Learning the Shape Manifolds using Diffusion Maps

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Outline

- Introduction
- Motivation
- Relevant Work
- The Proposed Framework
  - Feature Extraction
  - Sub-Manifold Embedding
  - Experimental Results
- Conclusions and Future Directions

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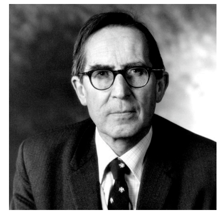
Shape Manifolds

- Kendall's shape spaces (1984)



5. *The manifold carrying the shapes of triangles*

We now know that there is a natural isometry between Σ_2^3, the space whose points are the shapes of labelled triangles, and the sphere $S^2(\frac{1}{2})$. The patch on which

- Manifolds of images and shapes exist due to:
  - Sparseness
  - Continuity

Example with Faces

Motivation

- The *curse of dimensionality*
- Recent surge in research on nonlinear dimensionality reduction (NLDR)

- Object recognition
- Shape-based classification of objects
- Image retrieval
- Object-based image/video coding

Relevant Work (Shape Manifolds)

- Kernel PCA for ASMs (*Twining & Taylor, 2001*)
- Statistical shape priors (*Cremers et al*., 2001)
- Image manifolds for retrieval (*He, Ma & Zhang, 2004*)
- Manifold clustering (*Souvenir & Pless, 2005*)
- Clustering of shape manifolds using Isomaps (*Yankov & Keogh, 2006*)
- Extension of the Laplacian Eigenmaps for interpolation between shape samples (*Etyngier, Keriven & Pons, 2007*)

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Relevant Work (NLDR)

- When the sub-manifold is linear, we can use standard DR methods, eg PCA, ICA, LDA etc.

- For nonlinear sub-manifolds, we need locality preserving DR methods, such as:
  - LLE (Roweis & Saul, 2000)
  - ISOMAPs (Tenenbaum, Silva & Langford, 2000)
  - Laplacian Eigenmaps (Belkin & Niyogi, 2002)
  - Hessian Eigenmaps (Donoho & Grimes, 2003)
  - Diffusion Maps (Coifman & Lafon, 2004)
  - Logmaps (Brun et al., 2005)

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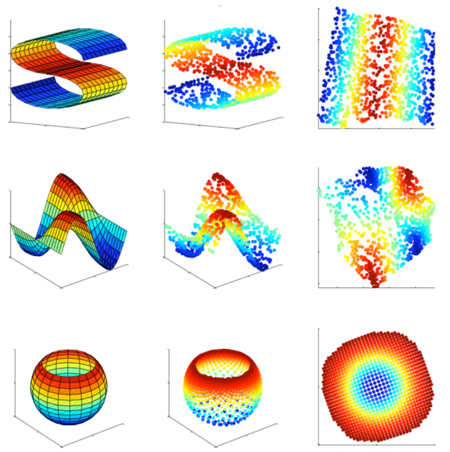
Locality Preservation



Source: Saul & Roweis, 2003

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Learning the Shape Manifolds

"Given a set $\Omega = \{\Omega_1, \Omega_2, \ldots, \Omega_k\}$, where $\Omega_i = \{C_{ij}\}, j = 1, 2, \ldots, n_i = |\Omega_i|$ and $C_{ij} \in \mathcal{C}^1$ is a connected closed curve, represented by N boundary points, in the Euclidean plane, find the intrinsic parameters of the k shape classes and the mapping

$$\Psi : \Re^{2N} \longmapsto \Re^m,$$

where $m << N$, such that clustering in $\Re^m$ yields a *plausible* grouping of similar shapes."

Problem Definition

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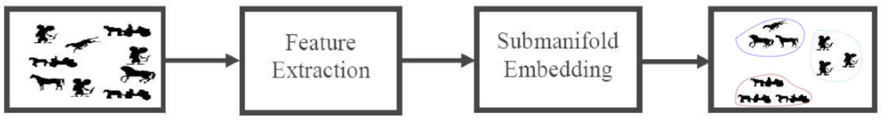
The Proposed Framework

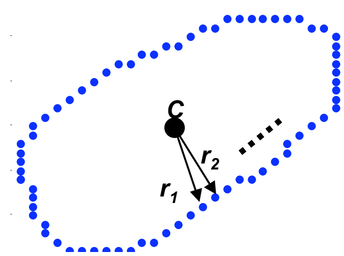


Our emphasis here is on the nonlinear embedding of sub-manifolds corresponding to shapes of different classes

