Differentiable Unsupervised Feature Selection based on a Gated Laplacian

Ofir Lindenbaum, Uri Shaham, Erez Peterfreund, Jonathan Svirsky, Nicolas Casey, Yuval Kluger

November 2021

Unsupervised Learning

Find structures in dataset $\tilde{X} \quad \mathrm{R}^{N \times D_c}$ (**no label information**)

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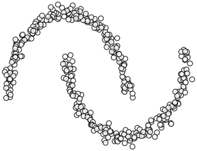

Two-moons

Find subsets
$C_1, ..., C_k \quad \tilde{X}$ so that
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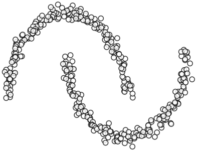

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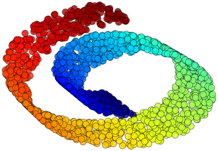
- Manifold Learning



Swiss-roll

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

Unsupervised Learning: Nuisance Variables

Consider an **informative** data $\tilde{X}$ concatenated with nuisance variables $X = \tilde{X}|\xi_1|...|\xi_{D_n}{}_{N\times(D_c+D_n)}$, where $\xi_{i,j}$ $N(0,1)$ and $D = D_c + D_n$

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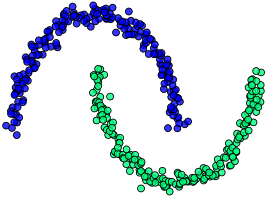

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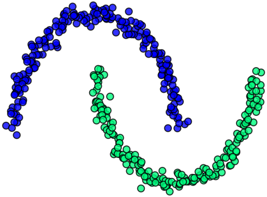

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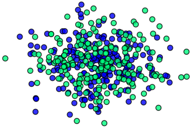

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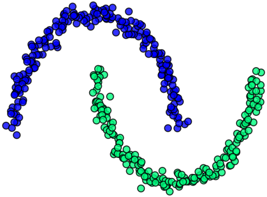

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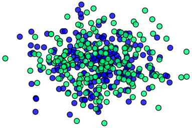

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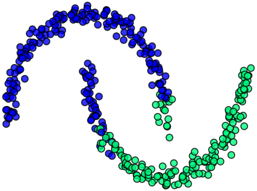

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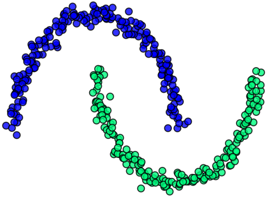

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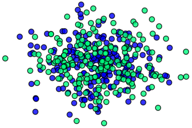

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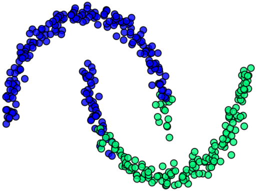

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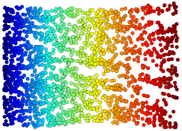

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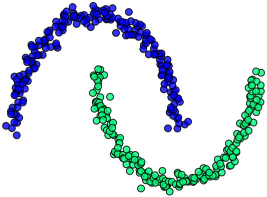

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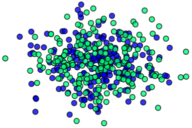

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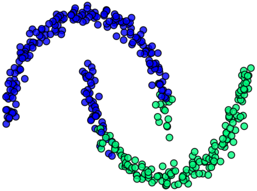

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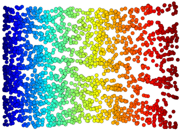

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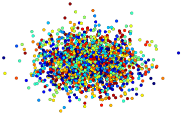

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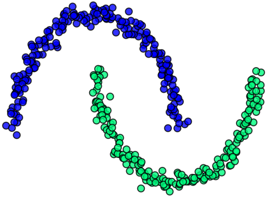

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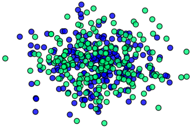

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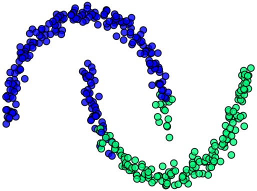

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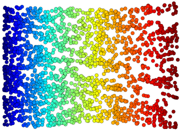

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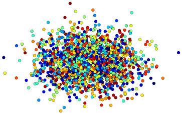

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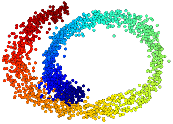

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Goal (informal)

Find a **subset** of *informative* variables $S \quad \{1, ..., D\}$ to improve clustering or manifold learning

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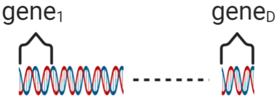
N- individuals, D- genes
Cluster traits/conditions



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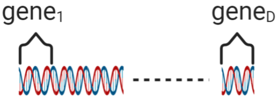

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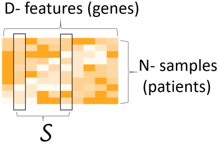

