Topological Regularizer

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Acknowledgment

Contents of the slide (including figures) are based on the paper:

- Chen, Chao, Xiuyan Ni, Qinxun Bai, and Yusu Wang. "A topological regularizer for classifiers via persistent homology." In The 22nd International Conference on Artificial Intelligence and Statistics, pp. 2573-2582. PMLR, 2019.

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- They also propose an algorithm to compute the *partial derivatives* (gradient) of such penalty
- They demonstrate the effectiveness of the topological regularizer on synthetic and real-world datasets

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- A particularly interesting category of methods is inspired by the geometry: design new penalty terms to enforce a geometric simplicity of the classifier (e.g., enforce the classification boundary to be smooth)
- But as claimed by the authors, the geometric regularizers are "structure agnostic"

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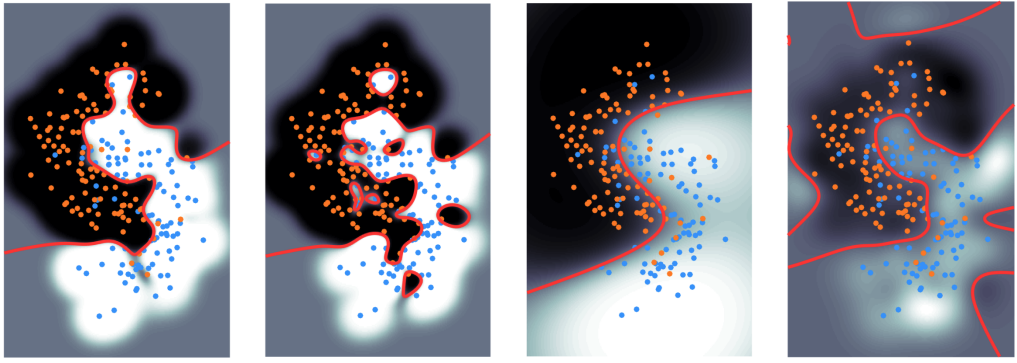
- Here, a regularizer aims at reducing the complexity of the classification boundary

Problem with geometric regularizer



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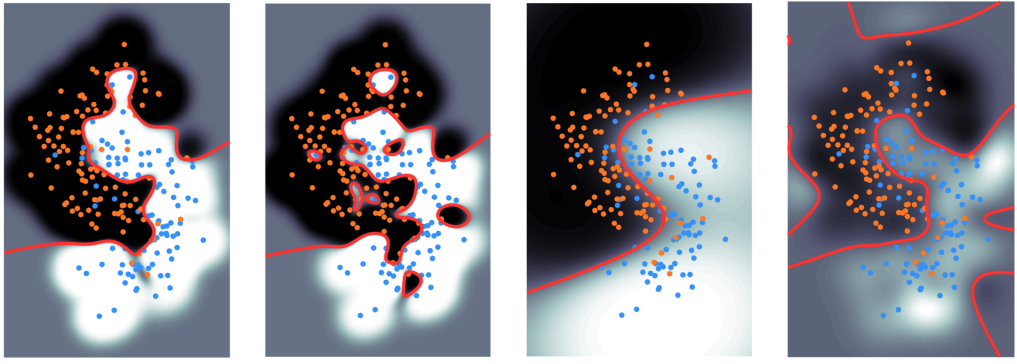

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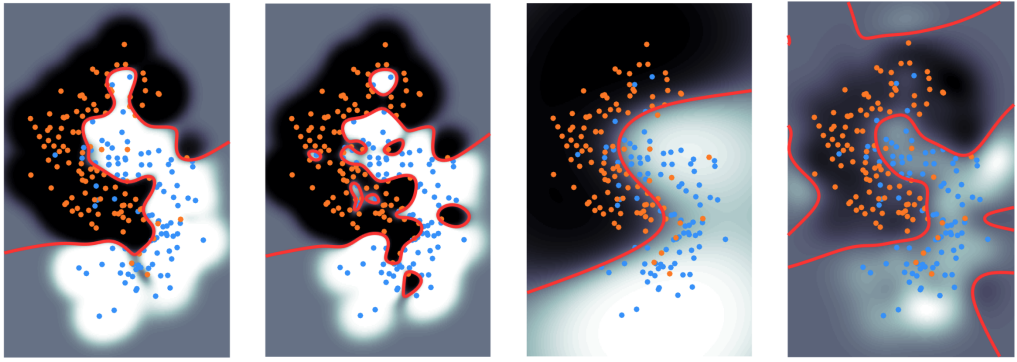

