Differentiable Unsupervised Feature Selection based on a Gated Laplacian

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Nicolas Casey, Yuval Kluger

November 2021

Unsupervised Learning

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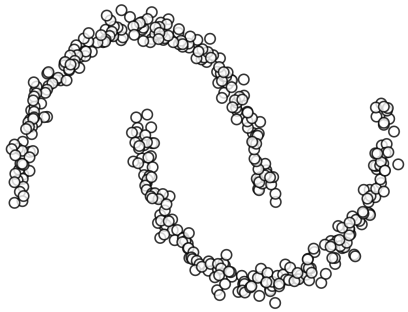

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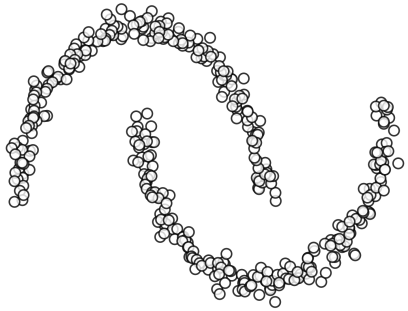

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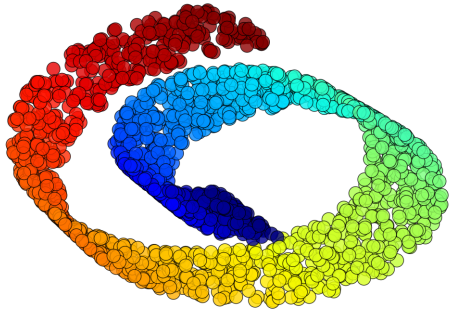

Swiss-roll

Embed $\tilde{\boldsymbol{X}}$ into a lower dimension without loosing much information

Unsupervised Learning: Nuisance Variables

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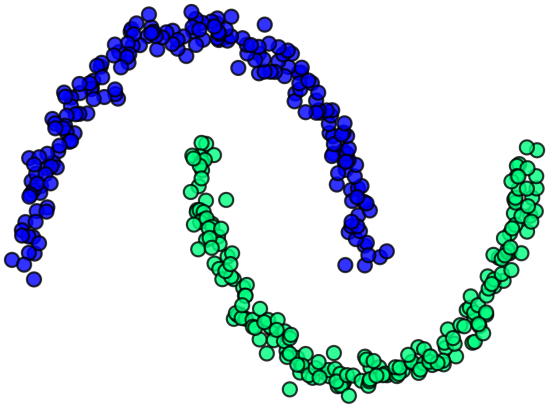

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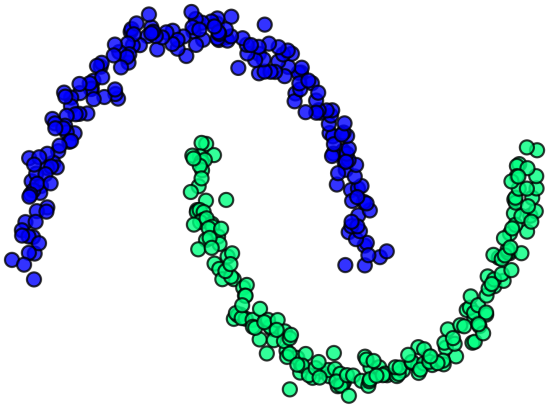

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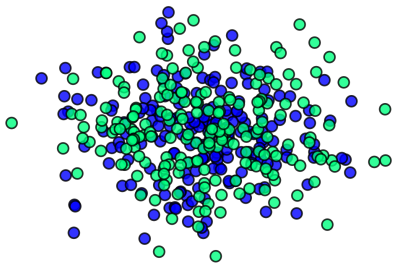

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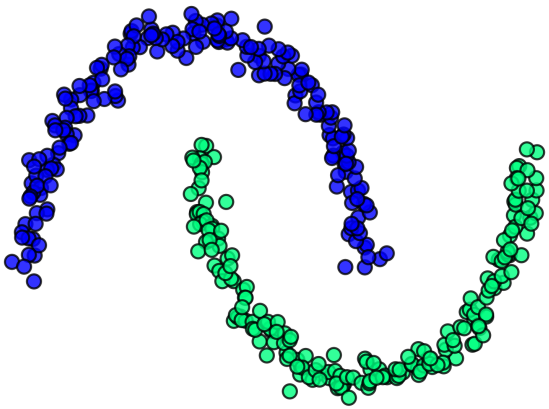

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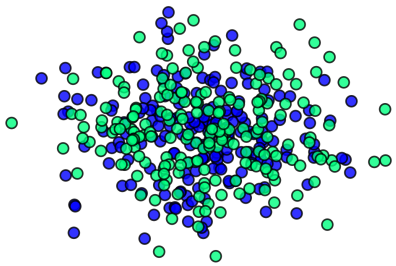

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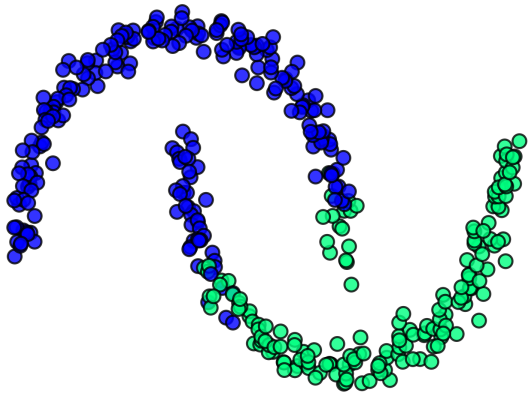

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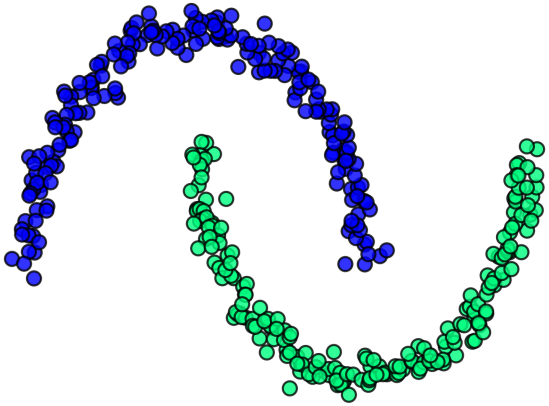

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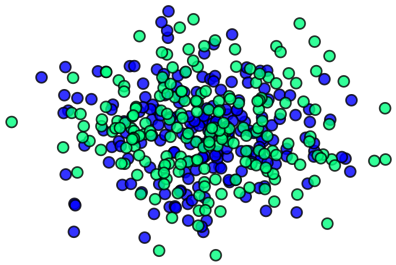

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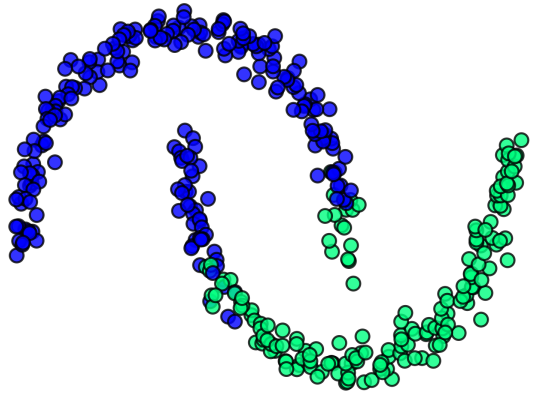

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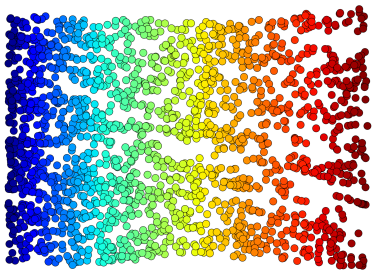