Feature Extraction

- Extract the boundaries of objects in the preprocessed images.
- Resample boundaries into an equal number of points, N.
- Compute centroidal distance function r_i, for $i=1,2,\ldots,N,$

$$r_i = \sqrt{([x_i - x_c]^2 + [y_i - y_c]^2)}$$



Feature Extraction

- The distance vector,

$$\mathbf{r}=\{r_1, r_2, \ldots r_N\}$$

- Rotation and scale invariant feature vector for each shape is obtained as follows,

$$\mathbf{f} = \left[\frac{|F_1|}{|F_0|}, \frac{|F_2|}{|F_0|}, \ldots, \frac{|F_{N/2}|}{|F_0|}\right]^T$$

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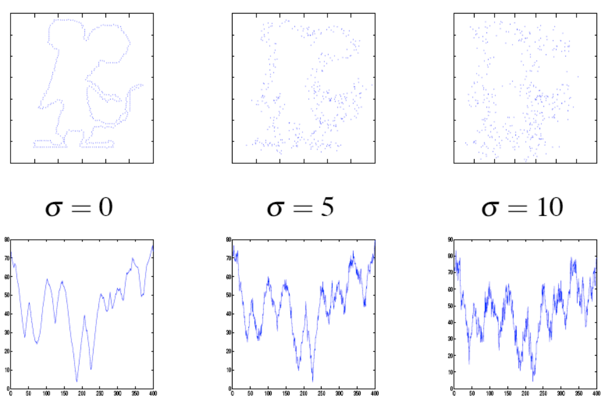
Feature Extraction



Centroidal Distance Vectors for a Rat image

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The Shape Distance

- The shape distance w_{ij} between two shape feature vectors $\mathbf{f}_i$ and $\mathbf{f}_j$ for $i,j=1,2,\ldots,n,$ is computed as follows:

$$w_{ij} = w(\mathbf{f}_i, \mathbf{f}_j) = \exp\left(-\frac{||\mathbf{f}_i - \mathbf{f}_j||^2}{2\varepsilon}\right)$$

where ε denotes the neighbourhood radius.

- The above distance measure can also be regarded as a similarity measure between shapes i and j.

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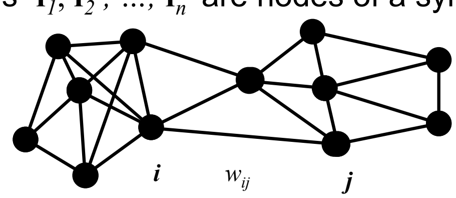
Diffusion Maps

- Diffusion based probabilistic interpretation of spectral methods.
- Feature vectors $\mathbf{f}_1, \mathbf{f}_2, \ldots, \mathbf{f}_n$ are nodes of a symmetric graph.



- Similarity matrix $\mathbf{W}=[w_{ij}]$ for $i,j=1,2,\ldots,n,$ where w_{ij} is given by:

$$w_{ij} = w(\mathbf{f}_i, \mathbf{f}_j) = \exp\left(-\frac{||\mathbf{f}_i - \mathbf{f}_j||^2}{2\varepsilon}\right)$$

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Markov Matrix

- The (i,j)th element of a Markov matrix $\mathbf{P}$ is computed as follows,

$$p_{ij} = \frac{w(\mathbf{f}_i, \mathbf{f}_j)}{d(\mathbf{f}_i)}$$

where

$$d(\mathbf{f}_i) = \sum_{\mathbf{z} \in \Omega} w(\mathbf{f}_i, \mathbf{z})$$

denotes the degree of node i in the graph, and

$$\Omega = \{\mathbf{f}_1, \mathbf{f}_2, \ldots, \mathbf{f}_n\}.$$

- The (i,j)th element of $\mathbf{P}^t$ gives the probability of going from node i to node j in t steps.

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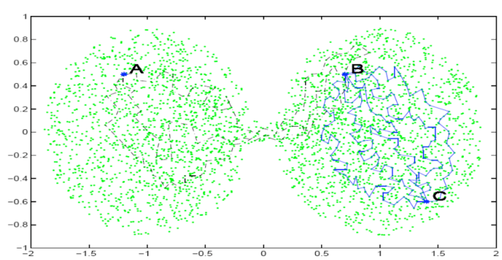
The Diffusion Distance

Diffusion distance between two points A and B is:

$$D(A,B) = \sqrt{\sum_y \frac{(p_{yA} - p_{yB})^2}{\phi_0(y)}}$$



Source : S. Lafon, "Diffusion Maps and Geometric Harmonics," *Ph.D. Dissertation*, Yale University, 2004

where

$$\phi_0(y) = \frac{d(y)}{\sum_{z \in \Omega} d(z)}$$

and ϕ_0 also denotes the top left eigenvector of $\mathbf{P}$.