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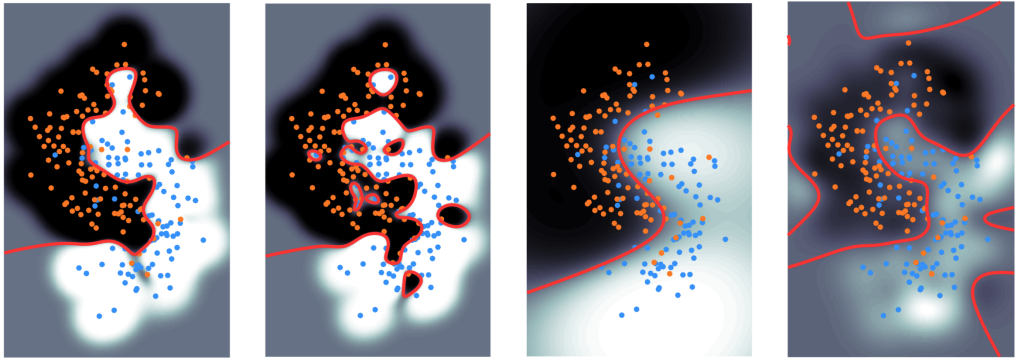

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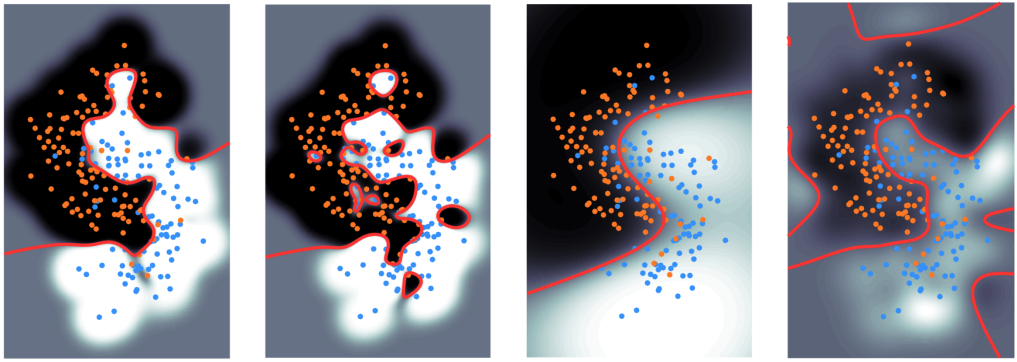
- (b) Overfitting to data without regularizer (aka. only minimize the empirical risk)
- (c) Geometry of model (smoothness of the classification boundary) is minimized
- (d) An actual classification boundary achieved with a geometric regularizer by [Bai, Q., Rosenberg, S., Wu, Z., and Sclaroff, S. (2016). Differential geometric regularization for supervised learning of classifiers.]

Advantage of topological regularizer



(a) (b) (c) (d)

- (a) By reducing the topological complexity of the classification boundary (in this case, the no. of connected components), we achieve structural simplicity without over-smoothing the classifier boundary

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- The "robustness" is roughly how easy it is to change the function value of f to make a component disappear

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- We could thus track almost all connected components in $f^{-1}(0)$ except one
- But this doesn't matter: we should always allow at least one connected component in $f^{-1}(0)$
- So as long as we are able to track all other connected components in $f^{-1}(0)$ and have a way of measuring their "robustness" and make those less robust ones disappear, we are good

Measuring the robustness of a connected component in $f^{-1}(0)$

- For an interval $[b, d) \in \Pi_f$: b is a local minimum of f below 0 creating a component, and d is a saddle above 0 merging two components
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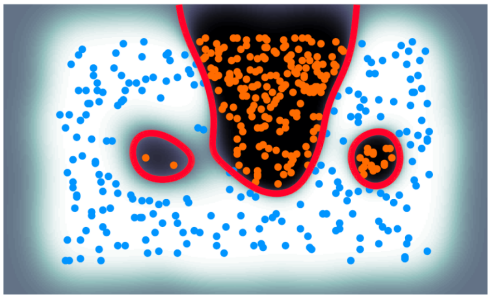
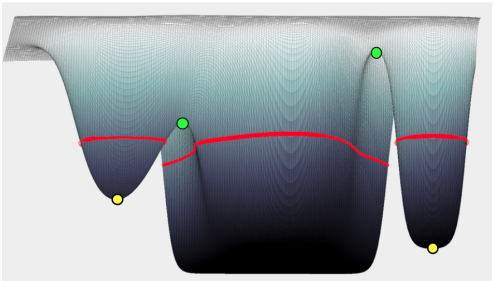


