Diffusion Maps for Changing Data

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How to compare images across sensors?

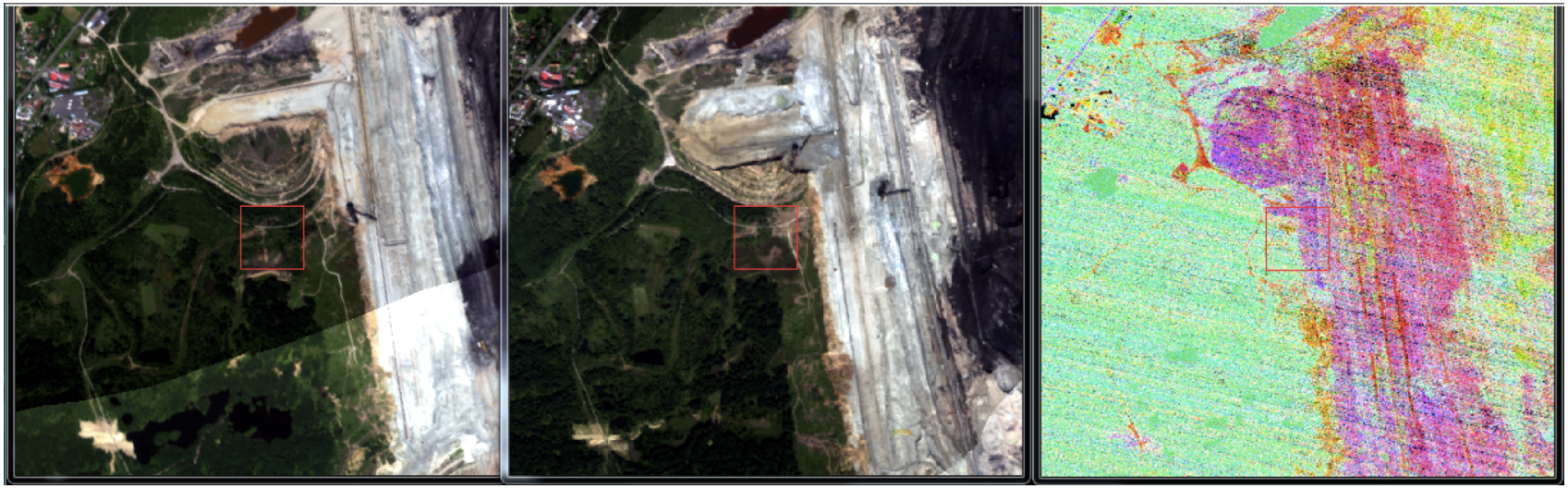

Figure: Sokolov Mine in 2009 and 2010 (during the day, visible range, HyMap sensor), as well as 2011 (at night, thermal range, AHS sensor)

Overview

1. High Dimensional Data, Low Dimensional Embeddings
   - Some Examples
   - Diffusion Maps
2. Diffusion Maps and Changing Graphs
   - Motivation
   - Generalizing the Diffusion Distance
3. Applications
   - Change Detection
   - Parameterized Difference Equations
4. Empirical Approximation

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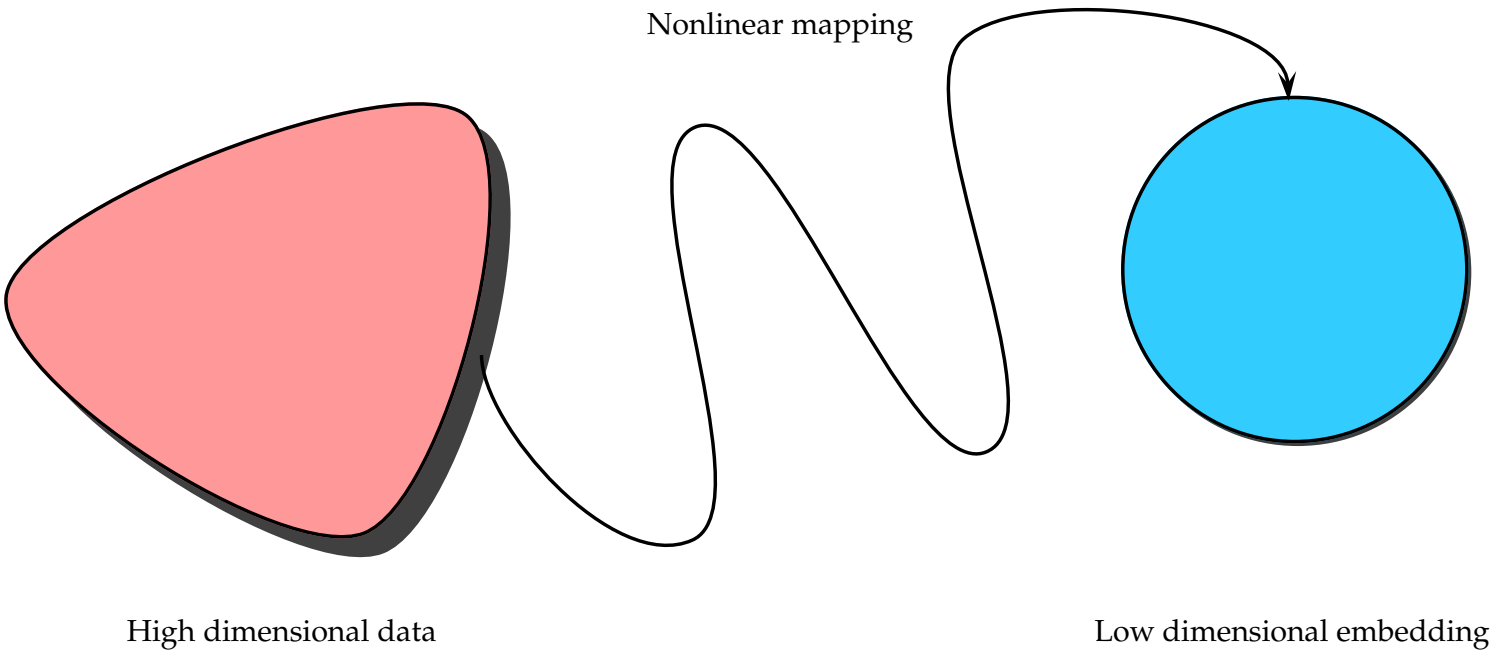
4 Empirical Approximation

