# COMPUTATIONAL METHODS IN MACHINE LEARNING: TRANSPORT MODEL, HAAR WAVELET, DNA CLASSIFICATION, AND MRI

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# Outline









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#### Overview

Introduction Transport by advection Experiments and results

# Outline



# 2 Introduction

3 Transport by advection



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# Overview

My dissertation includes the following topics:

• Haar approximation from within for  $L^{p}(\mathbb{R}^{d})$ , 0

#### Theorem (J. Benedetto and F. Njeunje)

Let  $f \in L^{p}(\mathbb{R})$ , where 0 suppose <math>f is a continuous function on  $\mathbb{R}$ , with supp  $f \subseteq [A, B]$ . Then, for all  $\epsilon > 0$ , there is an  $M = M(\epsilon)$ , and there is a sequence of sums,

$$f_{M,k} = \sum_{(i,j)\in \mathcal{S}_{M,k}} \tilde{a}_{i,j} \widetilde{\psi}_{i,j}, \quad \tilde{a}_{i,j} \in \mathbb{C},$$

indexed by  $k \ge 1$ , where  $S_{M,k} \subseteq \mathbb{Z} \times \mathbb{Z}$  and card  $S_{M,k} < \infty$ , with the following properties:

if 
$$(i,j) \in S_{M,k}$$
 then  $supp \widetilde{\psi}_{i,j} \subseteq supp f$ ,

and

$$\exists K = K(\epsilon) \text{ such that } \forall k > K, \ \|f - f_{M,k}\|_{\rho} < \epsilon.$$

# Overview

My dissertation includes the following topics:

#### Classification of multiton enhancers

- In collaboration with Dr. Ivan Ovcharenko and his research group at the National Institutes of Health (NIH).
- Enhancers are particular deoxyribonucleic acid (DNA) segments that increase or enhance the likelihood of gene expression.
- Singletons vs. multitons.
- We constructed a classifier using support vector machine to identify multitons having similar characteristics to singletons with high probability.

# • Analysis of *T*<sub>2</sub>-store-*T*<sub>2</sub> magnetic resonance relaxometry with *N* exchanging sites

- In collaboration with Dr. Richard G. Spencer and his research group at NIH.
- Magnetic resonance imaging (MRI) is a tool used for diagnosing anatomy and pathology, including osteoarthritis.
- We successfully extended the analysis of the magnetization signal from 2 sites to *N* sites.

#### Transport operator on graph

- In collaboration with Prof. Wojciech Czaja and Prof. Pierre-Emmanuel Jabin.
- This presentation contains material from this topic.

# Outline











# Introduction

- The curse of dimensionality
  - This expression was coined by Richard Bellman and refers to the problem caused by the exponential increase in volume associated with adding extra dimensions to a mathematical space.
  - In data science this means that the number of observations needed to obtain favorable results grows exponentially with the number of dimensions.
- Dimension reduction (DR):
  - Principal component analysis (PCA), by Pearson<sup>1</sup>.
    - Based on the covariance matrix.
    - Search of the orthogonal directions of greatest variance explaining as much of the data as possible.
  - Kernel PCA, by Schölkopf<sup>2</sup>.
    - Non-linear adaptation of PCA.
    - A great number of non-linear DR algorithms are special cases of kernel PCA.

<sup>2</sup>B. Schölkopf, A. Smola, and K-R. Müller, Kernel principal component analysis, International Conference on Artificial Networks, Springer, 1997, pp. 583-588.

<sup>&</sup>lt;sup>1</sup>K. Pearson, On lines and planes of closest fit to systems of point in space, Philosophical Magazine 2 (1901), no. 11, 559-572.

# Introduction

- Dimension reduction (DR):
  - Diffusion maps (DIF), by Coifman and Lafon<sup>3</sup>.
    - Diffusion maps are constructed using eigenfunctions of Markov matrices.
    - They generate efficient representations of complex geometric structures.
  - Isomap (ISO), by Tenenbaum<sup>4</sup>.
    - Based on the geodesic distance between points measured along the manifold.
  - Laplacian eigenmaps (LE), by Belkin and Niyogi<sup>5</sup>.
    - Preserves local information embedded in low dimensional manifold.
  - Schroedinger eigenmaps (SE), by Czaja and Ehler<sup>6</sup>.
    - Semi-supervised generalization of LE.
    - Uses barrier potential to stir the diffusion process.