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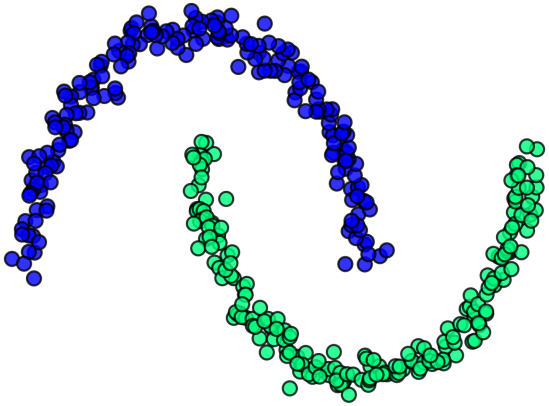

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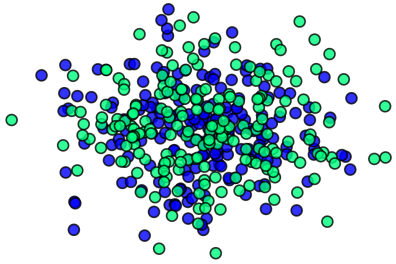

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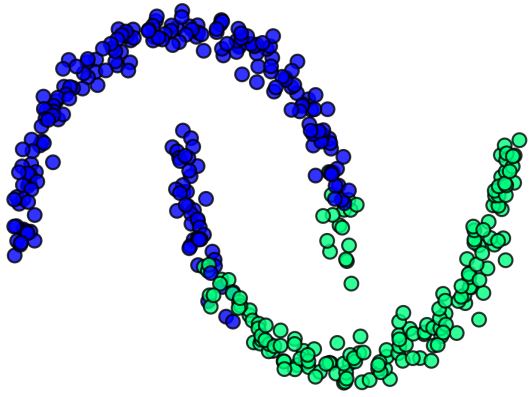

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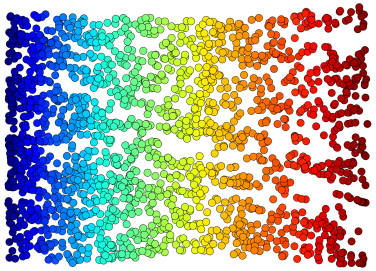

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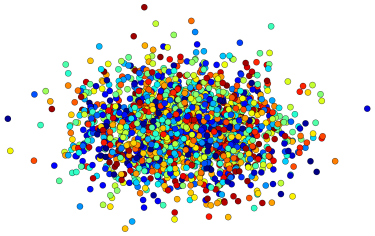

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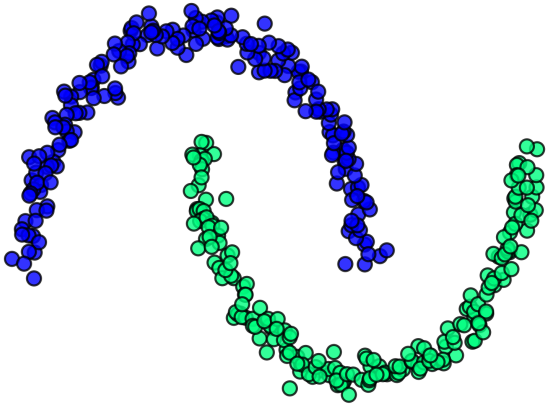

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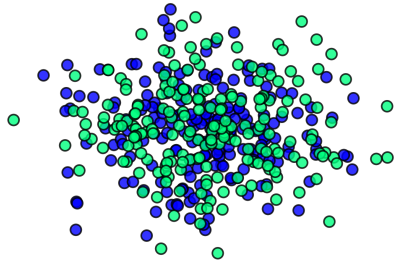

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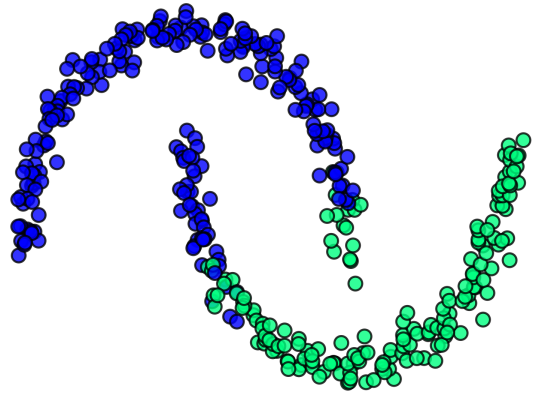

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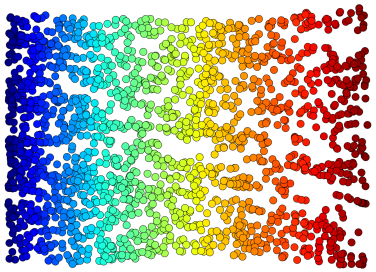

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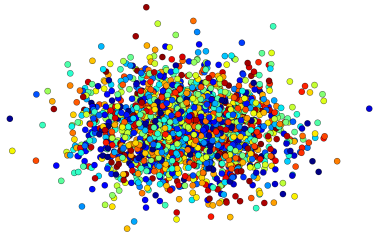

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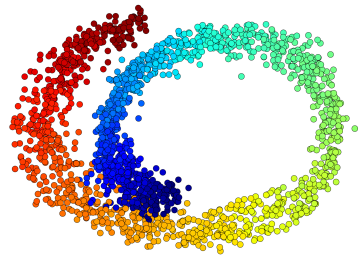

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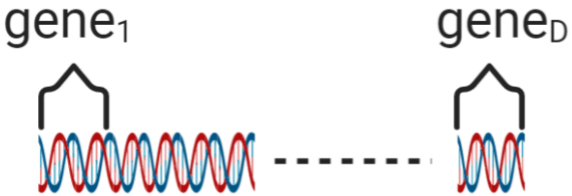

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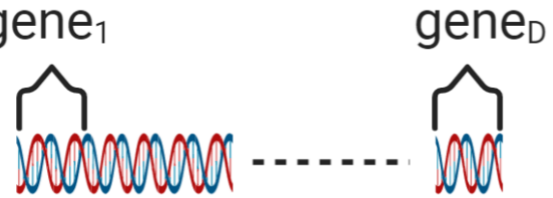

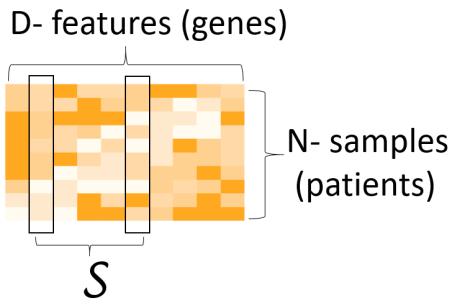

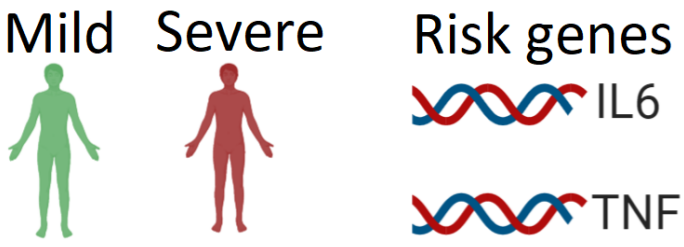

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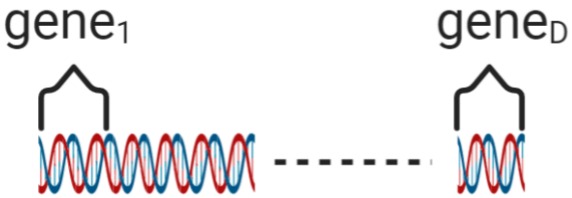