Cartoon


Nonlinear mapping
High dimensional data
Low dimensional embedding

Simple Example

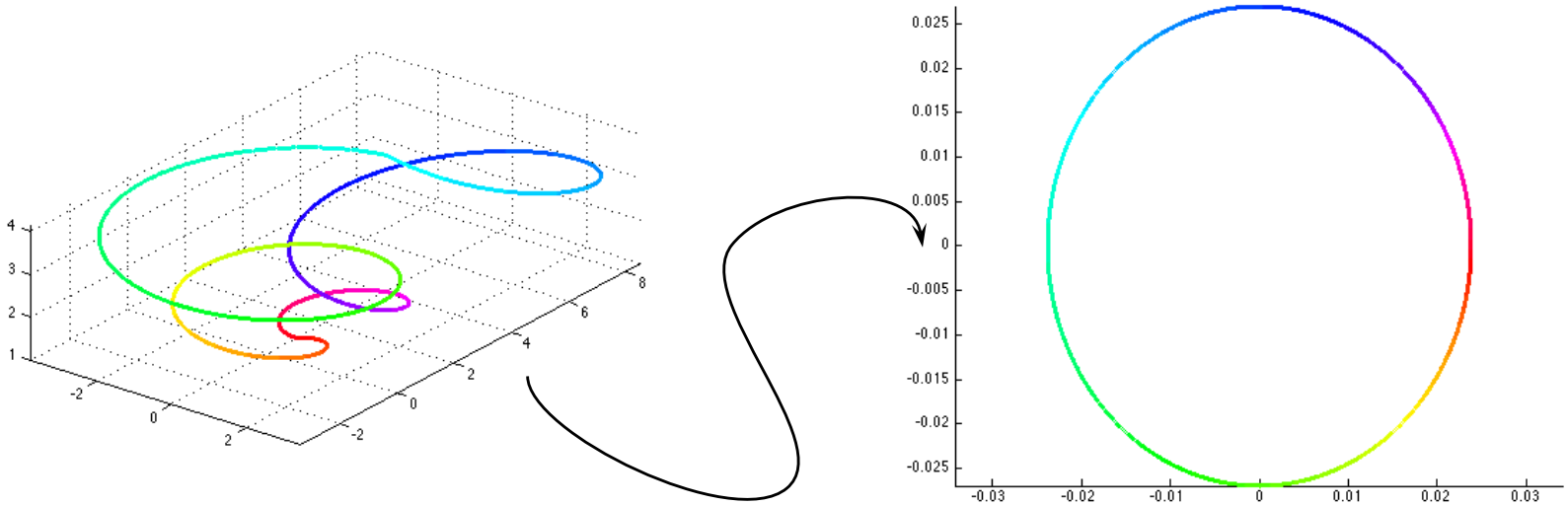
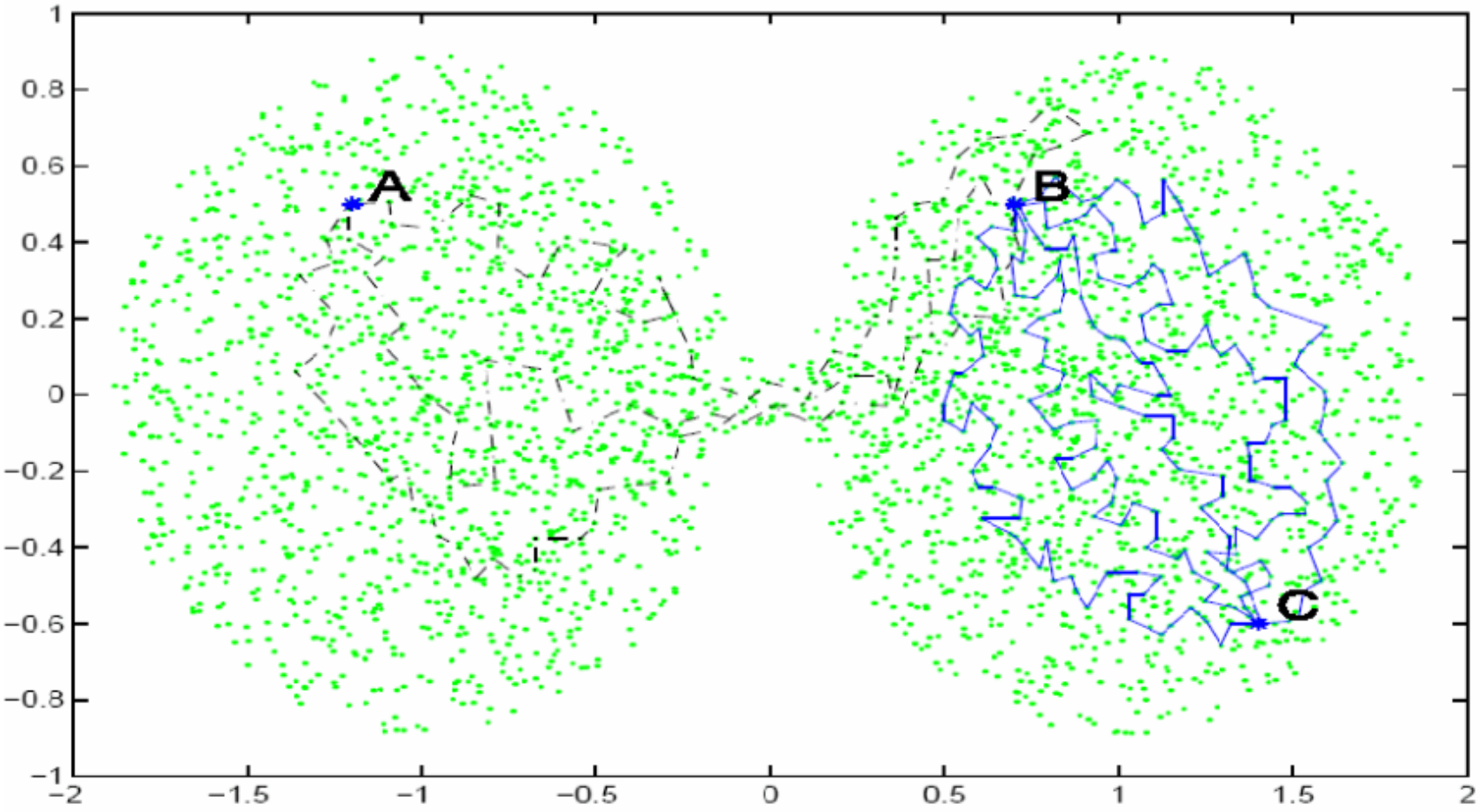


Figure: Left: A closed, non-self-intersecting curve in 3 dimensions. Right: Its embedding as a circle.

Euclidean vs Geodesic vs Diffusion



Created by Stéphane Lafon

Setup

- Let (X, μ) be a measure space.
  - The set X is our data set.
  - The measure μ represents the distribution of the points on X.
- Let $k : X \times X \to \mathbb{R}$ be a symmetric, positive kernel.
  - The value $k(x, y)$ measures the similarity between two points $x, y \in X$.
  - The kernel k should measure local similarities. For example,

$$k(x, y) = e^{-\|x-y\|^2/\varepsilon}.$$

- Let $G \triangleq (X, k)$ denote a weighted graph with:
  - Vertices given by our data set X.
  - Weighted edges with the weights given by k.

Facebook Graph

Created by Paul Butler
http://www.facebook.com/note.php?note_id=469716398919

Random Walk on G

- Define the density $d : X \to \mathbb{R}$ as

$$d(x) \triangleq \int_X k(x,y)\, d\mu(y).$$

- Define a new kernel $p : X \times X \to \mathbb{R}$ as:

$$p(x,y) \triangleq \frac{k(x,y)}{d(x)}.$$

- p is the transition kernel of a random walk on G. In particular, $p(x,y)$ is the probability of transition from x to y in one time step.

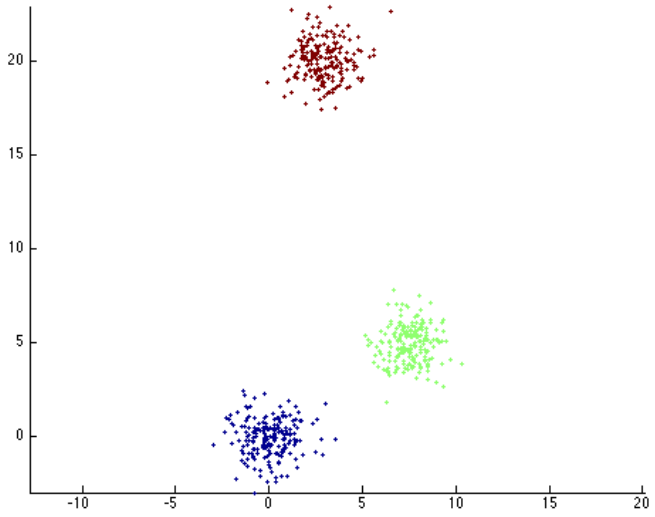
Diffusion Operator

- Define the diffusion operator $P : L^2(X, \mu) \to L^2(X, \mu)$ as:

$$(Pf)(x) \triangleq \int_X p(x, y) \cdot f(y)\, d\mu(y).$$

- Powers P^t, for t a positive integer, are equivalent to running the random walk forward in time t steps. Doing so reveals the relevant geometric structure of X at different scales.