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The Mapping Ψ

- Low-dimensional embedding (or diffusion map or DM) $\Psi : \Re^N \mapsto \Re^m$ of a feature vector $\mathbf{f}$ is given by:

$$\Psi(\mathbf{f}) = [\lambda_1\psi_1(\mathbf{f}), \lambda_2\psi_2(\mathbf{f}), \ldots, \lambda_m\psi_m(\mathbf{f})]^T$$

  where $m << N$ and λ_i, ψ_i for $, i = 1, 2, \ldots, m$ respectively denote the eigenvalues and eigenvectors of the Markov matrix $\mathbf{P}$.

- The mapping Ψ^t at time step t is computed as follows:

$$\Psi^t(\mathbf{f}) = [\lambda_1^t\psi_1(\mathbf{f}), \lambda_2^t\psi_2(\mathbf{f}), \ldots, \lambda_m^t\psi_m(\mathbf{f})]^T$$

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Properties of the DMs

- The diffusion distance as defined previously can also be written as follows:

$$D^t(\mathbf{f}_i, \mathbf{f}_j) = ||\Psi^t(\mathbf{f}_i) - \Psi^t(\mathbf{f}_j)||^2$$

- Diffuison Map: Diffusion distance $\mapsto$ Euclidean distance

- Spectral fall-off and time t of the random walk are the main factors contributing to dimensionality reduction.

- For large value of t, we can capture large-scale structures in the data with fewer coordinates.

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Case Study 1:
Clustering of Shapes

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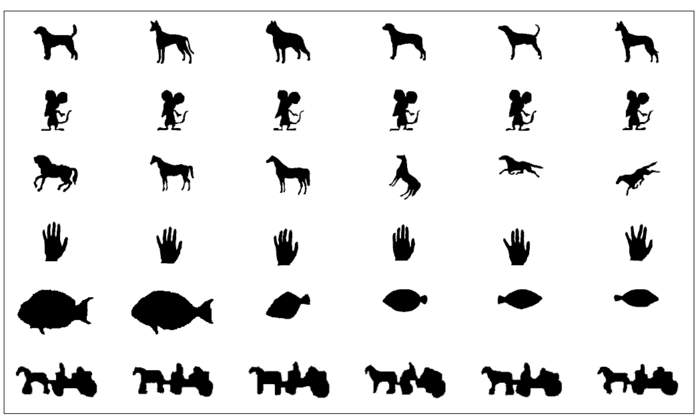
Kimia's Shape Dataset



6 classes, variable number of samples, a total of 157 samples.

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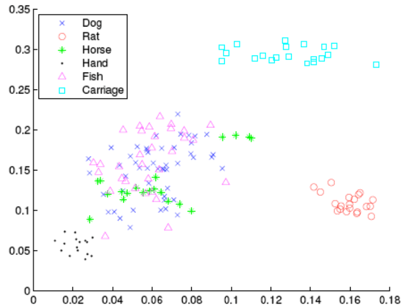
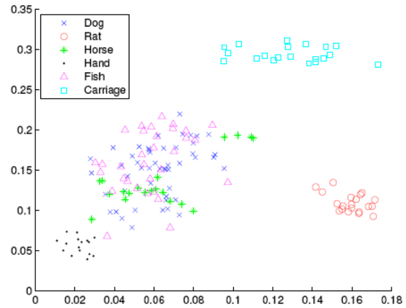
Raw Features





$\sigma = 0$ $\sigma = 10$

Two-dimensional feature space using top two (1st and 2nd) Fourier descriptors

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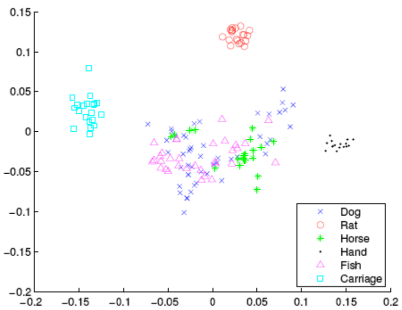
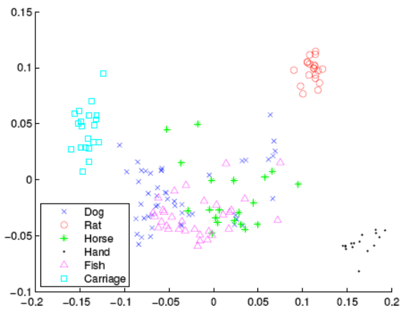
PCA Embedding