<sup>&</sup>lt;sup>3</sup>R. R. Coifman and S. Lafon, Diffusion maps, Applied and Computational Harmonic Analysis 21 (2006), no. 1, 5-30.

<sup>&</sup>lt;sup>4</sup> J. B. Tenenbaum, V. De Silva, and J. C. Langford, A global geometric framework for nonlinear dimensionality reduction, Science 290 (2000), no. 5500, 2319-2323.

<sup>&</sup>lt;sup>5</sup>M. Belkin and P. Niyogi, Laplacian eigenmaps and spectral techniques for embedding and clustering, Advances in Neural Information Processing Systems, 2002, pp. 585-591.

<sup>&</sup>lt;sup>6</sup>W. Czaja and M. Ehler, Schroedinger eigenmaps for the analysis of biomedical data, IEEE Transactions on Pattern Analysis and Machine Intelligence 35 (2013), no. 5, 1274-1280.

## Laplacian eigenmaps: optimization problem

Given a set of *n* points  $X = {\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_n}$  in  $\mathbb{R}^d$ , the goal is to find an optimal embedding for these points in a lower *m*-dimensional space where  $m \ll d$ , while preserving local information.

The embedding is given by the  $n \times m$  matrix  $\mathcal{Y} = [\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_m]$ , where the *i*<sup>th</sup> row corresponds to the embedded coordinates of the *i*<sup>th</sup> points  $\mathbf{x}_i$ . The objective to the minimization problem<sup>7</sup> is written as

$$\sum_{i,j} \|\mathbf{y}^{(i)} - \mathbf{y}^{(j)}\|^2 w_{ij} = \operatorname{tr} (\mathcal{Y}^T \mathcal{L} \mathcal{Y}),$$
(1)

where

- $\mathbf{y}^{(i)} = [\mathbf{y}_1(i), \dots, \mathbf{y}_m(i)]^T$  is the *m*-dimensional representation of the *i*<sup>th</sup> point  $\mathbf{x}_i$ .
- With the appropriate choice of weights *w*<sub>ij</sub>, minimizing (1) ensures that adjacent points remain close together after the mapping.

<sup>&</sup>lt;sup>7</sup>M. Belkin and P. Niyogi, Laplacian eigenmaps for dimensionality reduction and data representation, Neural Computation 15 (2003), no. 6, 1373-1396.

# Laplacian eigenmaps: algorithm

The LE algorithm we will be using in our work involves the following steps:

- Step 1: Construct the adjacency graph using the *k*-nearest neighbor (kNN) algorithm. This is done by putting an edge connecting nodes *i* and *j* given that **x**<sub>i</sub> is among the *k* nearest neighbors of **x**<sub>j</sub>.
- Step 2: Define a graph Laplacian, L, using the weight matrix, W. The weights in W are chosen using the heat kernel with parameter σ. If nodes i and j are connected,

$$w_{ij} = \exp\left(-rac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2}
ight);$$

otherwise,  $w_{ii} = 0$ . The graph Laplacian is given by

$$L=D-W,$$

where *D* is a diagonal matrix with entries  $d_{ii} = \sum_{i} w_{ij}$ .

# Laplacian eigenmaps: algorithm (continues)

• **Step 3:** Find the *m*-dimensional mapping by solving the generalized eigenvector problem,

$$L\mathbf{f} = \lambda D\mathbf{f},$$
 (2)

where **f** is a vector in  $\mathbb{R}^n$  and  $\lambda$  is a real number. Let {**f**<sub>0</sub>, **f**<sub>1</sub>, ..., **f**<sub>*n*-1</sub>} be the solution set to (2) written in ascending order according to their eigenvalues { $\lambda_0, \lambda_1, \ldots, \lambda_{n-1}$ }. The *m*-dimensional Euclidean space mapping is given by

$$\mathbf{x}_i \rightarrow [\mathbf{f}_1(i), \mathbf{f}_2(i), \dots, \mathbf{f}_m(i)].$$



# Example: LE vs PCA

- Laplacian eigenmaps is able to represent the data in a reasonable manner preserving local information.
- PCA fails to capture the true nature of the data and simply project it to a 2-dimensional space.