Multiscale Analysis of Gaussian Clouds using P



(a) 3 Gaussian clouds

(b) Powers of P

Symmetrize the Random Walk

- One can also use a symmetric version of the random walk, which will simplify things later.
- Let $a : X \times X \to \mathbb{R}$ be the symmetric version of p, where

$$a(x,y) \triangleq d(x)^{\frac{1}{2}} \cdot p(x,y) \cdot d(y)^{-\frac{1}{2}}.$$

- Define the symmetric diffusion operator $A : L^2(X,\mu) \to L^2(X,\mu)$ as

$$(Af)(x) \triangleq \int_X a(x,y) \cdot f(y)\, d\mu(y).$$

- Let $a^{(t)} : X \times X \to \mathbb{R}$ be the kernel of the operator A^t, so that

$$(A^t f)(x) = \int_X a^{(t)}(x,y) \cdot f(y)\, d\mu(y).$$

Diffusion Distance

Definition

For each positive integer t, let $D^{(t)} : X \times X \to \mathbb{R}$ denote the **diffusion distance** at time t, where

$$D^{(t)}(x,y)^2 \triangleq \int_X \left(a^{(t)}(x,s) - a^{(t)}(y,s)\right)^2 d\mu(s).$$

Comparing Diffusions

Spectral Decomposition of A

- Under some mild assumptions on G and A, the operator A will have a discrete sequence of orthonormal eigenfunctions $\{\psi^{(\ell)}\}_{\ell \geq 1}$ with corresponding eigenvalues $\{\lambda^{(\ell)}\}_{\ell \geq 1}$, that satisfy:
  - $(A\psi^{(\ell)})(x) = \lambda^{(\ell)} \cdot \psi^{(\ell)}(x)$.
  - $\langle \psi^{(\ell)}, \psi^{(m)} \rangle_{L^2(X,\mu)} = \delta(\ell - m)$.
  - $1 = \lambda^{(1)} > \lambda^{(2)} \geq \lambda^{(3)} \geq \ldots \geq 0$.
  - $\lim_{\ell \to \infty} \lambda^{(\ell)} = 0$.
  - $\psi^{(1)}(x) = \sqrt{d(x)}$.

Diffusion Map

Definition

- We use the spectral decomposition of A to define the **diffusion map** $\Psi^{(t)} : X \to \ell^2$ as:

$$\Psi^{(t)}(x) \triangleq \left(\left(\lambda^{(\ell)} \right)^t \cdot \psi^{(\ell)}(x) \right)_{\ell \geq 1} .$$

- For any positive integer d, one can also define an **approximate diffusion map** $\Psi^{(t,d)} : X \to \mathbb{R}^d$ as:

$$\Psi^{(t,d)}(x) \triangleq \left(\left(\lambda^{(\ell)} \right)^t \cdot \psi^{(\ell)}(x) \right)_{\ell=1}^{d} .$$

Diffusion Map and the Diffusion Distance

Theorem (Coifman and Lafon)

- The diffusion distance on X is equivalent to the ℓ^2 distance on $\Psi^{(t)}(X)$, i.e.,

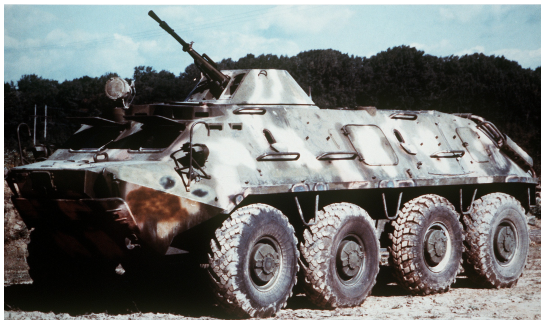
$$D^{(t)}(x,y) \triangleq \left\| a^{(t)}(x,\cdot) - a^{(t)}(y,\cdot) \right\|_{L^2(X,\mu)} = \left\| \Psi^{(t)}(x) - \Psi^{(t)}(y) \right\|_{\ell^2}.$$

- Furthermore, for any $\delta > 0$, there exists a positive integer d such that

$$D^{(t)}(x,y) \approx \left\| \Psi^{(t,d)}(x) - \Psi^{(t,d)}(y) \right\|_{\mathbb{R}^d},$$

to within accuracy δ.

Another Circle



(a) BTR-60

(b) BTR driving in a circle

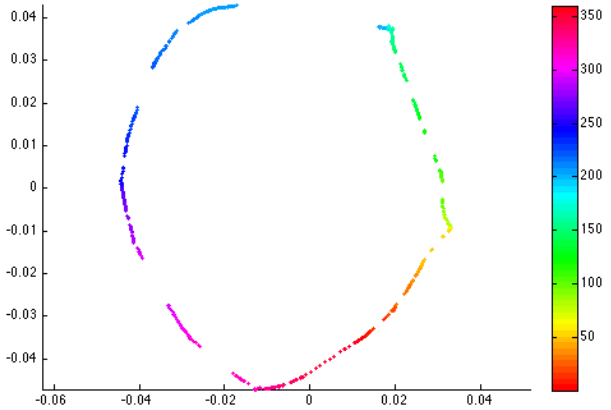


Figure: Embedding of the BTR video. The color corresponds to the angle on the circle at which the BTR is located.

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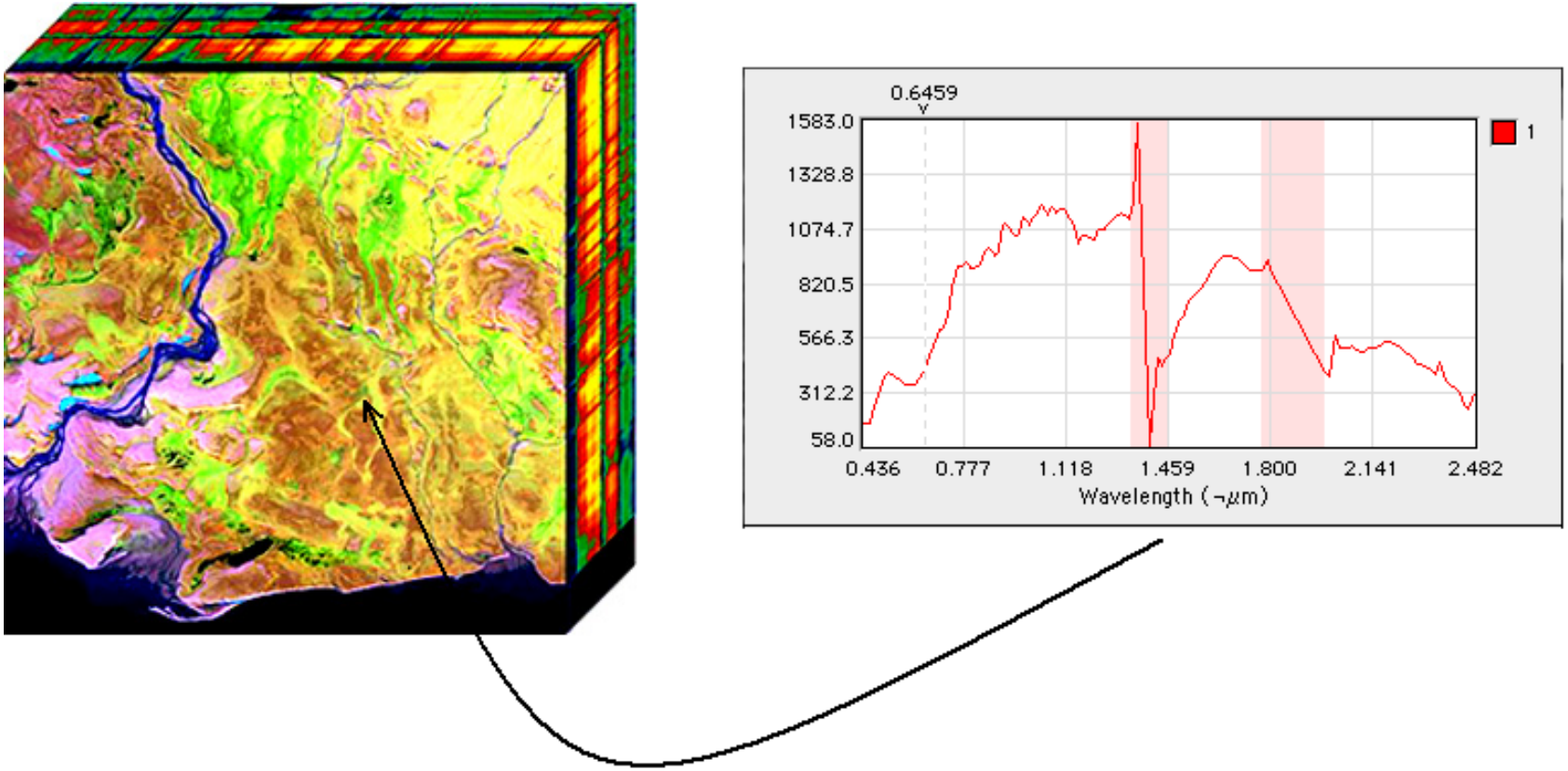
Hyperspectral Imagery