$\sigma = 0$ $\sigma = 10$

Scatter plots of top two PCA coordinates

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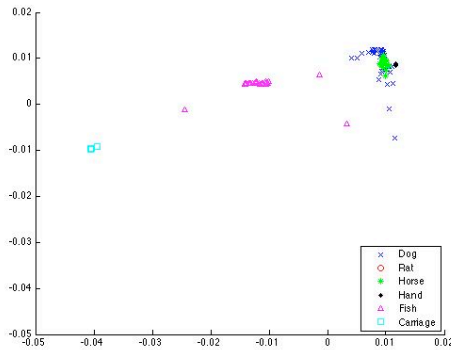
Laplacian Eigenmap



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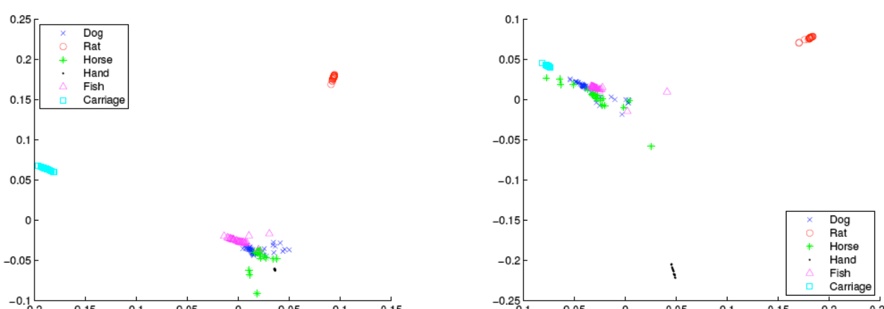
Diffusion Map



$\sigma = 0$ $\sigma = 10$

Scatter plots of top two diffusion coordinates

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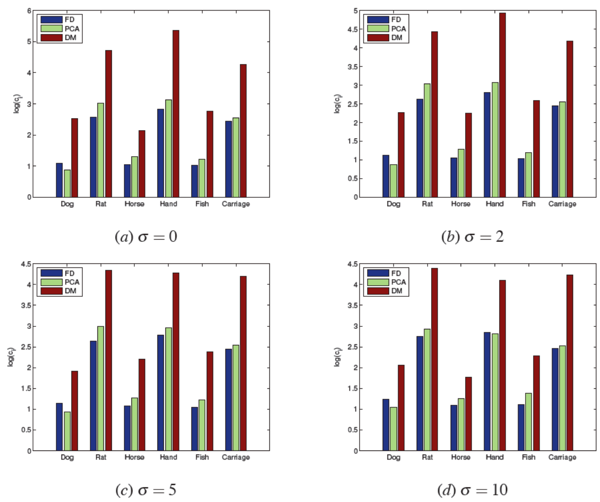
Class Separability Index (CSI)



$$c_i = \frac{\bar{d}_i}{\sqrt{\bar{\sigma_i^2}}}$$

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Clustering Validity Index (CVI)

- Commonly used to measure the performance of clustering algorithms and validate their outcome
- Some of the popular CVIs:
  - Dunn (Dunn, 1973)
  - DB (Davies & Bouldin, 1979)
  - DB* (Kim & Ramakrishna, 2005)

$$DB^*(nc) = \frac{1}{nc}\sum_{i=1}^{nc}\left(\frac{\max_{k=1,\ldots,k\neq i}\{S_i + S_k\}}{\min x_{l=1,\ldots,l\neq i}\{d_{i,l}\}}\right)$$

where $S_i = \frac{1}{n_i}\sum_{x\in c_i} d(x,c_i)$ and $d_{i,j} = d(c_i,c_j)$

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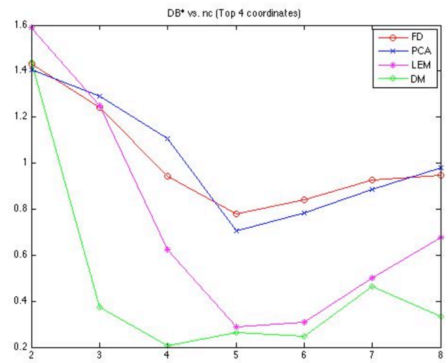
*DB** vs. *nc* (Top 4 Coordinates)



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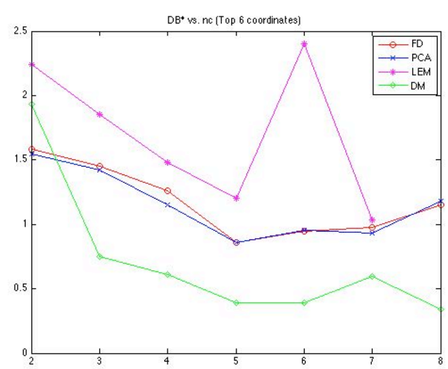
*DB** vs. *nc* (Top 6 Coordinates)