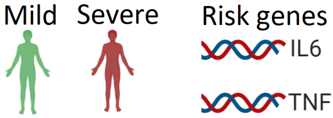

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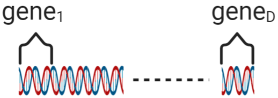

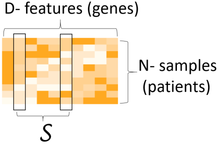

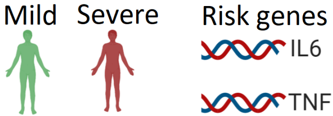

The idea: use "smoothness" to identify *informative* variables

Unsupervised Learning: Kernel Methods

The graph Laplacian[1] is a useful tool for unsupervised learning

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0 1 2 3 4

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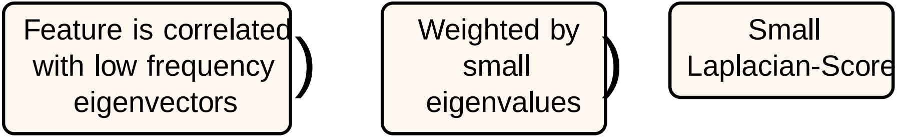
Feature is correlated with low frequency eigenvectors ⇒ Weighted by small eigenvalues ⇒ Small Laplacian-Score

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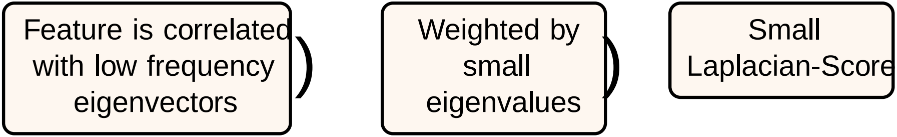

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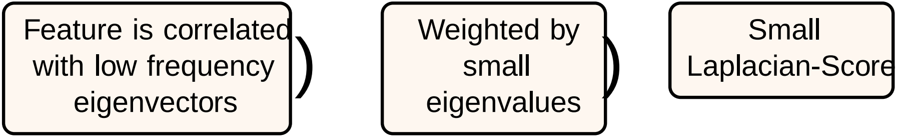
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e.g. (# nuisance variables) (cluster separation)^4 ! Laplacian "breaks"

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$$X = \left\langle f_1 z_1 \quad f_2 z_2 \quad \ldots \quad f_D z_D \right\rangle$$

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Identify smooth features by minimizing

$$L(\;) := \underbrace{\mathrm{Tr}\; X^T P_x X}_{\text{Smoothness}} + \underbrace{E_z \|z\|_0}_{\text{Regularization}}$$

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Gaussian STochastic Gates (STG)

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

- Truncate into $[0, 1]$

Gaussian STochastic Gates (STG)

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

Define the STochastic Gate (STG), denoted by z

Gaussian STochastic Gates (STG)

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

- Each gate is controlled by a trainable parameter

Gaussian STochastic Gates (STG)

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

Each gate is controlled by a trainable parameter

Learn model and gate parameters by minimizing

$$b = \arg\min_{2 R^D} \quad \mathrm{Tr} \ X^{T} P_{x} X \quad + \quad E_{z} kzk_{0}$$

$$+ \quad P^{D}_{d=1} \left(\quad \frac{d}{0:5} \right)$$

Gaussian STochastic Gates (STG)

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

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Learn model and gate parameters by minimizing

$$b = \arg\min_{2\, R^{D}} \mathrm{Tr}\ X^{T} P_{x} X + E_{z} kzk_{0}$$

$$+ \sum_{d=1}^{D} \left(\frac{d}{0{:}5} \right)$$

GaussianSTochasticGates (STG)

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Each gate is controlled by a trainable parameter

Learn model and gate parameters by minimizing

$$b = \arg\min_{2 R^D} \mathrm{Tr}\ X^{T} P_{x} X + E_{z} kzk_{0}$$

$$+ \overset{D}{\underset{d=1}{P}} \left(\frac{d}{0:5} \right)$$

Gaussian STochastic Gates (STG)

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

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Learn model and gate parameters by minimizing

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$$+ \; \mathrm{P}_{d=1}^{D} \left(\frac{d}{0{:}5} \right)$$

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$$+$$

$$\mathrm{P}_{d=1}^{D} \left(\ \frac{d}{0:5} \right)$$

Results: Noisy Two-moons

Consider an informative data $\tilde{X}$ concatenated with nuisance variables $X = \tilde{X} | _1 | \ldots | _{D_n}$ N (D), where $D = D_c + D_n$, and $_{i;j}$ $N(0;1)$

Results: Noisy Two-moons

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DUFS performance for different number of nuisance variables (d)

Results: MNIST

Use digits of3s and8s from noisy MNIST

Results: MNIST

Use digits of 3s and 8s from noisy MNIST

Results: MNIST

Selected features and clustering accuaracy

Results: MNIST

Selected features and clustering accuaracy

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Results: MNIST

Selected features and clustering accuaracy

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