Figure 1: The leftmost plot represents a set of 2000 3-dimensional points sitting on a swiss roll; the middle plot represents the embedding in 2-dimension using principal component analysis (PCA); and the rightmost plot represents the same embedding using Laplacian eigenmaps (LE) with k = 12 (number of neighbors per node) and  $\sigma = 1$ .

# Schroedinger eigenmaps: optimization problem

Czaja and Ehler proposed the Schroedinger eigenmaps (SE) algorithm:

- Semi-supervised generalization to the LE algorithm using partial knowledge about the ground truth of the data set.
- The minimization problem<sup>8</sup>

$$\min_{\mathcal{Y}^{T} \mathcal{D} \mathcal{Y} = \mathbf{I}} \frac{1}{2} \sum_{i,j} \|\mathbf{y}^{(i)} - \mathbf{y}^{(j)}\|^2 w_{ij} + \alpha \sum_{i} V(i) \|\mathbf{y}^{(i)}\|^2,$$
(3)

where V is the diagonal matrix with entries V(1) through V(n).

- The second component of the sum (3) add an extra level of clustering on the representation  $\mathbf{y}^{(i)}$  which are associated with large value of V(i).
- Partial knowledge about the data is used to build barrier potential, encoded in the matrix *V*, to stir the diffusion process in order to obtain suitable results

<sup>&</sup>lt;sup>8</sup>W. Czaja and M. Ehler, Schroedinger eigenmaps for the analysis of biomedical data, IEEE Transactions on Pattern Analysis and Machine Intelligence 35 (2013), no. 5, 1274-1280.

Schroedinger eigenmaps: algorithm

Given a set of *n* points  $X = {\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_n}$  in  $\mathbb{R}^d$  and a function  $\mu$ ,

 $\mu: X \to \mathbb{R},$ 

containing the extra information over the set of points X, the SE algorithm we will be using in our work involves the following steps:

- Step 1: Construct the adjacency graph.
- Step 2: Define a graph Laplacian, L, using the weight matrix, W.
- Step 3: Define the Schrodinger matrix, S, using the extra information,  $\mu$ .

$$S = L + \alpha V$$
,

where  $\alpha$  is a real number, and V is the diagonal potential matrix given by

$$V = \begin{bmatrix} \mu_1 & & & \\ & \mu_2 & & \\ & & \ddots & \\ & & & & \mu_n \end{bmatrix},$$
(4)

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where  $\mu_i = \mu(\mathbf{x}_i)$  for all  $i = 1, \ldots, n$ .

Schroedinger eigenmaps: algorithm (continues)

• Step 4: Find the *m*-dimensional mapping by solving the generalized eigenvector problem,

$$Sf = \lambda Df,$$
 (5)

where **f** is a vector in  $\mathbb{R}^n$  and  $\lambda$  is a real number. Let {**f**<sub>0</sub>, **f**<sub>1</sub>, ..., **f**<sub>*n*-1</sub>} be the solution set to (5) written in ascending order according to their eigenvalues { $\lambda_0, \lambda_1, \ldots, \lambda_{n-1}$ }. The *m*-dimensional Euclidean space mapping is given by

$$\mathbf{x}_i \rightarrow [\mathbf{f}_1(i), \mathbf{f}_2(i), \dots, \mathbf{f}_m(i)].$$

# Outline









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# Continuous model: notations

We consider a graph as a set of points  $X = {\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_n}$  in  $\mathbb{R}^d$ , or equivalently as a set of indices *i* in  $I = {1, 2, ..., n}$ .