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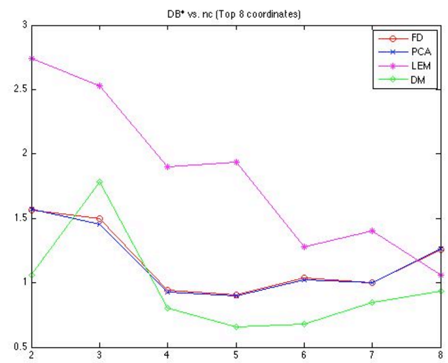
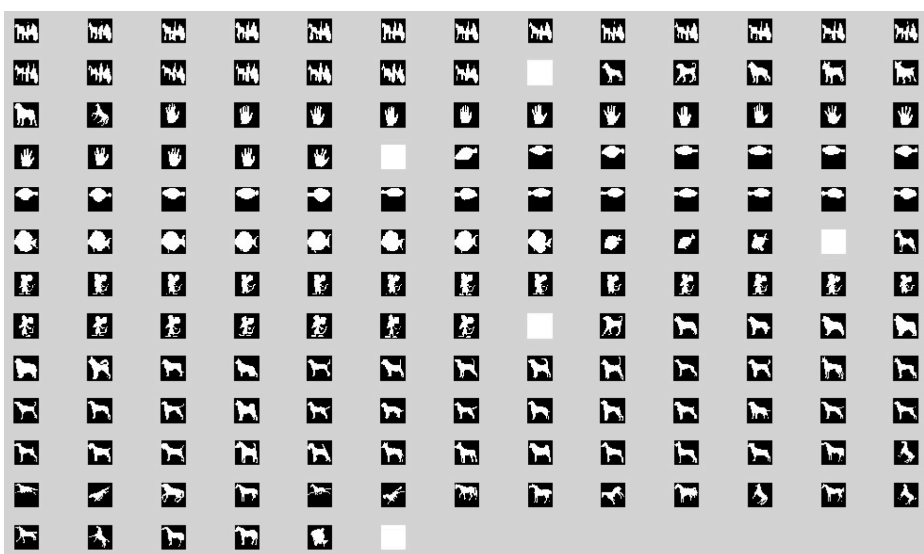
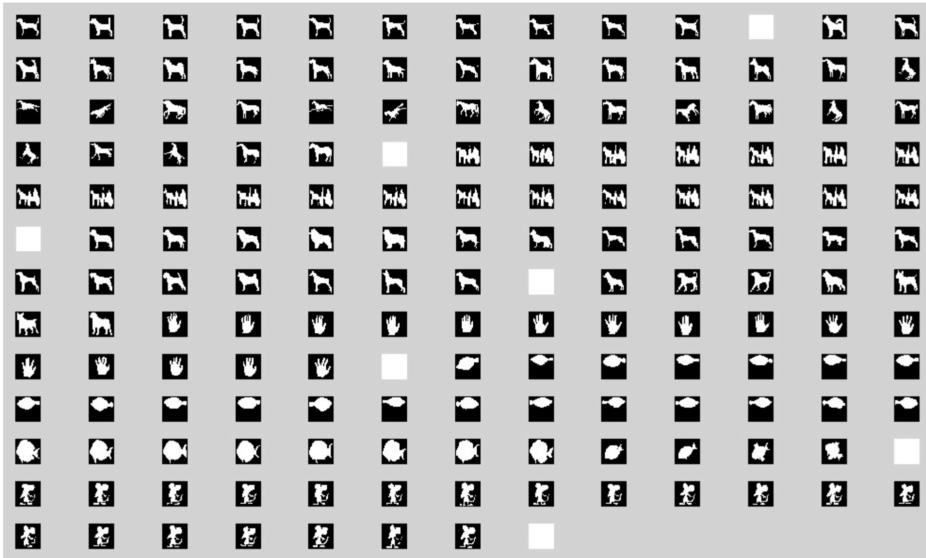
*DB** vs. *nc* (Top 8 Coordinates)