(a)



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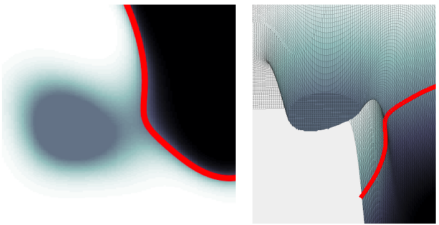

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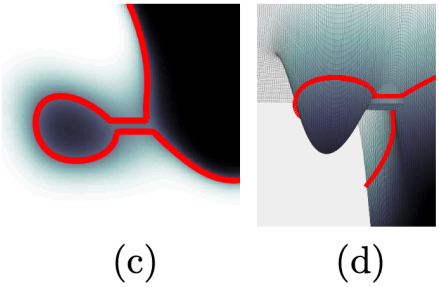
- If we "pull" the death (saddle) down, the left component merges with the right one:



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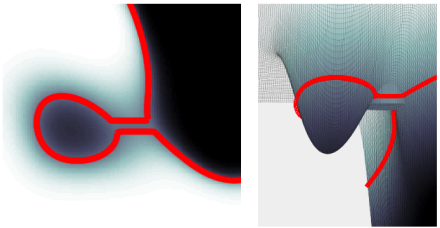

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- So the robustness of the connected component (min. effort to remove it) is:

$$\min\{|b|, |d|\}$$

Topological penalty of the classifier

- The topological penalty of the classifier is then sum of the squared robustness of each interval (connected component) in $\Pi_f \cup \Pi_{-f}$, excluding the one with the maximum robustness (we should always ensure there is at least one major component in the classification boundary)

$$\mathcal{R}_T(f) = \sum_{[b,d) \in \Pi_f \cup \Pi_{-f} \setminus \max(\Pi_f \cup \Pi_{-f})} (\min\{|b|, |d|\})^2$$

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- They then show that $\mathcal{R}_T(f)$ is *differentiable almost everywhere* (except some isolated points), which should be good enough for gradient descent

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- also compare with two state-of-the-art methods based on geometric regularizers: the Eulers Elastica classifier (EE) and the Classifier with Differential Geometric Regularization (DGR)
- In order to thoroughly evaluate the behavior of the model, especially in large noise regime, created synthetic data with various noise levels: beside feature space noise, also inject different levels of label noise, e.g., randomly perturb labels of 0%, 5%, 10% and 20% of the training data
- also evaluate their method on real world data

Synthetic							
	KNN	LG	SVM	EE	DGR	KLR	TopoReg
Blob-2 (500,5)	7.61	8.20	7.61	8.41	7.41	7.80	**7.20**
Moons (500,2)	20.62	20.00	19.80	19.00	19.01	18.83	**18.63**
Moons (1000,2,Noise 0%)	19.30	19.59	19.89	17.90	19.20	17.80	**17.60**
Moons (1000,2,Noise 5%)	21.60	19.29	19.59	22.00	22.30	**19.00**	**19.00**
Moons (1000,2,Noise 10%)	21.10	**19.19**	19.89	24.40	26.30	20.00	19.70
Moons (1000,2,Noise 20%)	23.00	19.79	**19.40**	30.60	30.20	19.50	**19.40**
AVERAGE	18.87	17.68	17.70	20.39	20.74	21.63	**16.92**
UCI							
	KNN	LG	SVM	EE	DGR	KLR	TopoReg
SPECT (267,22)	17.57	17.20	18.68	**16.38**	23.92	18.31	17.54
Congress (435,16)	5.04	4.13	4.59	4.59	4.80	**4.12**	4.58
Molec. (106,57)	24.54	19.10	19.79	17.25	16.32	19.10	**12.62**
Cancer (286,9)	29.36	28.65	28.64	28.68	31.42	29.00	**28.31**
Vertebral (310,6)	15.47	15.46	23.23	17.15	13.56	12.56	**12.24**
Energy (768,8)	0.78	0.65	0.65	0.91	0.78	**0.52**	**0.52**
AVERAGE	15.46	14.20	15.93	14.16	15.13	13.94	**11.80**
Biomedicine							
	KNN	LG	SVM	EE	DGR	KLR	TopoReg
KIRC (243,166)	30.12	28.87	32.56	31.38	35.50	31.38	**26.81**
fMRI (1092,19)	46.70	74.91	74.08	82.51	**31.32**	34.07	33.24