Change Detection

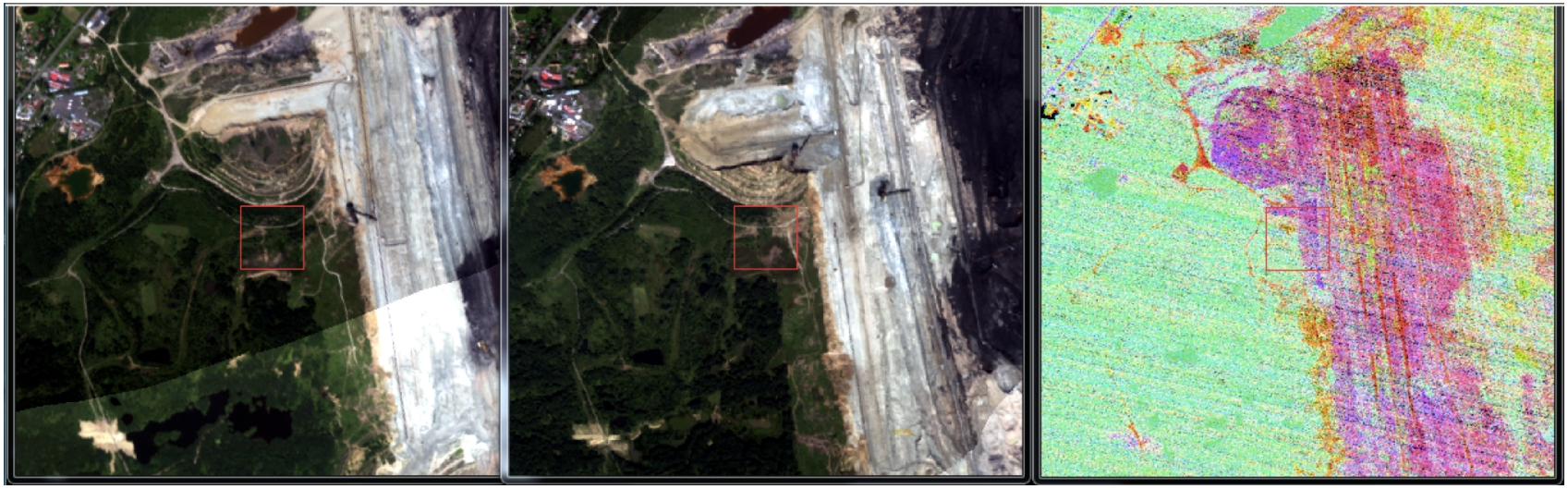
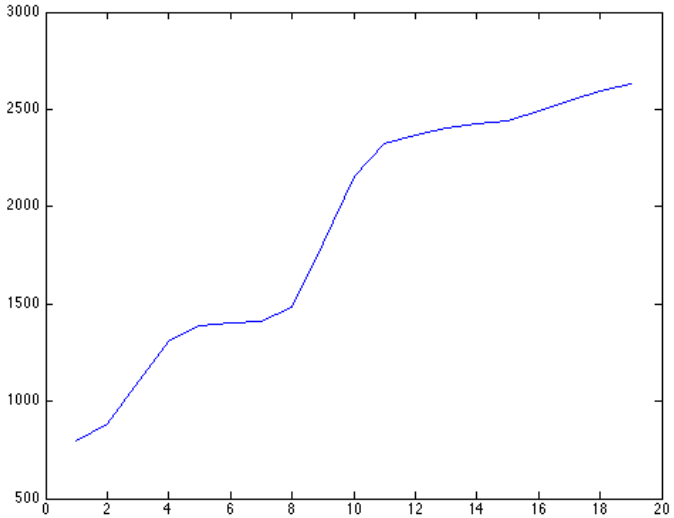
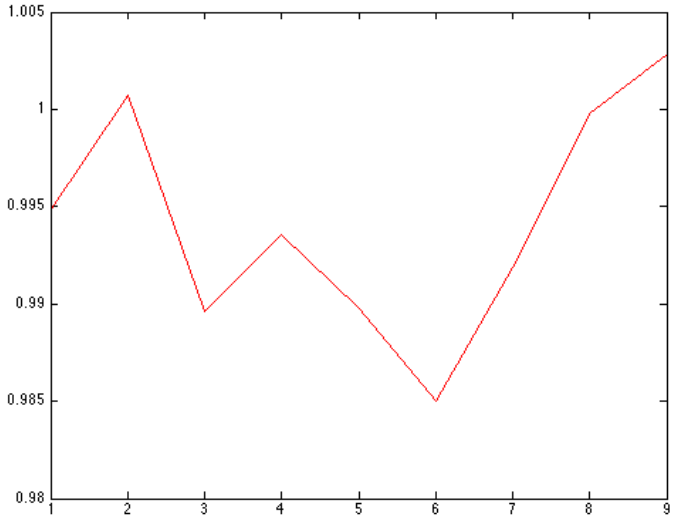


Figure: Sokolov Mine in 2009 and 2010 (during the day, visible range, HyMap sensor), as well as 2011 (at night, thermal range, AHS sensor)