Results of unsupervised FCM clustering using top 8 PCA coordinates



Results of unsupervised FCM clustering using top 6 LEM coordinates

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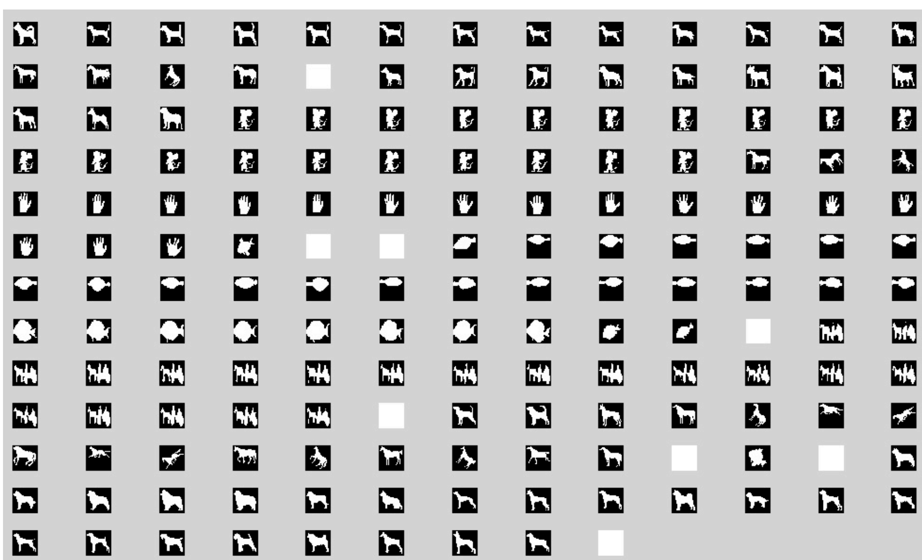

Results of unsupervised FCM clustering using top 8 LEM coordinates

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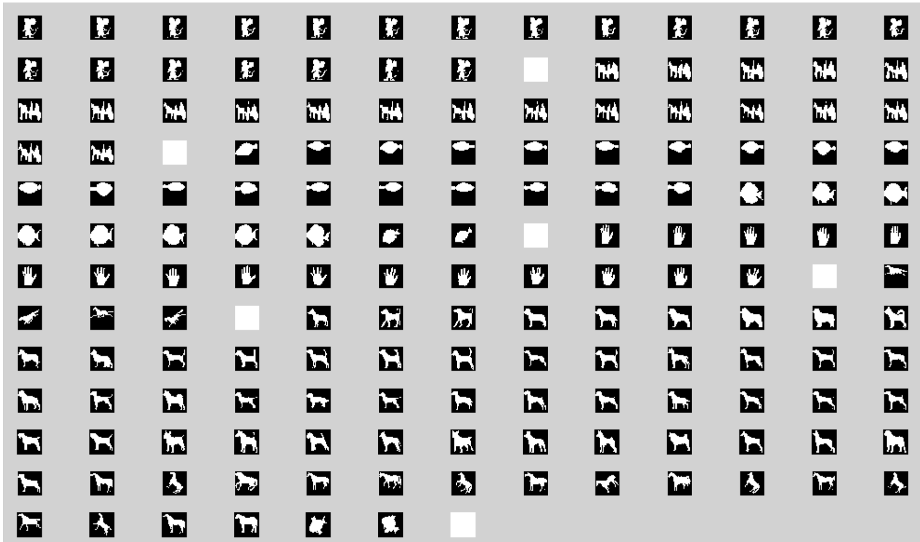

Results of unsupervised FCM clustering using top 7 DM coordinates; 88.54% accuracy

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Case Study 2: Detection of Nuclei

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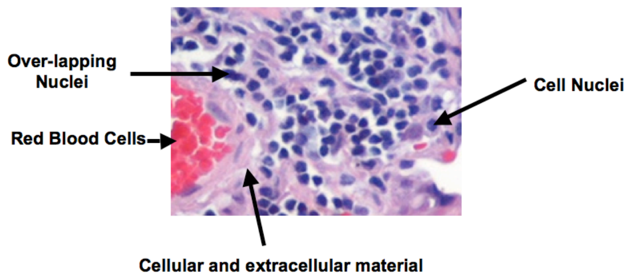
Problem Definition



"Detecting nuclei in a histology image by posing it as a problem of classification of closed objects using unsupervised shape manifold learning"