- We denote A<sub>i</sub> as the set of adjacent indices to i
- We denote  $A = \{(i, j) : j \in A_i\}$  as the set of edges of the graph
- We denote  $\mathcal P$  as the set of probability distributions  $\mu$  from / to  $\mathbb R^+,\,\mu$  is such that

$$\mu \in \mathcal{P} \Rightarrow \sum_{i} \mu_{i} = \mathbf{1}.$$

- We denote  $\mathcal{E}$  as the set of functions from A to  $\mathbb{R}$ , and
- We denote  $\mathcal{E}_a$  as the set of functions v in  $\mathcal{E}$  that are antisymmetric, that is

$$v_{ij} = -v_{ji}$$

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# Continuous model: definition

Let  $\mu \in \mathcal{P}$ , and  $v \in \mathcal{E}_a$  a velocity field that is itself a function of  $\mu$ . The transport model we consider is also known as the transport by advection; it refers to the active transportation of a distribution,  $\mu$ , by a flow field, v.

We define the transport operator, T, acting on  $\mu$  as follows:

$$T\mu = \triangle \mu - \operatorname{div}(\mathbf{v}\mu). \tag{6}$$

- $\triangle$  denotes the Laplacian defined as the divergence of the gradient acting on a distribution  $\mu$ .
- div denotes the divergence, a vector operator that produces a scalar field quantifying a vector field's source at each point.
- We denote  $\nabla$  as the gradient acting on a scalar field.
- A comprehensive study of the operator in (6) is found in related materials by Benamou et al.<sup>9</sup> and Hundsdorfer et al.<sup>10</sup>.
- Given an appropriately chosen flow field, v, we are able to direct the diffusion process in order to form desirable clusters.

<sup>&</sup>lt;sup>9</sup> J-D. Benamou, B. D. Froese, and A. M. Oberman, Numerical solution of the optimal transportation problem using the Monge-Ampèere equation, Journal of Computational Physics 260 (2014), 107-126.

<sup>&</sup>lt;sup>10</sup>W. Hundsdorfer and J. G. Verwer, Numerical solution of time-dependent advection-diffusion-reaction equations, vol. 33, Springer Science & Business Media, 2013.

# Discrete model: discretization

We propose the following discretization as well as matrix formulation:

• Given a function  $\mu$  on *I*, we define the gradient of  $\mu$  as  $\nabla \mu$  by

$$(\nabla \mu)_{ij} = \mathbf{W}_{ij}(\mu_j - \mu_i).$$

• We also define the Laplacian of  $\mu$  as  $riangle \mu = \textit{div}(
abla \mu)$  by

$$( riangle \mu)_i = \sum_{j \in A_i} w_{ij}(\mu_j - \mu_i).$$

• The centered discretization of *v*µ is given by:

$$(\mathbf{v}\mu)_{ij}^{\mathbf{c}} = \mathbf{v}_{ij}rac{\mu_i + \mu_j}{2}.$$

Our choice of discretization schemes is motivated by its well-defined analytic properties.

#### Discrete model and derivative

We consider a purely local type of flow by taking  $v = \beta \nabla \mu$ , where  $\beta$  is a real number. Using the central discretization, we obtain the following equation:

$$(T\mu)_i = \sum_{j \in A_i} w_{ij}(\mu_j - \mu_i) - \beta \sum_{j \in A_i} w_{ij}(\mu_j^2 - \mu_i^2), \quad \text{for each} \quad i \in I$$
  
$$= (F_i(\mu))_i - \beta (F_d(\mu))_i, \quad \text{for each} \quad i \in I.$$

The derivatives of  $F_l$  and  $F_d$  with respect to  $\mu$  are:

$$F'_l(\mu) = L$$
 and  $F'_d(\mu) = 2C_\mu \circ L$ ,

where the operation  $\circ$  is the element-wise multiplication, and the matrix  $\textit{C}_{\mu}$  is given by

$$C_{\mu} = \begin{bmatrix} \vdots & \vdots & \vdots & \vdots \\ \mu_1 & \mu_2 & \dots & \mu_n \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix}.$$

# Linearization

We finally write the linearization,  $\tilde{\mathcal{T}},$  of the transport operator around any given distribution  $\mu$  as

$$\tilde{T}(u) = [L - 2\beta C_{\mu} \circ L](u) \quad \forall u \in \mathcal{P}.$$
(7)

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Transport eigenmaps algorithm