Sample Spectra

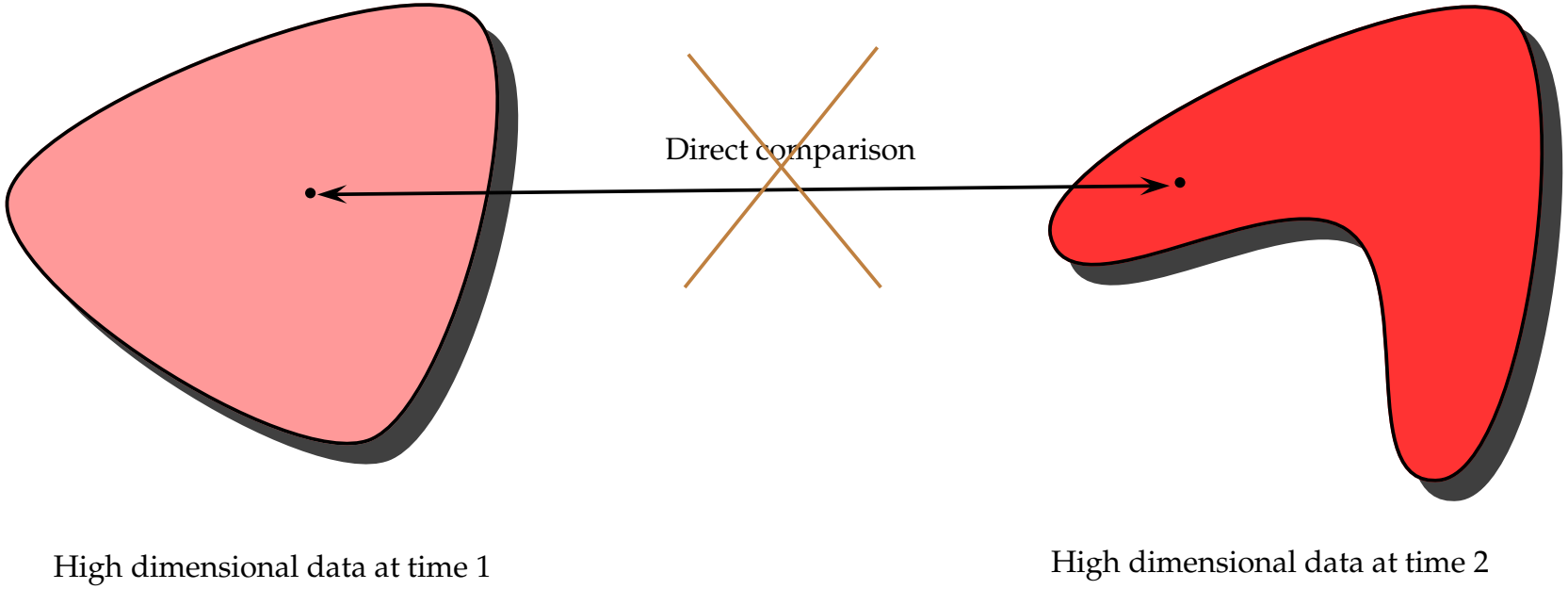


(a) Spectral signature of a pixel, 2009, during the day, visible range

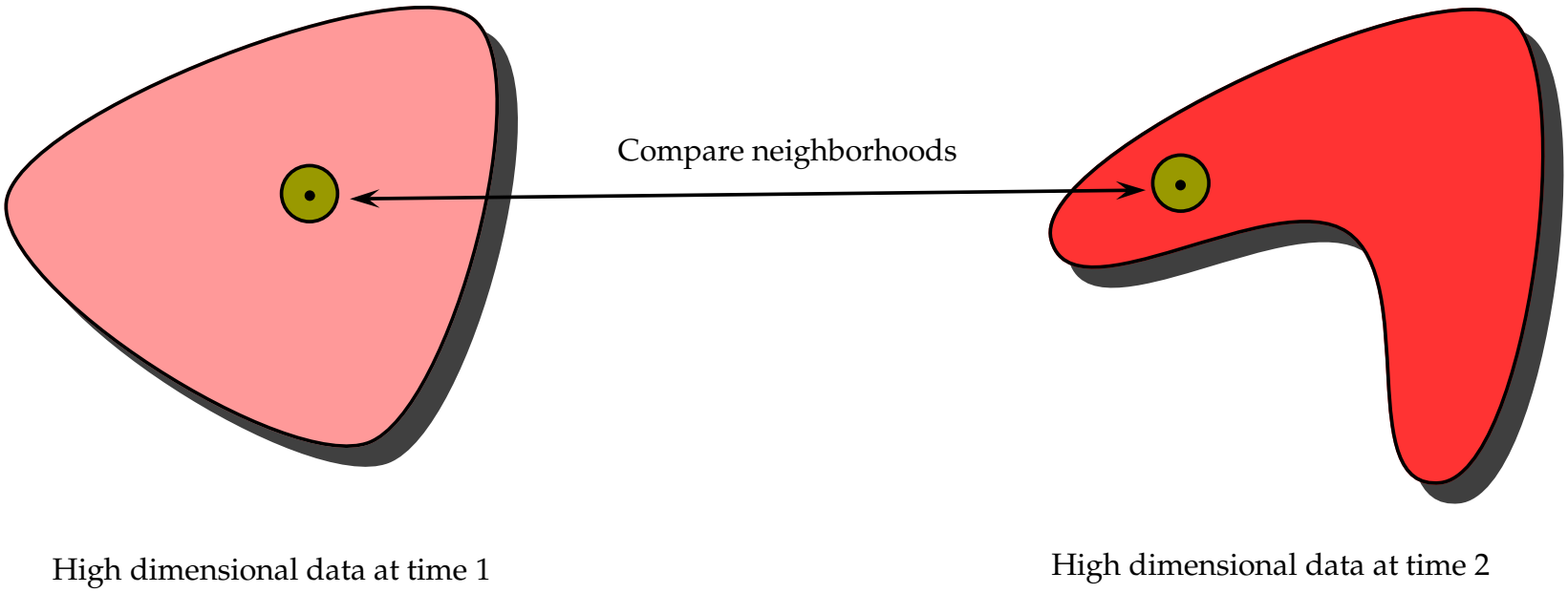


(b) Spectral signature of the same pixel, 2011, at night, thermal range

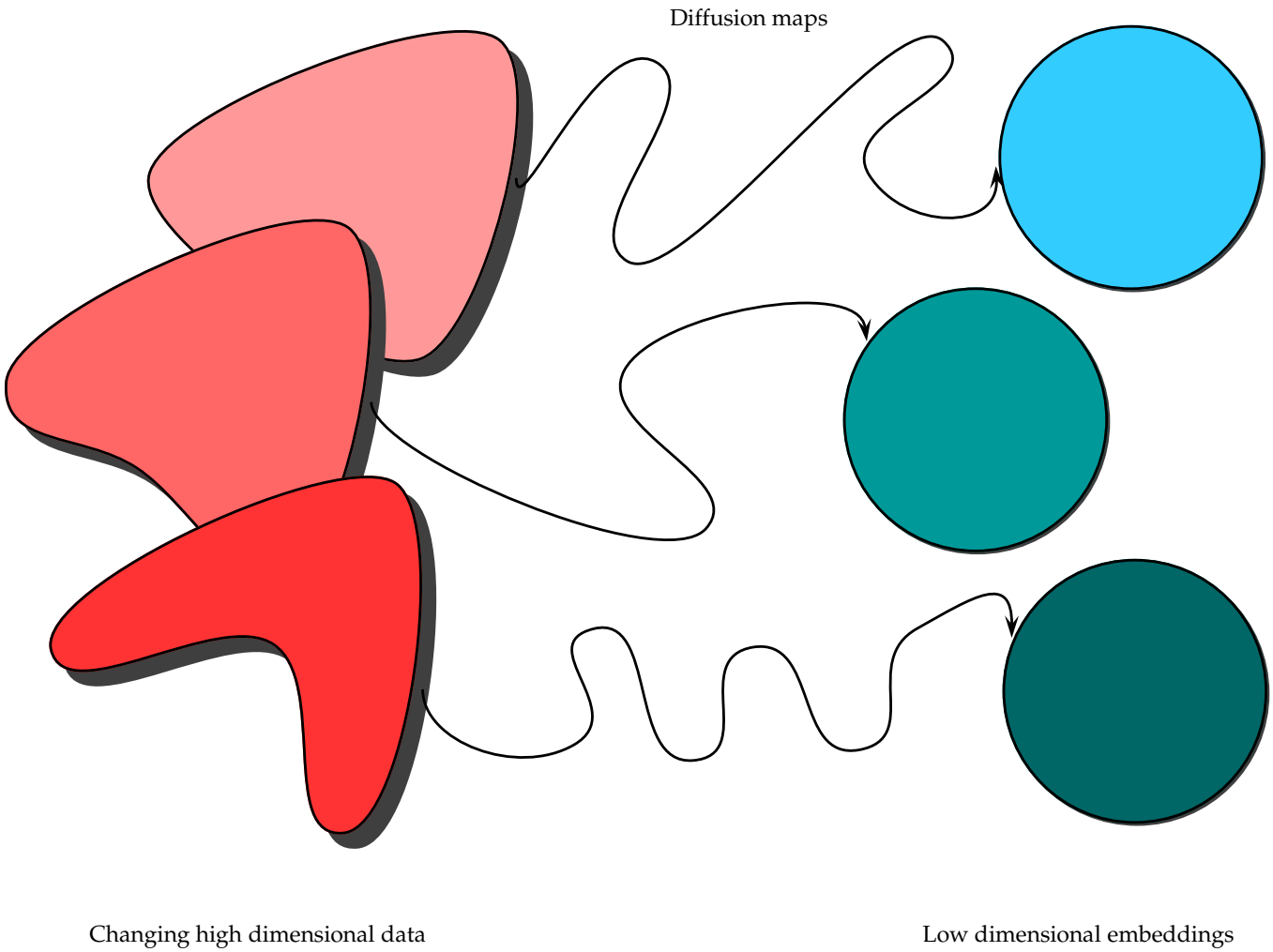
Compare Neighborhoods



Compare Neighborhoods



Multiple Low Dimensional Embeddings



Changing Data Model

- Once again let (X, μ) be the data set.
- Let $\mathcal{I}$ denote the set of parameters (or times) for which we view/measure/observe (X, μ).
- Encode the changes in (X, μ) across $\mathcal{I}$ in a family of kernels $\{k_\alpha : X \times X \to \mathbb{R} \mid \alpha \in \mathcal{I}\}$.
- Let $G_\alpha \triangleq (X, k_\alpha)$ denote the corresponding weighted graph for each $\alpha \in \mathcal{I}$.

Symmetric Diffusion Operators, Revisited

- For each $\alpha \in \mathcal{I}$, we have the symmetric transition kernels $a_\alpha^{(t)} : X \times X \to \mathbb{R}$ for the random walk on G_α, along with their corresponding symmetric diffusion operators:

$$(A_\alpha^t f)(x) = \int_X a_\alpha^{(t)}(x,y) \cdot f(y)\, d\mu(y).$$

- Let $\{\psi_\alpha^{(\ell)}\}_{\ell \geq 1}$ be the eigenfunctions of A_α with corresponding eigenvalues $\{\lambda_\alpha^{(\ell)}\}_{\ell \geq 1}$.

Generalized Diffusion Distance

- Set $x_\alpha \triangleq (x, \alpha) \in X \times \mathcal{I}$.

Definition