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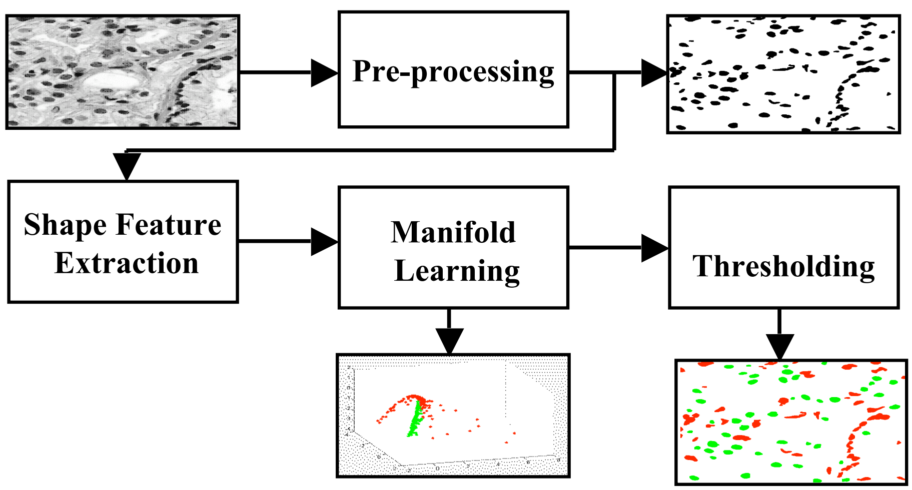
The Proposed Algorithm



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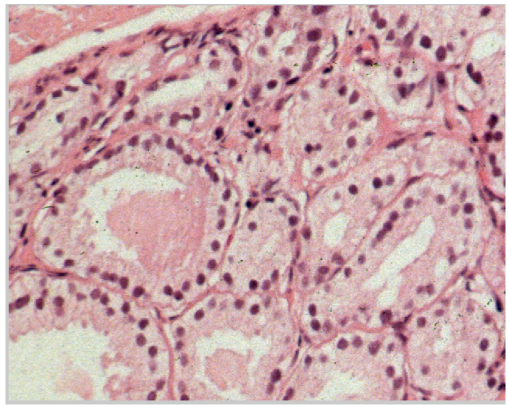
Pre-processing



H&E stained colour image of prostate tissue

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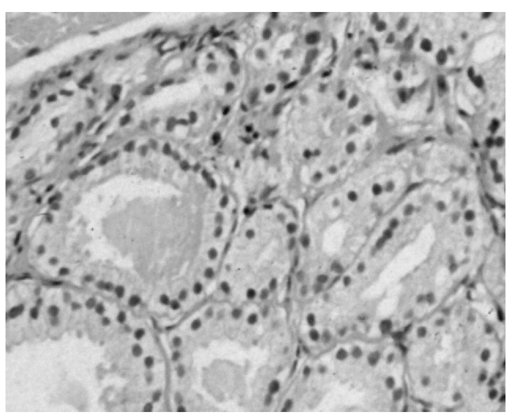
Pre-processing



Result of greyscale conversion and smoothing by bilateral filtering

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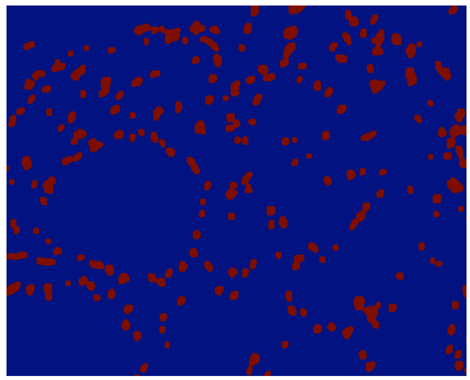
Preprocessing



Result of k-means clustering and morphological operations

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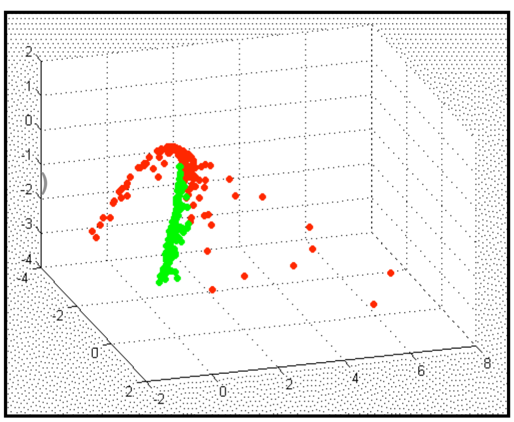
Towards the Nuclei Detection



Diffusion maps in 3D

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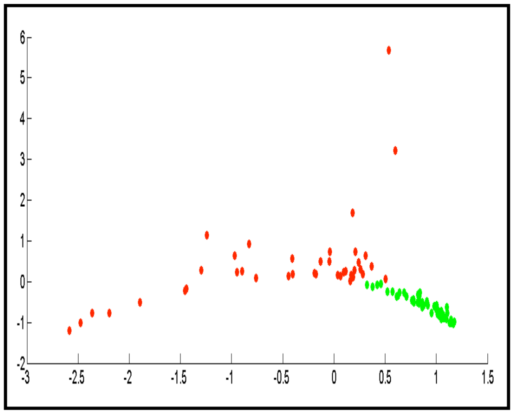
Towards the Nuclei Detection