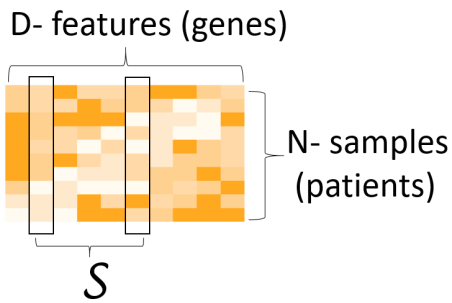

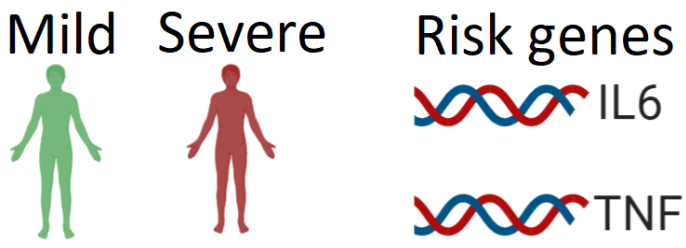

The idea: use "smoothness" to identify *informative* variables

Unsupervised Learning: Kernel Methods

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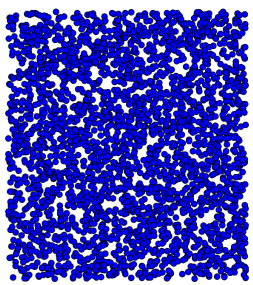
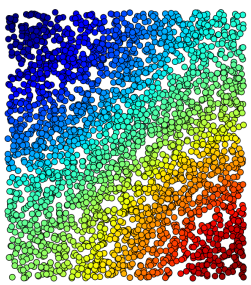
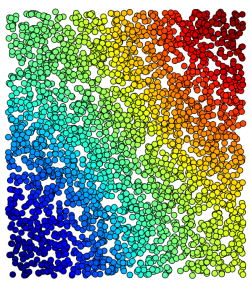
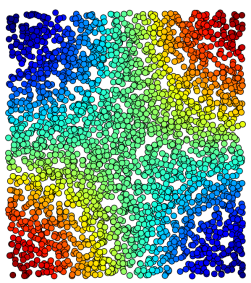
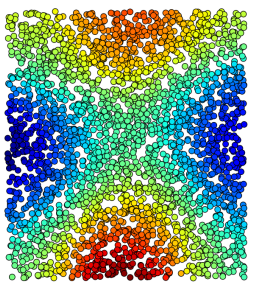

$\boldsymbol{\psi}_0$


$\boldsymbol{\psi}_1$


$\boldsymbol{\psi}_2$


$\boldsymbol{\psi}_3$


$\boldsymbol{\psi}_4$

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Feature is correlated with low frequency eigenvectors

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- Normalize each feature $\bar{\boldsymbol{f}}_d = \frac{\boldsymbol{f}_d}{\|\boldsymbol{f}_d\|_2}$, where $\boldsymbol{f}_d = (x_1^{(d)}, ..., x_N^{(d)})^\top$
- Compute the Rayleigh quotient

$$\text{Laplacian-Score}(d) \stackrel{\triangle}{=} \bar{\boldsymbol{f}}_d^\top \boldsymbol{L} \bar{\boldsymbol{f}}_d = \sum_{n=0}^{N-1} \lambda_n \langle \boldsymbol{\psi}_n, \bar{\boldsymbol{f}}_d \rangle^2,$$

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e.g. (# nuisance variables)$\sim$ (cluster separation)^4 $\rightarrow$ Laplacian "breaks"

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Differentiable Unsupervised Feature Selection (DUFS)

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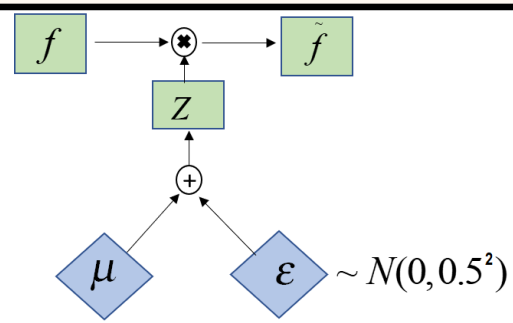
1. Filter features using stochastic gates



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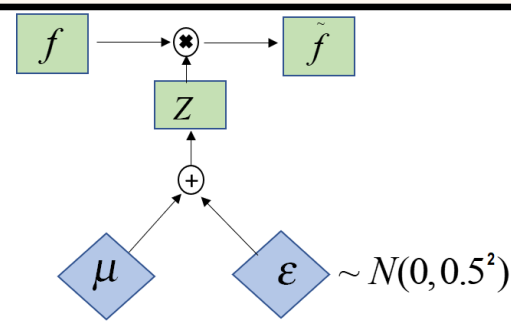

2. Define the **gated** measurement matrix

$$\bar{\boldsymbol{X}} = \left[\bar{\boldsymbol{f}}_1 \cdot \mathrm{z}_1 \middle| \quad \bar{\boldsymbol{f}}_2 \cdot \mathrm{z}_2 \middle| \quad \ldots \quad \middle| \bar{\boldsymbol{f}}_D \cdot \mathrm{z}_D\right]$$

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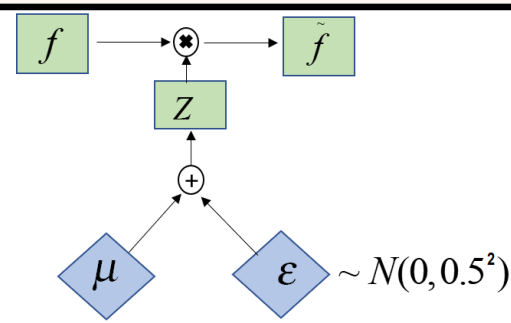

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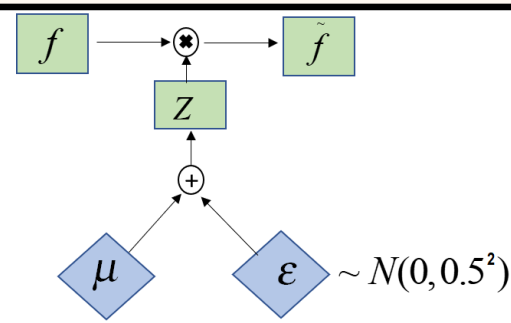

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4. Identify **smooth** features by minimizing

$$L(\boldsymbol{\mu}) := \underbrace{-\mathrm{Tr}\left[\bar{\boldsymbol{X}}^T \boldsymbol{P}_{\bar{x}} \bar{\boldsymbol{X}}\right]}_{\text{Smoothness}} + \lambda \underbrace{\mathbb{E}_{\mathsf{z}} \|\mathbf{z}\|_0}_{\text{Regularization}}$$

Gaussian **ST**ochastic **G**ates (**STG**)

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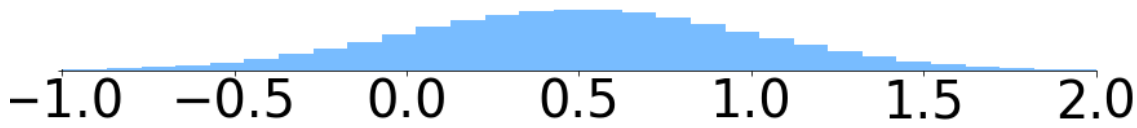
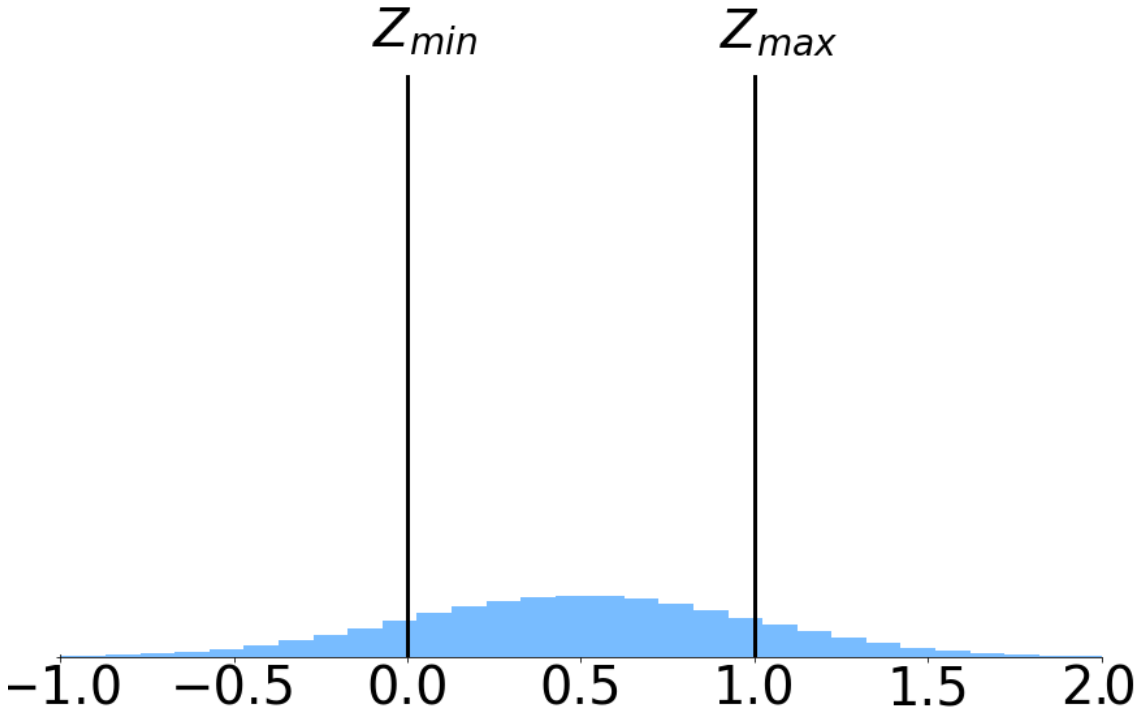


