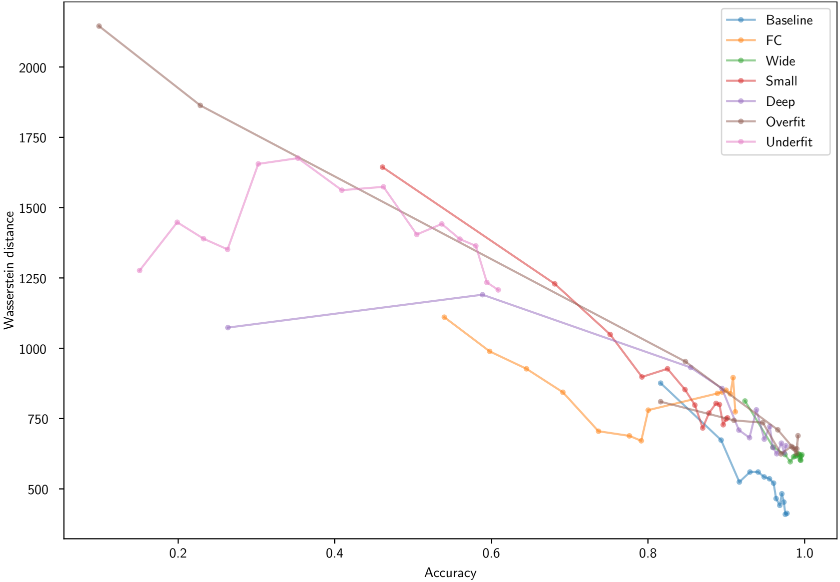
Results: multiclass classification

Clear indication of overfit in the overfit model's trajectory



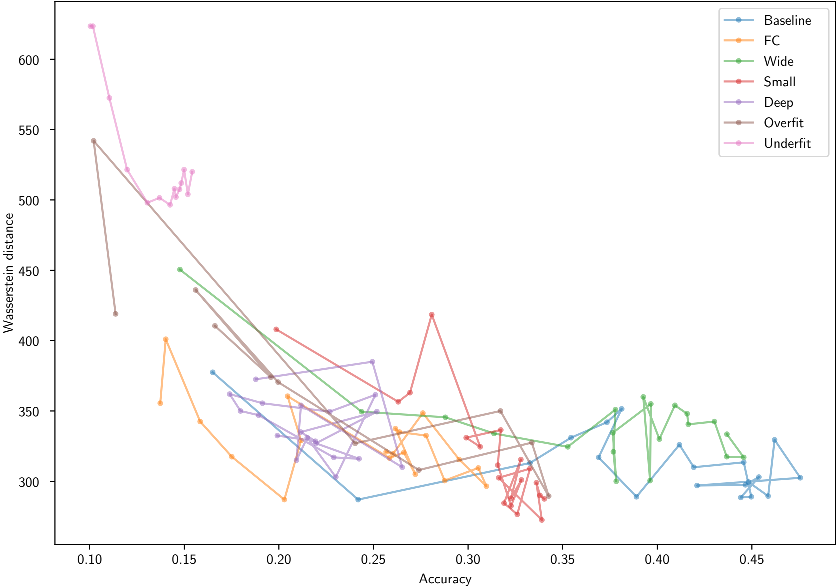
Results: multiclass classification, train data

TDA on training data, accuracy on test data



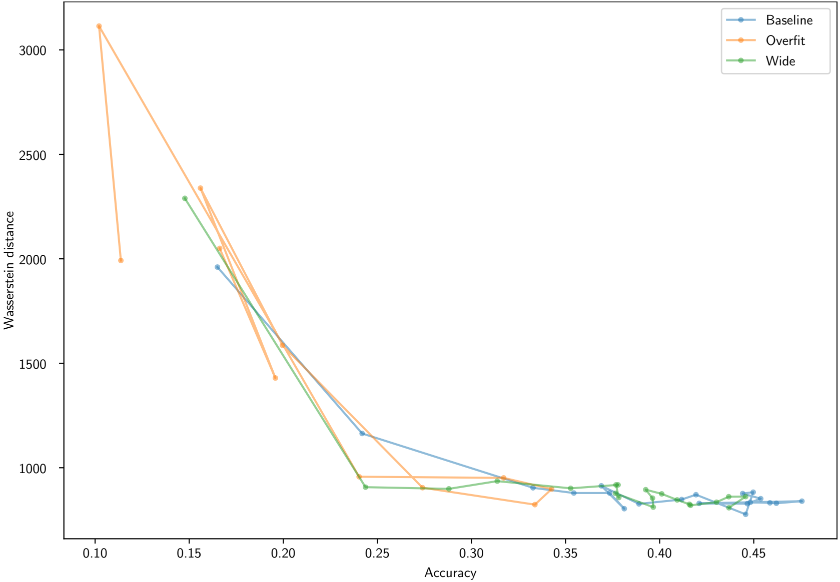
Results: multiclass classification, CIFAR10, 2000 points

