# An Unsupervised Material Learning Method for Imaging Spectroscopy

Johannes Jordan, Elli Angelopoulou, Antonio Robles-Kelly University of Erlangen-Nuremberg; National ICT Australia







FRIEDRICH-ALEXANDER JNIVERSITÄT ERLANGEN-NÜRNBERG

TECHNISCHE FAKULTÄT

# Multispectral Imaging / Imaging Spectroscopy



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- feature-rich
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## Challenges:

- high-dimensional
- highly correlated, but noisy

# Contribution

#### Application: Material Learning

- False-colour visualisation of scene materials
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  - Common application in remote sensing: Spectral unmixing

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## Methodology:

- Unsupervised manifold learning
- Fast clustering using established methods





# Manifold Learning vs Dimensionality Reduction



Original data (image spectral gradient)



Principal Component Analysis

# Manifold Learning vs Dimensionality Reduction



Principal Component Analysis



## Concept

- graph G<sub>M</sub> = (Y, E<sub>M</sub>), node set Y comprises of y<sub>i</sub> ∈ ℝ<sup>m</sup>
- determining  $E_M$  is a hard problem
- graph G<sub>Q</sub> = (X, E<sub>Q</sub>), constructed to help derive the manifold topology





# Concept

- graph  $G_M = (Y, E_M)$ , node set Y comprises of  $y_i \in \mathbb{R}^m$
- determining *E<sub>M</sub>* is a hard problem
- graph G<sub>Q</sub> = (X, E<sub>Q</sub>), constructed to help derive the manifold topology
- X, Y are linked via  $x_j = \sum_{y_k \in Y} \mathbb{I}(x_j \sim y_k) \Gamma(y_k)$
- $\Gamma : \mathbb{R}^m \mapsto \mathbb{R}^q$ ,  $\mathbb{I}(x_j \sim y_k)$  indicator function for adjacency





# Concept (1)

- G<sub>Q</sub> is a Gibbs Field
- conditional probability of vertex  $x_i$ :  $P(x_i \mid C_{x_i}) = \frac{1}{Z_Q} \prod_{x_i \in C_{x_i}} f_Q(x_j, x_i)$
- $C_{x_i}$  clique centered at  $x_i$
- Z<sub>Q</sub> partition function, f<sub>Q</sub>(x<sub>j</sub>, x<sub>i</sub>) potential function, also edge weight between x<sub>i</sub> and x<sub>i</sub>





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- maximum-likelihood estimation (MLE) on the vertex-set *Y* ∈ *G<sub>M</sub>* based upon the vertices *X* ∈ *G<sub>Q</sub>*





# Concept (2) Q Qí $C_{x_i}$ Μ Μ

We introduce the parameter set  $\xi_i$  with correspondence to  $x_i$ .



# Concept (3)

- $x_j = \sum_{y_k \in Y} \eta_j \mathcal{K}(y_k, \xi_j)$
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#### **Potential function:**

• Gibbs distribution:

$$f_Q(x_j, x_i) = \sum_{y_k \in Y} \alpha_{i,j} \exp\left\{-\frac{1}{T} d_M(y_k, \xi_j)^2\right\}$$



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#### **Algorithm:** Expectation-Maximization on $\xi_j$ , $\alpha_{i,j}$



# **Relation to Self-Organizing Maps**

Consider a sampling process in *M*,

• 
$$\alpha_{i,j} = \mathbb{I}(x_j \sim \rho) h\left(\frac{1}{T} d_Q(x_i, x_j)^2\right)$$

- $\rho$  resembles the *best-matching unit* in a SOM
- I(x<sub>j</sub> ~ ρ) indicates the vertex x<sub>j</sub> connected to ξ<sub>j</sub> with minimum distance to the input sample



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Observations:

- Clique size eq. SOM neighborhood size
- Gibbs temperature *T* eq. SOM learning rate
- More general formulation, but binary neighborhood function



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#### Visualization:

$$u = \sum_{\substack{y_k \in Y \\ x_j \in \mathcal{C}_\rho}} \mathbb{I}(x_j \sim y_k) \exp\left\{-\frac{1}{T} d_Q(x_j, \rho)^2\right\} \exp\left\{-\frac{1}{T} (y_k - \xi_\rho)^2\right\}$$



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#### Material clustering:

- cluster on parameters  $\xi_j$
- fast-adaptive mean shift algorithm
- hill-climbing to find material prototypes

# **Results: Learning process**

Input



Pseudocolor



PCA

## SOM-Euclidean SOM-Constant Our method



Visualisation

Visualisation



Visualisation

# **Results: Visualisation**



Input in pseudocolour

Visualisation using only the best matching unit

Visualisation recovered using clique information

# **Results: Material clustering**



Input in pseudocolour

Huynh and Robles-Kelly

Our method



# **Results: Material clustering (2)**





## **Results: Dimensionality Reduction**





## **Results: Dimensionality Reduction**



# Timing Results Training: 3 s, mapping: 12 s, clustering: 3 s, total 17.7 s



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- · We model the problem of manifold learning with two linked graphs
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- Our method is shown to be effective for:
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- Our method is computationally efficient in terms of computing power and memory use
- We improve over state-of-the-art in speed and performance