Diffusion maps in 2D

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Experimental Results

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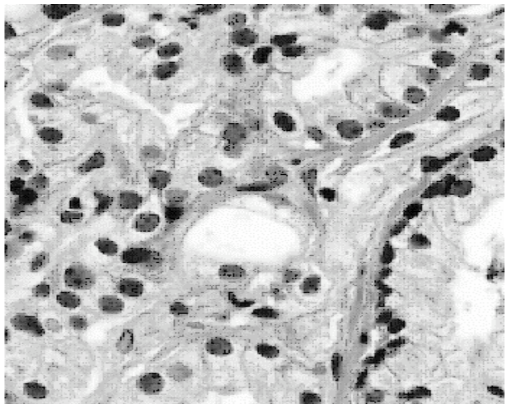
Experimental Results



A typical prostate tissue specimen

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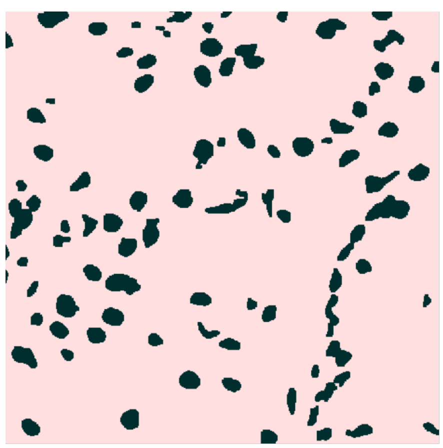
Experimental Results



Binary image

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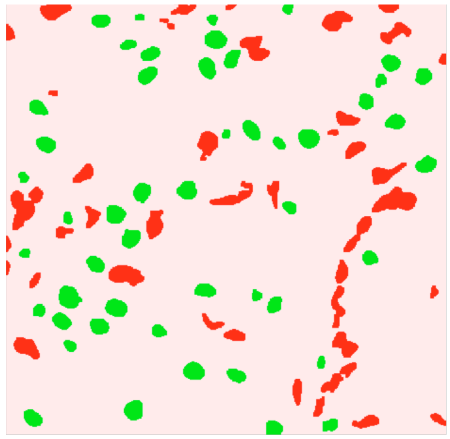
Experimental Results



Nuclei detected (shown in green) by our detection algorithm

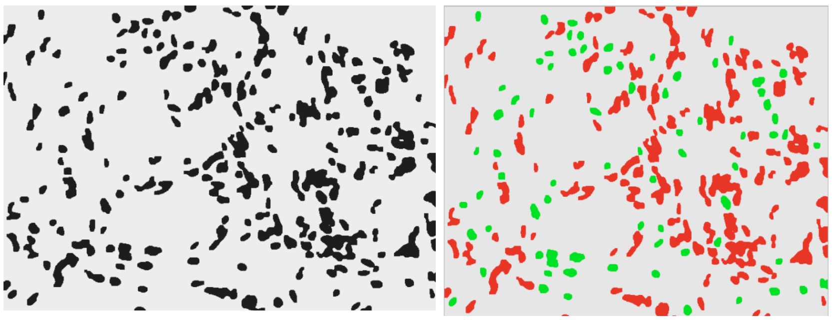
Out-of-Sample Extention

Nyström's Formula:

$$x_i = [\Psi(\mathbf{f})]_i = \frac{1}{\lambda_i} \sum_{j=1}^{m} \psi_{ij}\, p(\mathbf{f}_i, \mathbf{f})$$

where x_r is *rth* Nystrom sample estimator and ψ_{ij} is j*th* coordinate of i*th* eigenvector.

Experimental Results



Detection of potential nuclei using the out-of-sample extension

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Conclusions

- Presented a framework for unsupervised learning of shape manifolds
- Diffusion maps were used to:
  - Preserve the local diffusion distance (a geodesic) on shape manifolds
  - Learn the global structure of the manifolds
- Results for unsupervised shape clustering (and detection of nuclei) are quite encouraging
- Currently limited to:
  - Connected closed curves in 2D
  - Computation of similarity matrix is expensive

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Learning the Shape Manifolds using Diffusion Maps

a. *Arif & Rajpoot*, "Classification of Potential Nuclei in Prostate Histology Images using Shape Manifold Learning", ***ICMV'2007***
b. Rajpoot, Arif & Bhalerao, "Unsupervised Learning of Shape Manifolds", ***BMVC'2007***
c. *Arif & Rajpoot*, Detection of Nuclei by Unsupervised Manifold Learning, ***MIUA'2007***

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