Gaussian **ST**ochastic **G**ates (**STG**)

The idea: use a truncated Gaussian to relax the Bernoulli distribution

- Truncate into $[0, 1]$



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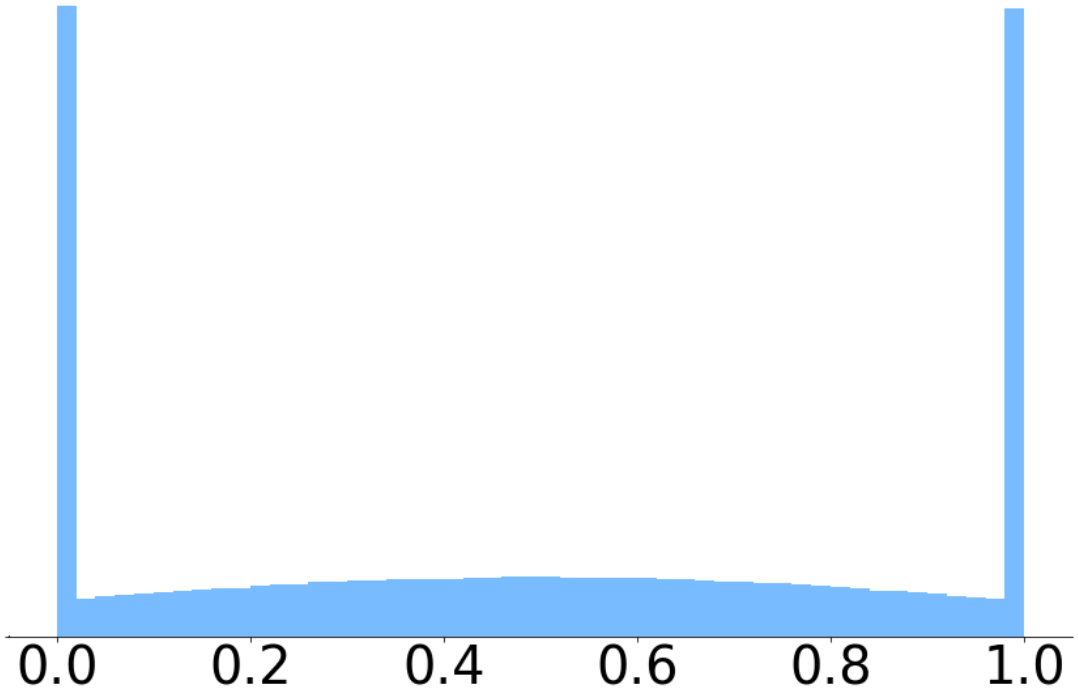
- Define the STochastic Gate (STG), denoted by z



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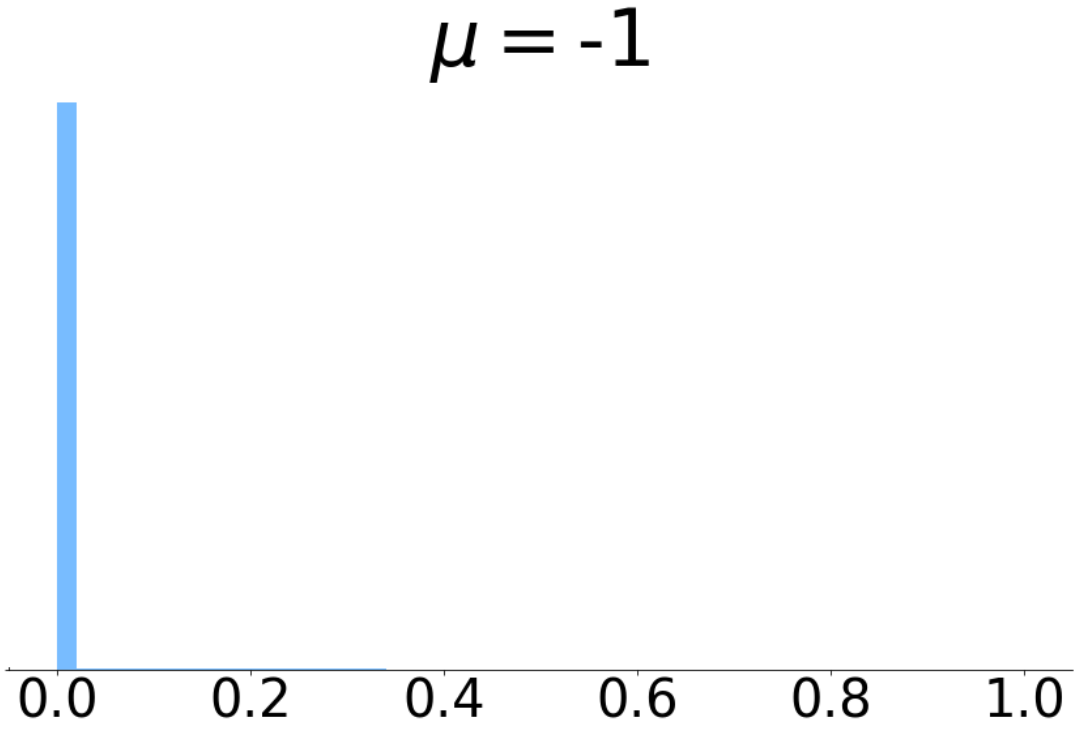
- Each gate is controlled by a trainable parameter μ



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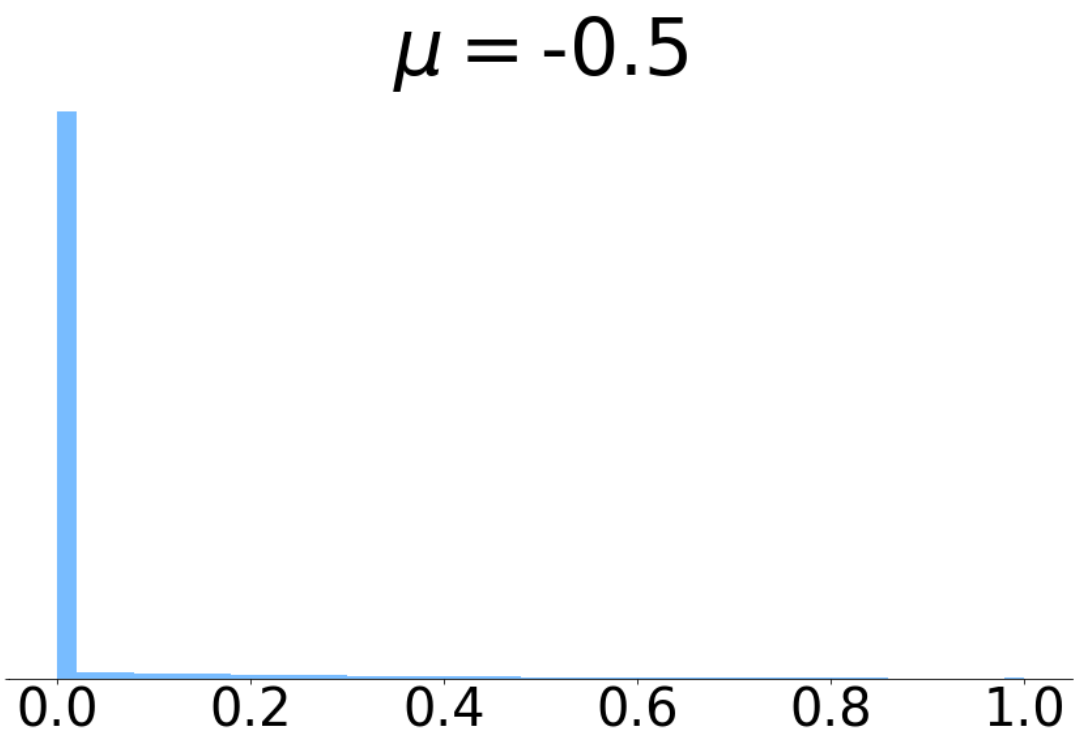