For each positive integer t, let $D^{(t)} : (X \times \mathcal{I}) \times (X \times \mathcal{I}) \to \mathbb{R}$ denote the **diffusion distance** at time t, where

$$D^{(t)}(x_\alpha, y_\beta)^2 \triangleq \int_X \left(a_\alpha^{(t)}(x, s) - a_\beta^{(t)}(y, s) \right)^2 d\mu(s).$$

Diffusion Maps, Revisited

- For each $\alpha \in \mathcal{I}$ we have the diffusion map $\Psi_\alpha^{(t)} : X \to \ell^2$, which gives
$$D^{(t)}(x_\alpha, y_\alpha) = \left\| \Psi_\alpha^{(t)}(x) - \Psi_\alpha^{(t)}(y) \right\|_{\ell^2}.$$
- On the other hand, if $\alpha, \beta \in \mathcal{I}$ and $\alpha \neq \beta$, then
$$D^{(t)}(x_\alpha, y_\beta) \neq \left\| \Psi_\alpha^{(t)}(x) - \Psi_\beta^{(t)}(y) \right\|_{\ell^2}.$$
- In particular, the ℓ^2 space $\Psi_\alpha^{(t)}(X)$ is different than the ℓ^2 space $\Psi_\beta^{(t)}(X)$.

Mapping $\Psi_\alpha^{(t)}(X)$ into $\Psi_\beta^{(t)}(X)$

- Let $u = (u_\ell)_{\ell \geq 1} \in \ell^2$.
- For each $\alpha, \beta \in \mathcal{I}$, define the map $O_{\alpha \to \beta} : \ell^2 \to \ell^2$ as:

$$O_{\alpha \to \beta}(u) \triangleq \left(\sum_{m \geq 1} u_m \cdot \langle \psi_\alpha^{(m)}, \psi_\beta^{(\ell)} \rangle_{L^2(X,\mu)} \right)_{\ell \geq 1}.$$

- The map $O_{\alpha \to \beta}$ has the effect of mapping $\Psi_\alpha^{(t)}(X)$ into $\Psi_\beta^{(t)}(X)$.

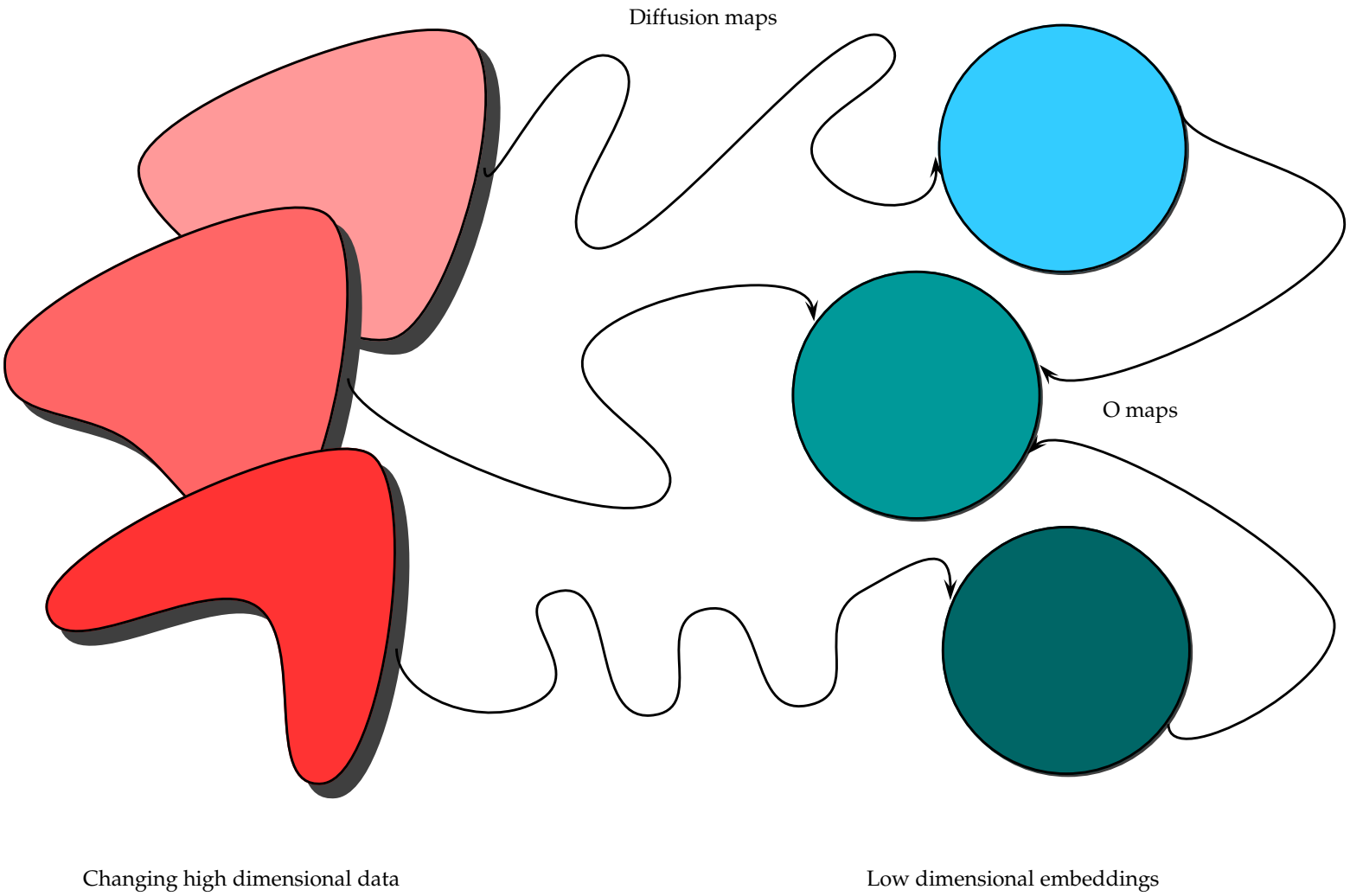
Composing the Two Maps

Theorem (Coifman and H.)