Given a set of *n* points  $X = {\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n}$  in  $\mathbb{R}^d$  and a function  $\mu$ 

 $\mu: \pmb{X} \to \mathbb{R}$ 

over the set of points X. The transport eigenmaps algorithm involves the following steps:

- Step 1: Construct the adjacency graph.
- Step 2: Define a graph Laplacian, *L*, using the weight matrix, *W*.
- Step 3: Define the linearized transport matrix, *T̃*, using the extra information, μ.

$$\tilde{T} = L - 2\beta C_{\mu} \circ L,$$

where  $\beta$  is a real number, the operation  $\circ$  is the element-wise multiplication and

$$C_{\mu} = \begin{bmatrix} \vdots & \vdots & \vdots & \vdots \\ \mu_{1} & \mu_{2} & \dots & \mu_{n} \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix},$$
 (8)

where  $\mu_i = \mu(\mathbf{x}_i)$  for all  $i = 1, \ldots, n$ .

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# Transport eigenmaps algorithm (continues)

• **Step 4:** Find the *m*-dimensional mapping by solving the generalized eigenvector problem,

$$\tilde{T}\mathbf{f} = \lambda D\mathbf{f},$$
 (9)

where **f** is a vector in  $\mathbb{R}^n$  and  $\lambda$  is a real number. Let  $\{\mathbf{f}_0, \mathbf{f}_1, \dots, \mathbf{f}_{n-1}\}$  be the solution set to (9) written in ascending order according to their eigenvalues  $\{\lambda_0, \lambda_1, \dots, \lambda_{n-1}\}$ . The *m*-dimensional Euclidean space mapping is given by

$$\mathbf{x}_i \rightarrow [\mathbf{f}_1(i), \mathbf{f}_2(i), \dots, \mathbf{f}_m(i)].$$

# Outline









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#### Example: Laplacian, transport, and Schroedinger mapping



Figure 2: The first plot represents a set of points, 300 points grouped in 3 clusters of 100 points each, in the order blue, green, then yellow. The rest represents various mapping using the first and second eigenvectors with corresponding non-zero eigenvalue.

The adjusted Rand index (ARI)

Given a set *X* of *n* points and two partitions, e.g., clusterings, of these points, viz.,  $P = \{P_1, P_2, \ldots, P_r\}$  and  $Q = \{Q_1, Q_2, \ldots, Q_s\}$ , the adjusted Rand index<sup>1112</sup> is defined as

$$ARI = \frac{\sum_{ij} \binom{n_{ij}}{2} - \left[\sum_{i} \binom{a_{i}}{2} \sum_{j} \binom{b_{j}}{2}\right] / \binom{n}{2}}{\frac{1}{2} \left[\sum_{i} \binom{a_{i}}{2} + \sum_{j} \binom{b_{j}}{2}\right] - \left[\sum_{i} \binom{a_{i}}{2} \sum_{j} \binom{b_{j}}{2}\right] / \binom{n}{2}},$$
(10)

where  $n_{ij} = |P_i \cap Q_j|$ ,  $a_i = |P_i|$ , and  $b_j = |Q_j|$ , for i = 1, ..., r and j = 1, ..., s.

The adjusted Rand index:

- Quantifies the similarities between two clusterings from 0 to 1.
- A 0 indicates that the clusterings do not agree on any pair of points and a 1 indicates that the clusterings are exactly the same.
- ARI is robust against random chance assignments.

<sup>&</sup>lt;sup>11</sup> W. M. Rand, Objective criteria for the evaluation of clustering methods, Journal of the American Statistical Association, 66.336, 1971, pp. 846-850.

<sup>&</sup>lt;sup>12</sup>J. M. Santos and M. Embrechts, On the use of the adjusted Rand index as a metric for evaluating supervised classification, International Conference on Artificial Neural Networks, Springer, 2009, pp. 175-184.

# Representation experiment: setup

We demonstrate the strength of our algorithm in its ability to faithfully represent the data using a large number of experiments.