- Learn model and gate parameters by minimizing

$$\widehat{\boldsymbol{\mu}} = \underset{\boldsymbol{\mu}\in\mathbb{R}^D}{\arg\min} -\mathrm{Tr}\left[\bar{\boldsymbol{X}}^T \boldsymbol{P}_{\bar{x}} \bar{\boldsymbol{X}}\right] + \lambda \mathbb{E}_{\mathbf{z}} \|\mathbf{z}\|_0$$

$$\Downarrow$$

$$\sum_{d=1}^{D} \Phi\left(\frac{\mu_d}{0.5}\right)$$

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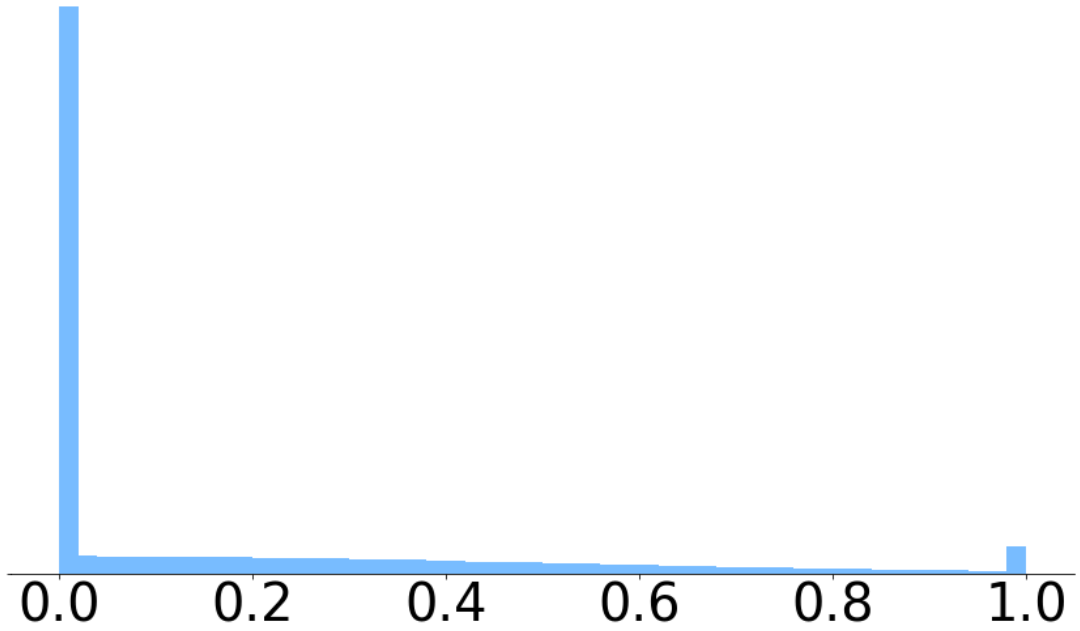
$$\mu = 0$$



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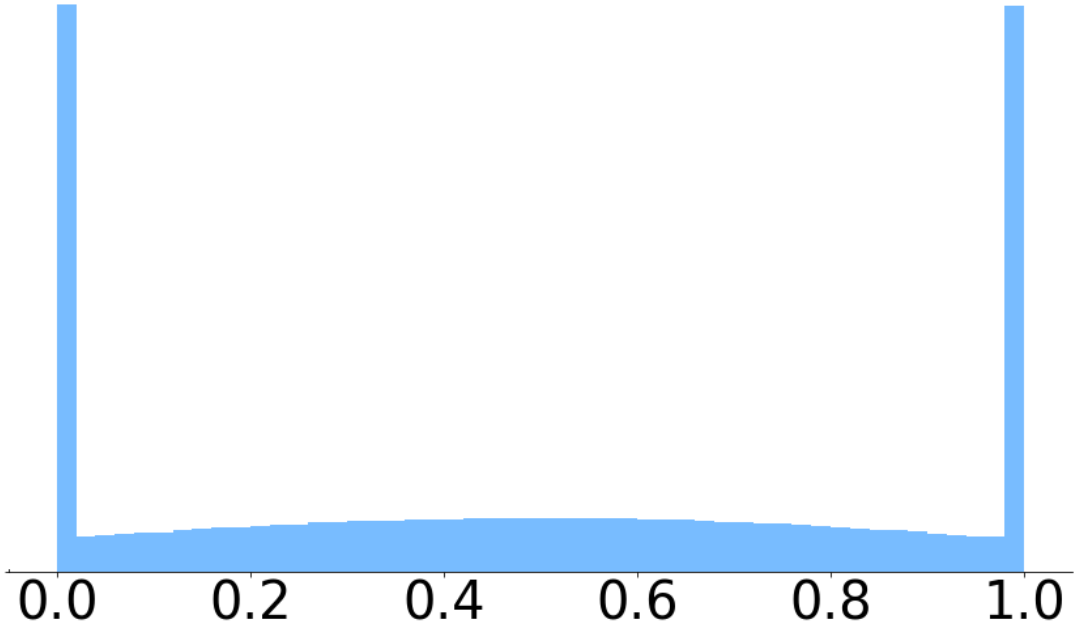

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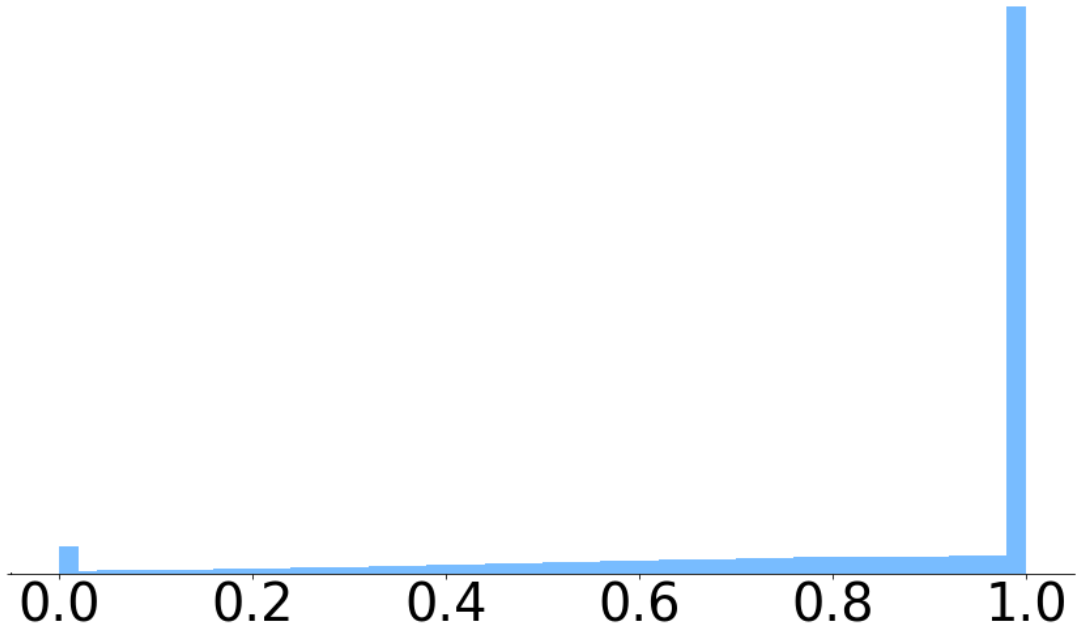
$$\mu = 1$$