Weak correlation as dimensionality of data increases, number of datapoints is unchanged



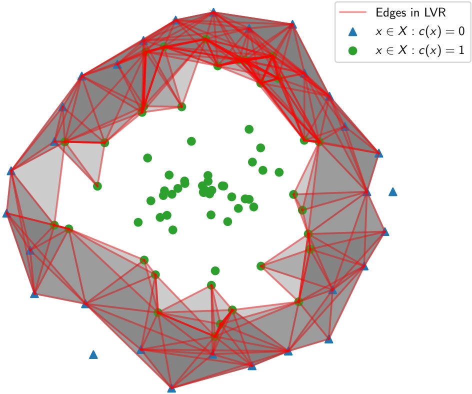
Results: multiclass classification, CIFAR10, 8000 points

Increasing number of points improves correlation



Conclusion

- Multiclass LVR complex is better
  - Preserves more topological information
  - Stronger correlation
  - More computationally efficient



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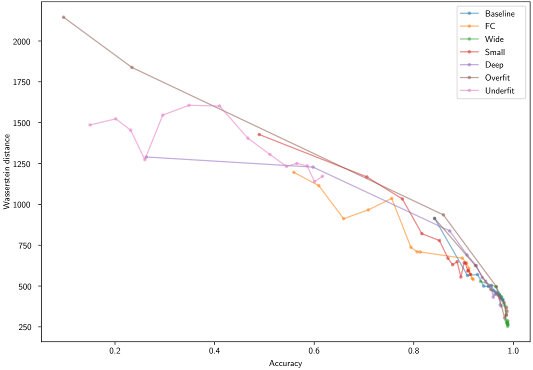
- Multiclass LVR complex is better
- TDA provides insights into classifier behavior
  - Strong correlation between Wasserstein distance and model accuracy
  - Wasserstein distance increases during overfitting



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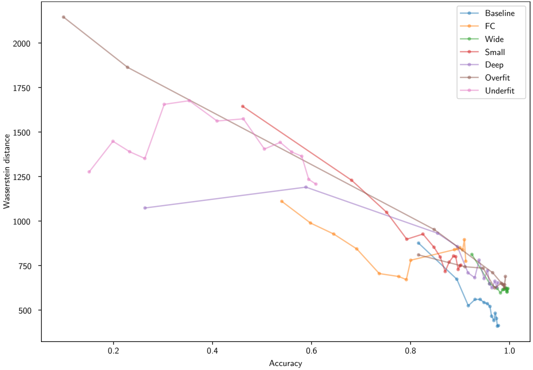
- Training data decision boundary topology correlates with test performance
  - Enables model evaluation without separate test sets
  - Could serve as early overfitting detection



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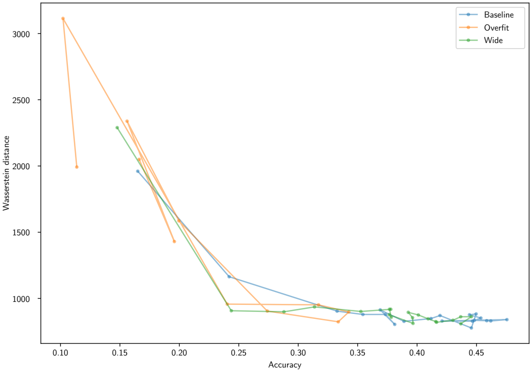
- Dimensionality scaling from CIFAR-10 experiments
  - Initial effectiveness decrease in higher dimensions
  - Performance restored by increasing sample size
  - Limitation: too many points required for very high-dimensional X



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