- Clusters are arranged in 2 or 3 dimensions increasing in difficulty.
- We increase the difficulty by changing the parameters used to generate the data set: position, spread or standard deviation, added Gaussian noise, and number of clusters.
- Example: changing the position



• We use the adjusted Rand index (ARI) to quantify the representation of the data set.

# Representation experiment: procedure

For each individual run, the following operations are performed:

- Step 1: Generate the data set, *X*, and corresponding labels.
- Step 2: We cluster the data set before and after dimension reduction using the k-means algorithm.
- Step 3: We compute the adjusted Rand index before and after dimension reduction and store the difference.

The following dimension reduction algorithms are used in the experiment:

- Principal components analysis (PCA),
- Laplacian eigenmaps (LE),
- Diffusion maps (DIF),
- Isomap (ISO),
- Schroedinger eigenmaps (SE),
- Transport eigenmaps (TE).

### Representation experiment: result - overall

A positive change in ARI implies a better representation of the data after dimension reduction:

 The rightmost position of the box plot corresponding to TE in relation to the other DR algorithms implies that in general, TE produces the best representation of the data.



Figure 3: Box plot for the change of ARI, all  $162 \times 20 = 3240$  cases.



#### Representation experiment: result - complex and simple

The dominant performance of TE is more apparent on difficult cases, see Figure 4, than it is on simple cases, see Figure 5.



Figure 4: Box plot for the change of adjusted Rand index,  $126 \times 20 = 2520$  difficult cases.



Figure 5: Box plot for the change of adjusted Rand index,  $36 \times 20 = 720$  simple cases.

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# Hyperspectral dataset: Indian Pines

In this section, we work with the Indian Pines<sup>1314</sup> data set:

- Gathered by AVIRIS (Airborne Visible/Infrared Imaging Spectrometer) sensor.
- Over the Indian Pines test site in North-western Indiana: 145  $\times$  145  $\times$  200.
- Hyperspectral bands covering the region of water absorption have been removed.



Figure 6: Ground truth (left) and sample band: 170 (right.)

<sup>&</sup>lt;sup>13</sup>M. F. Baumgardner, L. L. Biehl, and D. A. Landgrebe, 220 band AVIRIS hyperspectral image data set: June 12, 1992 Indian Pines test site 3, September 2015.

<sup>14</sup> Hyperspectral remote sensing scenes, http://www.ehu.eus/ccwintco/index.php/Hyperspectral.Remote.Sensing.Scenes, Accessed: 2018-04-04.

# Indian Pines: ground truth

| #  | Class                        | Sample |  |
|----|------------------------------|--------|--|
| 0  | Empty-space                  | 10776  |  |
| 1  | Alfalfa                      | 46     |  |
| 2  | Corn-notill                  | 1428   |  |
| 3  | Corn-mintill                 | 830    |  |
| 4  | Corn                         | 237    |  |
| 5  | Grass-pasture                | 483    |  |
| 6  | Grass-trees                  | 730    |  |
| 7  | Grass-pasture-mowed          | 28     |  |
| 8  | Hay-windrowed                | 478    |  |
| 9  | Oats                         | 20     |  |
| 10 | Soybean-notill               | 972    |  |
| 11 | Soybean-mintill              | 2455   |  |
| 12 | Soybean-clean                | 593    |  |
| 13 | Wheat                        | 205    |  |
| 14 | Woods                        | 1265   |  |
| 15 | Buildings-Grass-Trees-Drives | 386    |  |
| 16 | Stone-Steel-Towers           | 93     |  |

Table 1: Indian Pines classes.

# Indian Pines grouped: ground truth

| #  | Class                        | Sample |  |
|----|------------------------------|--------|--|
| 0  | Empty-space                  | 10776  |  |
| 1  | Alfalfa                      | 46     |  |
| 2  | Corn                         | 2495   |  |
| 5  | Grass                        | 1241   |  |
| 8  | Hay-windrowed                | 478    |  |
| 9  | Oats                         | 20     |  |
| 10 | Soybean                      | 4020   |  |
| 13 | Wheat                        | 205    |  |
| 14 | Woods                        | 1265   |  |
| 15 | Buildings-Grass-Trees-Drives | 386    |  |
| 16 | Stone-Steel-Towers           | 93     |  |

Table 2: Indian Pines-G classes, ground truth with corresponding grouped labels.