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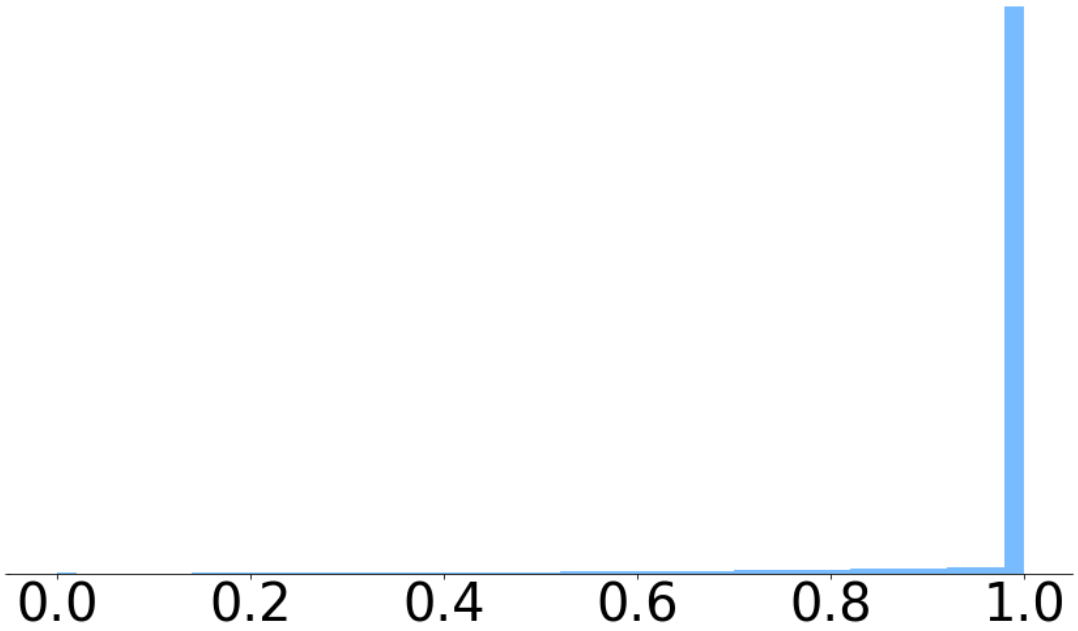
$$\mu = 1.5$$



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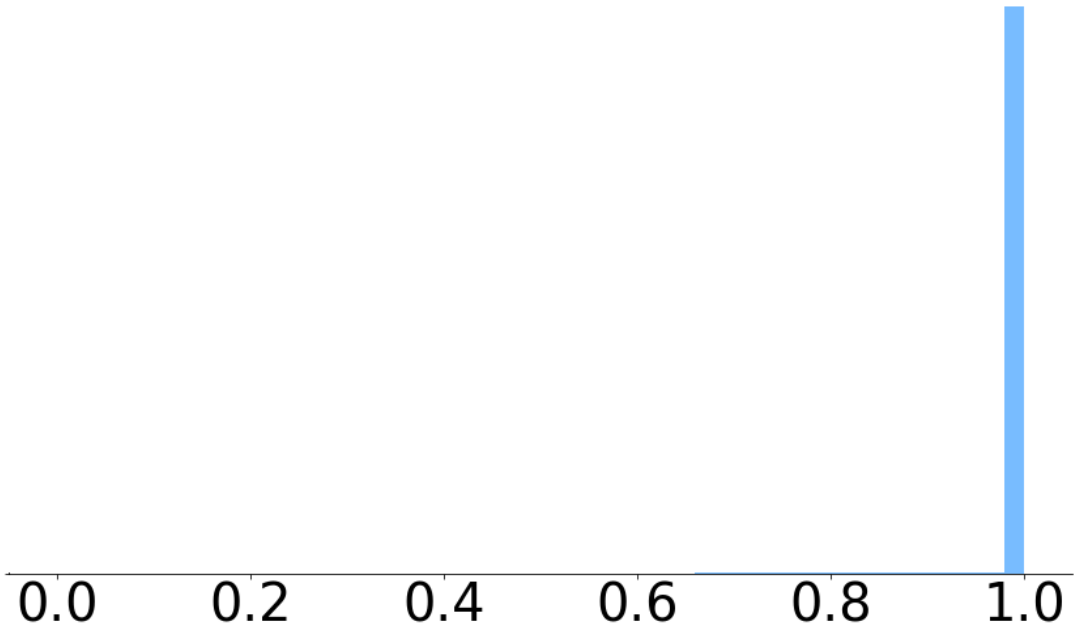
$$\mu = 2$$



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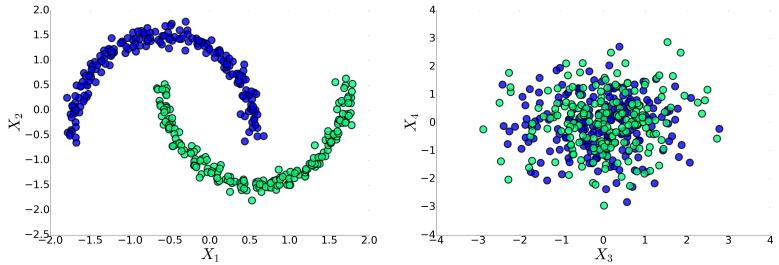
Results: Noisy Two-moons

Consider an **informative** data $\tilde{\boldsymbol{X}}$ concatenated with nuisance variables $\boldsymbol{X} = \left[\tilde{\boldsymbol{X}}|\boldsymbol{\xi}_1|...|\boldsymbol{\xi}_{D_n}\right]_{N\times(D)}$, where $D = D_c + D_n$, and $\xi_{i,j} \sim N(0,1)$



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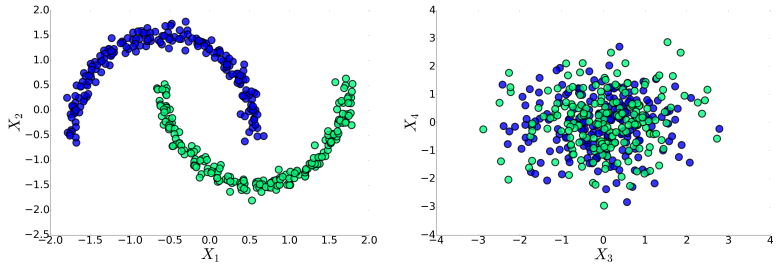
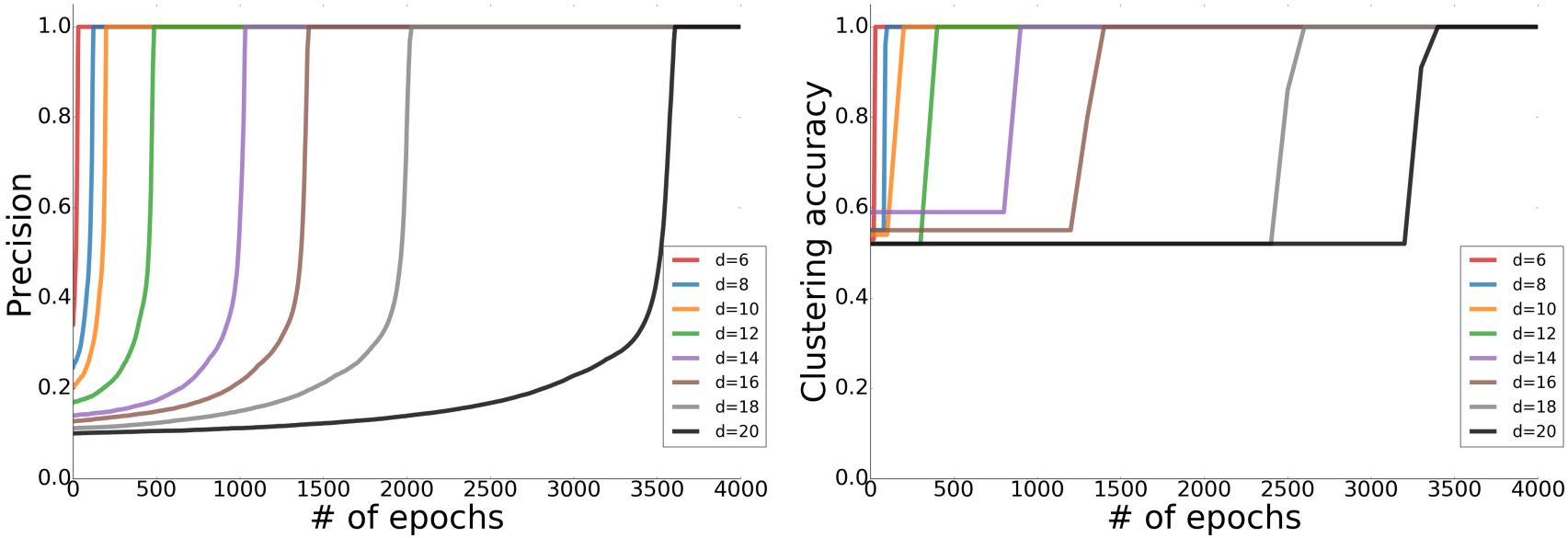