Fix $\gamma \in \mathcal{I}$. Then, for any positive integer t and $x_\alpha, y_\beta \in X \times \mathcal{I}$,

$$\begin{aligned} D^{(t)}(x_\alpha, y_\beta) &\triangleq \left\| a_\alpha^{(t)}(x,\cdot) - a_\beta^{(t)}(y,\cdot) \right\|_{L^2(X,\mu)} \\ &= \left\| O_{\alpha\to\gamma}\Psi_\alpha^{(t)}(x) - O_{\beta\to\gamma}\Psi_\beta^{(t)}(y) \right\|_{\ell^2}. \end{aligned}$$

Final Cartoon



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Sokolov Mine

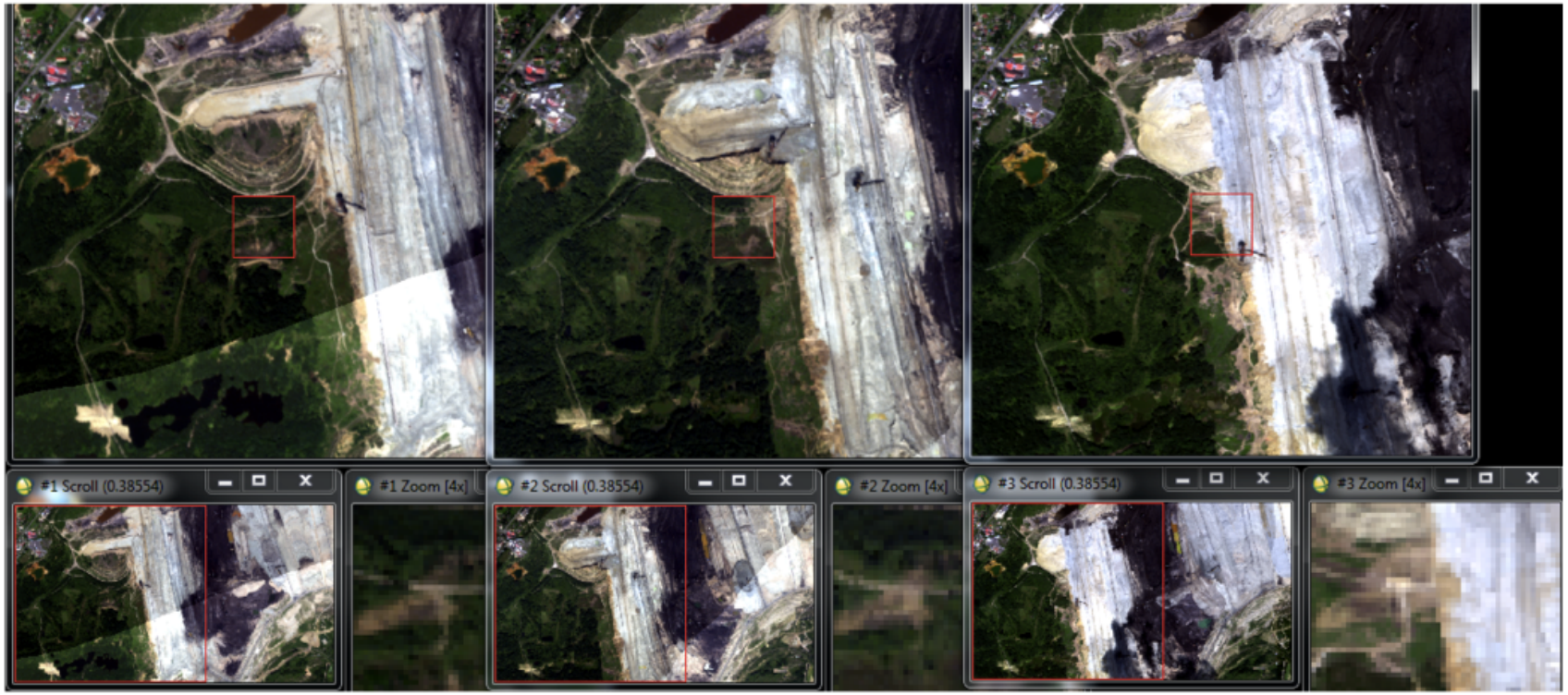
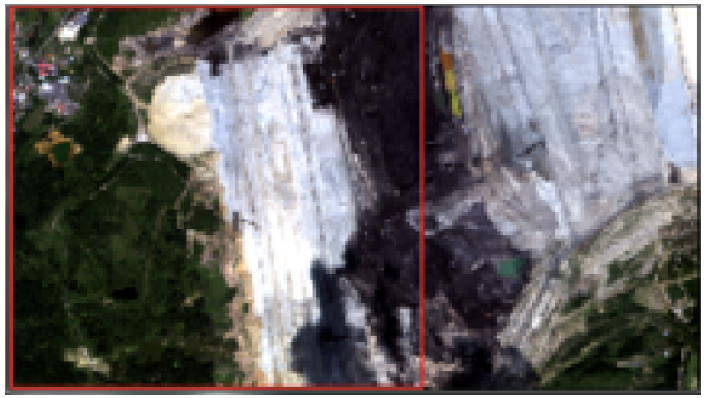


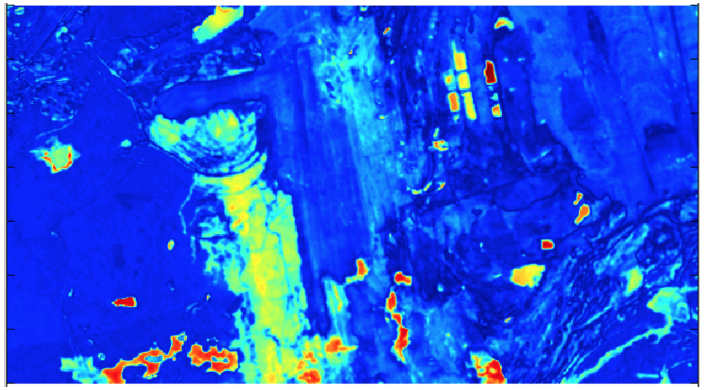
Figure: Sokolov Mine in 2009 and 2010 (during the day, visible range, HyMap sensor), as well as 2011 (during the day, visible range, AHS sensor)