#### Extra information and parameters

 Given prior knowledge about class 11–soybean-mintill in the Indian Pines data set, we would place a potential for SE or an advection for TE on class 11–soybean-mintill using the function μ defined as follows:

$$\mu(\mathbf{x}) = egin{cases} 1, & ext{if } \mathbf{x} \in ext{Class 11-soybean-mintill}, \ 0, & ext{elsewhere.} \end{cases}$$

- We ran a set of experiments to obtain the following parameters:
  - We set m = 50 (Indian Pines), k = 12, and  $\sigma = 1$ .
  - We set  $\beta = 10$  and  $\hat{\alpha} = 10^4$ , where the parameter  $\hat{\alpha}$  such that  $\alpha = \hat{\alpha} \cdot \text{tr}(L)/\text{tr}(V)$ .

# Classification and validation metric

#### After the embedding:

- We use the 1-nearest neighbor algorithm to classify the data sets.
- We use 10% of the data from each class to train the classifier and the rest,  $N_{\nu}$ , as the validation set.
- We took an average of ten runs to produce the confusion matrices, C.

#### We following validation metrics are reported:

- The adjusted Rand index (ARI) between the predicted labels and the ground truth.
- The overall accuracy (OA).
- The Cohen's kappa coefficient<sup>1516</sup> ( $\kappa$ ) is defined by

$$\kappa = rac{N_v \sum_i (C_{i,i})^2 - \omega}{N_v^2 - \omega},$$

where  $\omega = \sum_{i} C_{i,i}$ . Similar to ARI,  $\kappa$  measures the agreement between clusterings, a 0 indicates no agreement while a 1 indicates complete agreement.

<sup>16</sup>Galton, F, Finger Prints Macmillan, 1892.

<sup>&</sup>lt;sup>15</sup>Smeeton, N. C., Early history of the kappa statistic, 1985, pp. 795-795.

## **Results: Indian Pines**

The best representation and accuracy come from TE, with SE as a close second, see Table 3.

| IP       | PCA    | LE     | DIF    | ISO    | SE-2   | SE-11  | TE-2   | TE-11  |
|----------|--------|--------|--------|--------|--------|--------|--------|--------|
| ARI      | 0.4426 | 0.3694 | 0.4210 | 0.3929 | 0.5520 | 0.6955 | 0.5735 | 0.7085 |
| OA       | 0.6761 | 0.6081 | 0.6556 | 0.6308 | 0.7138 | 0.7353 | 0.7281 | 0.7418 |
| $\kappa$ | 0.6301 | 0.5532 | 0.6065 | 0.5785 | 0.6732 | 0.6981 | 0.6900 | 0.7055 |

Table 3: Classification results for Indian Pines (IP).



Figure 7: Classification map.

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### Results: TE vs SE vs % of information

- With lesser information provided from a particular class, SE is slightly ahead of TE.
- As a more complete information is provided, TE outperforms SE.



Figure 8: Classification performance measures for TE (red diamonds) and SE (blue squares) as a function of the amount of information provided. The Indian Pines-G data set is used with the advection and potential is placed on class 10–soybean.



## Results: robustness against noise

- The added Gaussian noise has a mean of 0, we selected 20 logarithmically spaced values for the standard deviation from 10<sup>0</sup> to 10<sup>5</sup>.
- In general, TE is the most robust algorithm against noise.



Figure 9: TE (red diamonds), SE (blue boxes), PCA (green x's), and LE (black circles). The Indian Pines-G data set is used with the advection and potential is placed on class 10–soybean.

# Conclusion

- We constructed a novel semi-supervised non-linear dimension reduction algorithm based on a transport model by advection.
- We used advection, the active transportation of a distribution by a flow field, to stir the diffusion process in order to get better or more desirable results.
- We provided a set of experiments based on artificially generated data sets and on publicly available hyperspectral data set to show that our algorithm exhibits superior/competitive performance.
- We believe that the performance of our algorithm can be improved by choosing alternative flow fields and/or using different linearization techniques.

# Thank You!

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