DUFS performance for different number of nuisance variables (d)



Results: MNIST

Use digits of 3s and 8s from noisy MNIST

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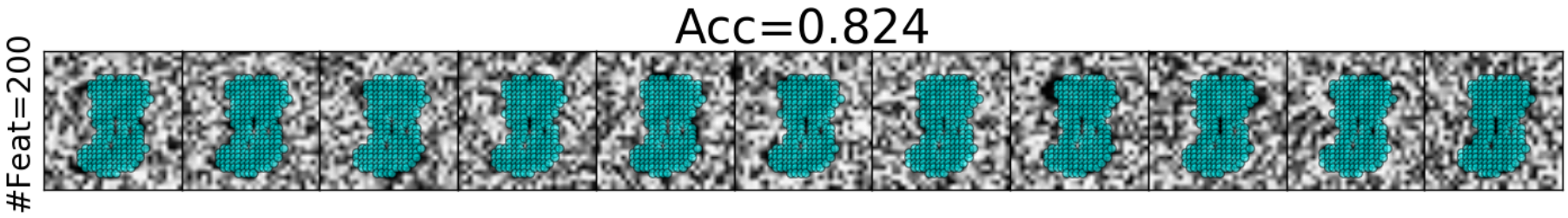
Selected features and clustering accuaracy



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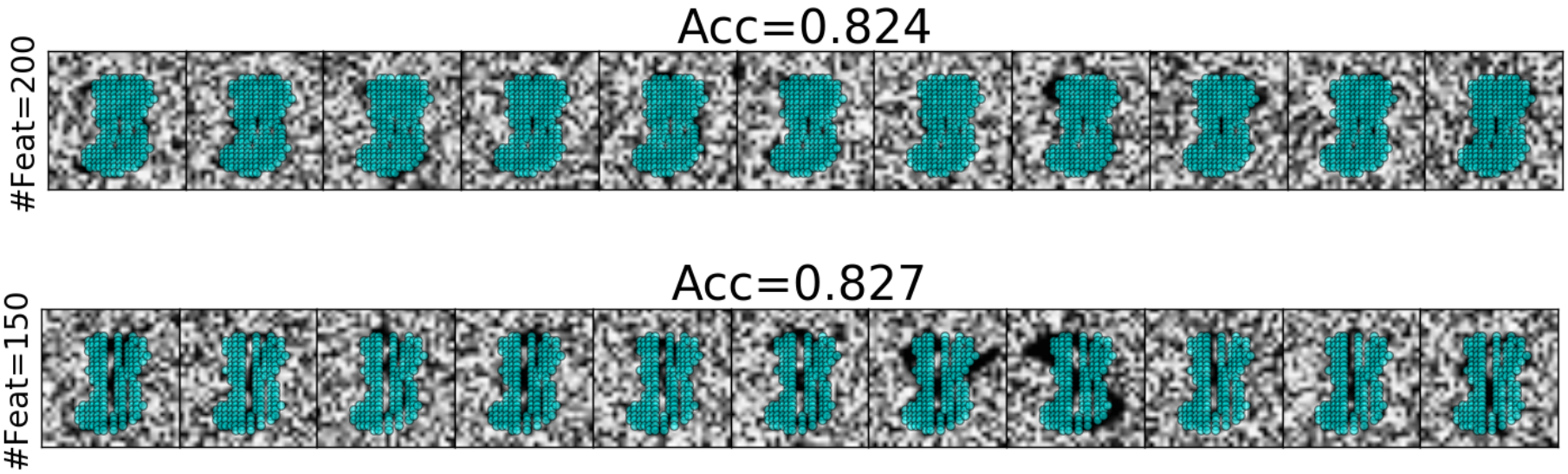

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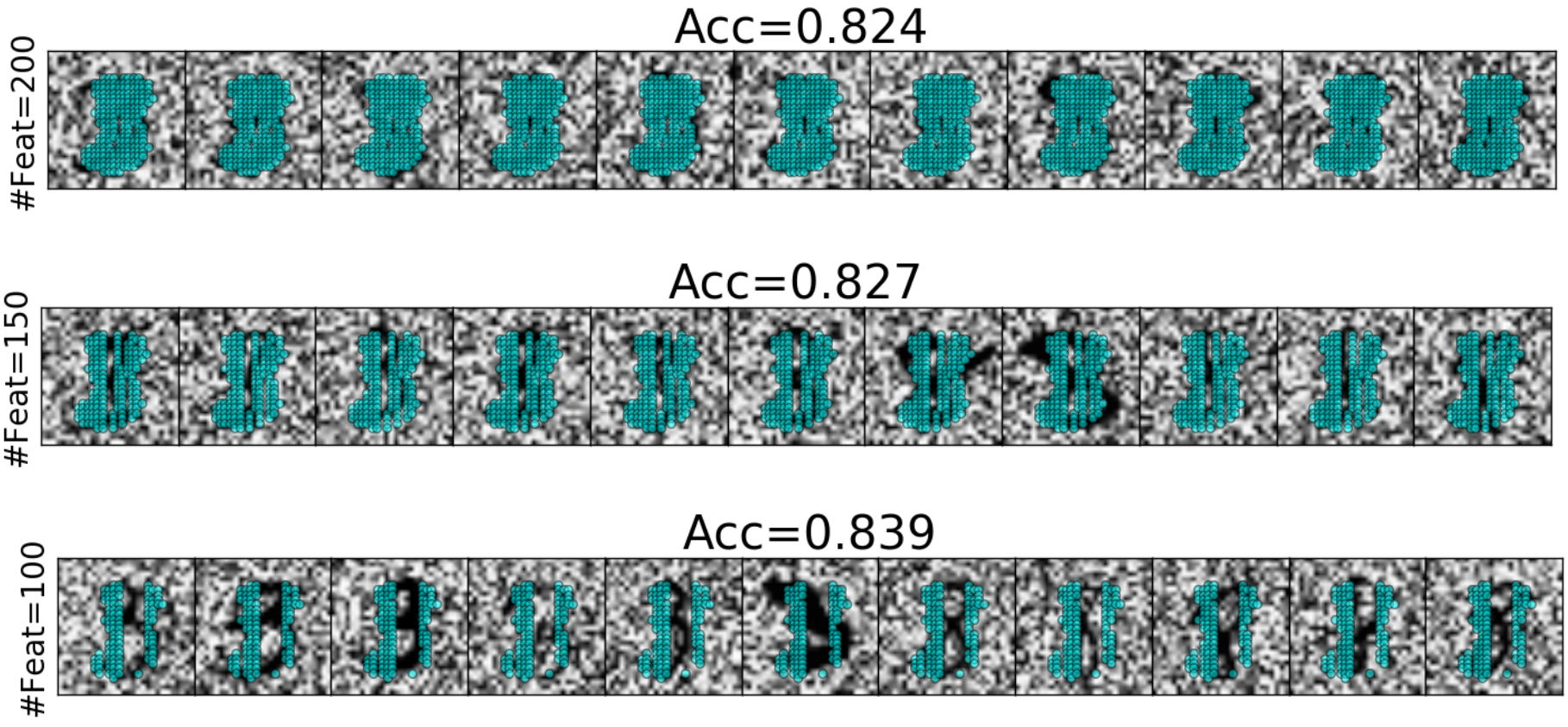

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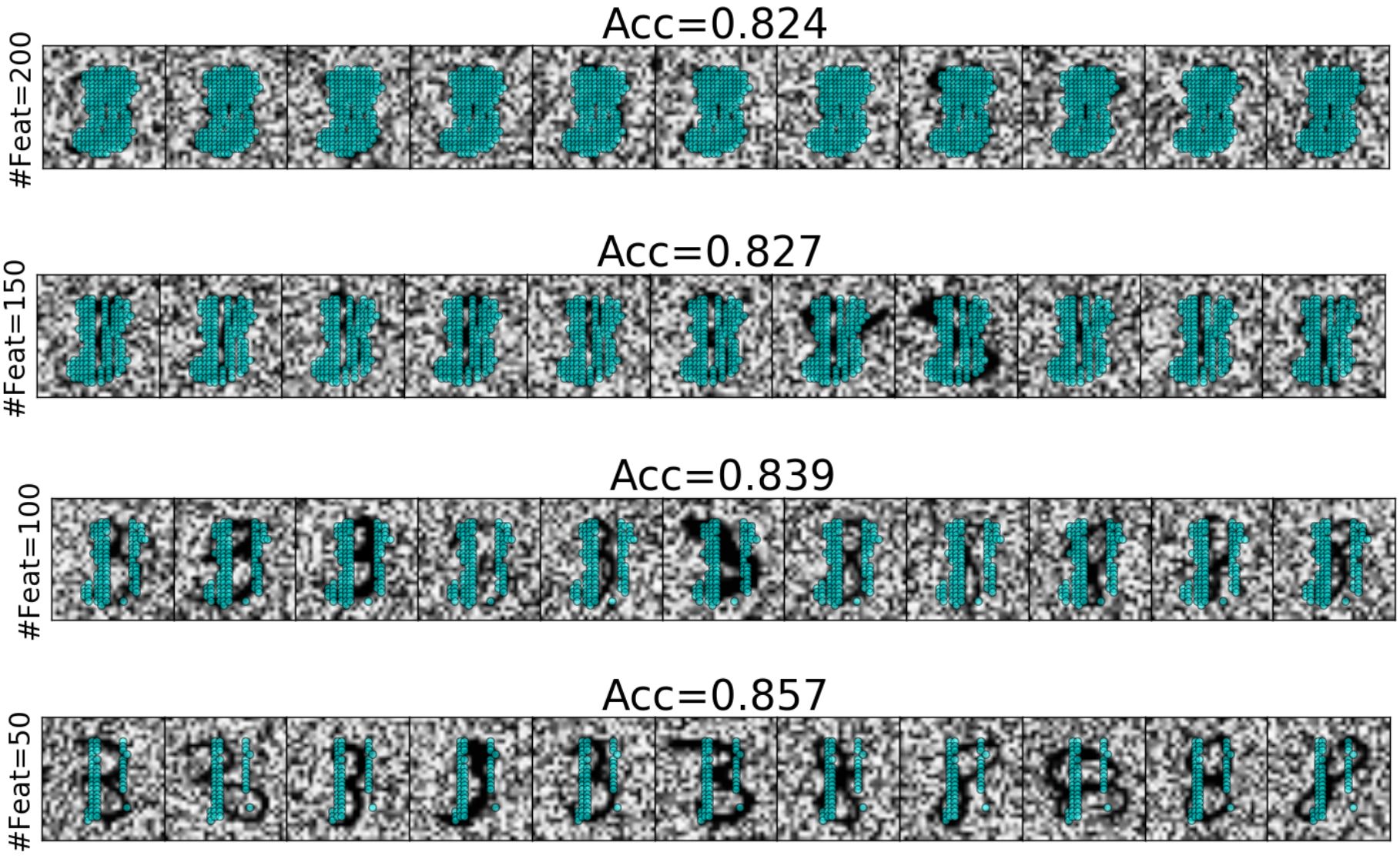

Results: Real Data

K-means accuracy on benchmark datasets[3] (# of selected features)

Datasets	LS	MCFS	NDFS	LLCFS	SRCFS	CAE	**DUFS**	All	Dim/Samples/Classes
GISETTE	75.8 (50)	56.5 (50)	69.3 (250)	72.5 (50)	68.5 (50)	77.3 (250)	**99.5 (50)**	74.4	4955 / 6000 / 2
PIX10	76.6 (150)	75.9 (200)	76.7 (200)	69.1 (300)	76.0 (300)	**94.1 (250)**	88.4 (50)	74.3	10000 / 100 / 10
COIL20	55.2 (250)	59.7 (250)	60.1 (300)	48.1 (300)	59.9 (300)	65.6 (200)	**65.8 (250)**	53.6	1024 / 1444 / 20
Yale	42.7 (300)	41.7 (300)	42.5 (300)	42.6 (300)	46.3 (250)	45.4 (250)	**47.9 (200)**	38.3	1024 / 165 / 15
TOX-171	47.5 (200)	42.5 (100)	46.1 (100)	46.7 (250)	45.8 (150)	44.4 (150)	**49.1 (50)**	41.5	2000 / 62 / 4
ALLAML	73.2 (150)	68.4 (100)	69.4 (100)	**77.8 (50)**	67.7 (250)	72.2 (200)	74.5 (100)	67.3	7192 / 72 / 2
PROSTATE	57.5 (300)	57.3 (300)	58.3 (100)	57.8 (50)	60.6 (50)	56.9 (250)	**64.7 (150)**	58.1	5966 / 102 / 2
RCV1	54.9 (300)	50.1 (150)	55.1 (150)	55.0 (300)	53.7 (300)	54.9 (300)	**60.2 (300)**	50.0	47236 / 21232 / 2
SRBCT	41.1(300)	43.7(250)	41.0(50)	34.6(150)	33.49(50)	**62.6 (200)**	51.7 (50)	39.6	2308 / 83 / 4
BIASE	83.8 (200)	95.5 (300)	100 (100)	52.2 (300)	50.8 (50)	85.1 (250)	**100 (50)**	41.8	25683 / 56 / 4
INTESTINE	43.2 (300)	48.2 (300)	42.3 (100)	63.3 (200)	58.1 (300)	51.9 (50)	**71.9 (250)**	54.8	3775 / 238 / 13
FAN	42.9 (150)	45.5 (150)	48.8 (100)	29.0 (50)	29.0 (100)	35.2 (300)	**49.0 (50)**	37.5	25683 / 56 / 8
POLLEN	46.9 (150)	**66.5 (300)**	48.9 (50)	35.0 (100)	34.9 (300)	58.0 (250)	60.2 (50)	54.9	21810 / 301 / 4
Median rank	4	6	4	4	5	3	**1**		
Mean rank	4.1	6	3.9	4.6	4.7	3.4	**1.3**		

[3] https://jundongl.github.io/scikit-feature/

Conclusion and Future Work

- "Cleaning" the Laplacian prior to calculation of the LS is cruical
- DUFS is also applicable for Manifold Learning
- Potential applications in computational biology, medicine
- Extending the method to handle correlated features
- Code available at https://github.com/Ofirlin/DUFS