Change Detection using Diffusion Maps

(a) Sokolov Mine 2009 / Day / Visible / HyMap sensor

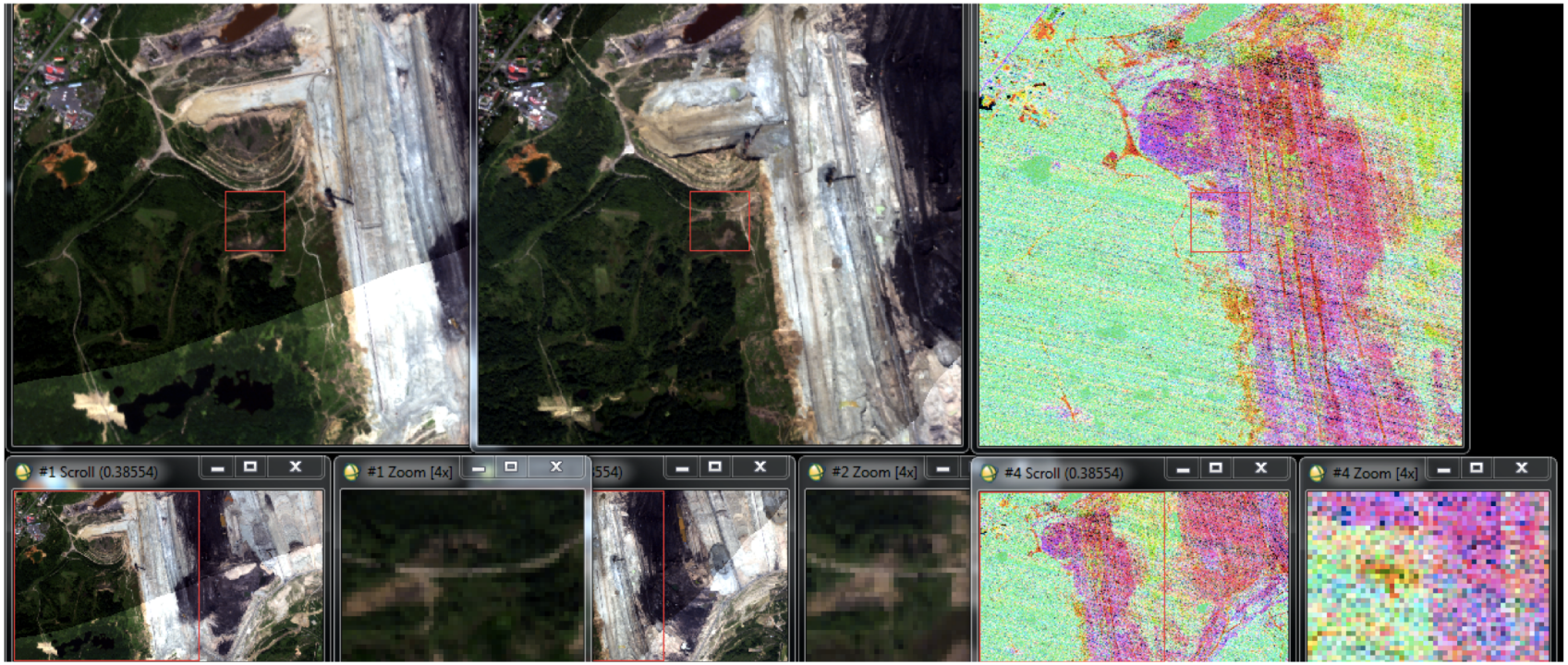


(b) Sokolov Mine 2011 / Day / Visible / AHS sensor



(c) Change Map using Diffusion Maps

Sokolov Mine



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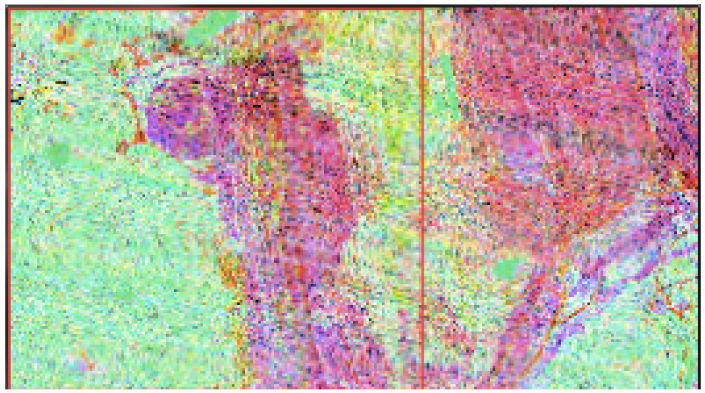
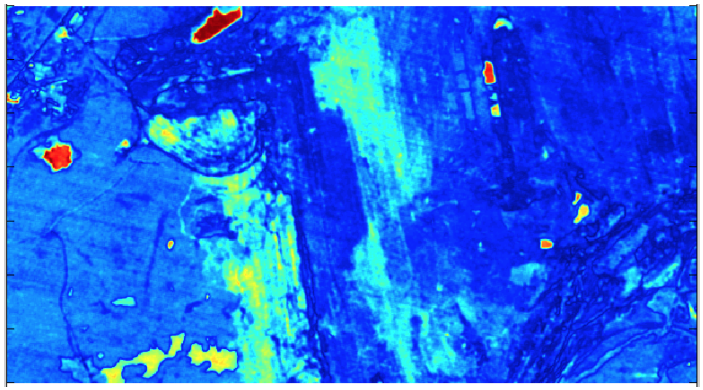
Change Detection using Diffusion Maps

(a) Sokolov Mine 2009 / Day / Visible / HyMap sensor

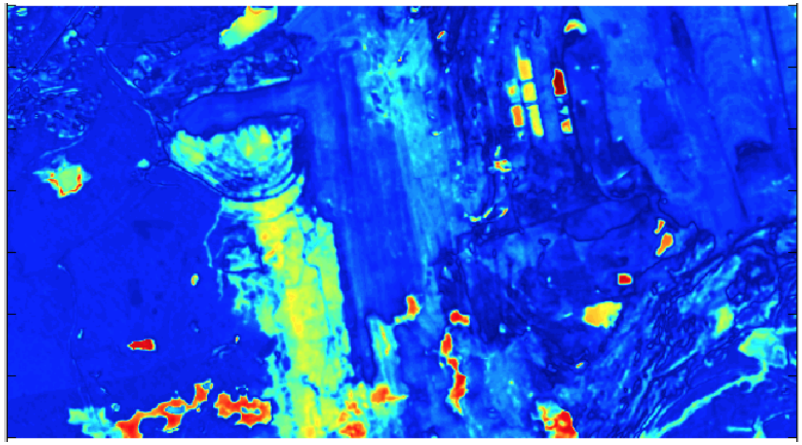


(b) Sokolov Mine 2011 / Night / Thermal / AHS sensor

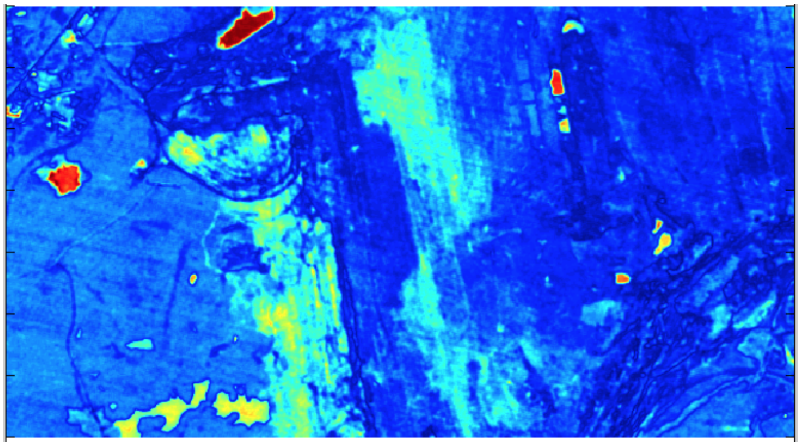


(c) Change Map using Diffusion Maps

Comparison of Change Maps



(a) 2009 / Day / Visible / HyMap sensor vs. 2011 / Day / Visible / AHS sensor



(b) 2009 / Day / Visible / HyMap sensor vs. 2011 / Night / Thermal / AHS sensor

Change Detection via Diffusion Maps as $t \to \infty$

(a) September

(b) October

(c) $D^{(t)}(x_{\text{Sep}}, x_{\text{Oct}})$ as $t \to \infty$

The Standard Map

- The standard map is an area preserving chaotic map from a square with side length 2π onto itself.
- It is defined as:

$$p_{n+1} = p_n + K \cdot \sin(\theta_n)$$
$$\theta_{n+1} = \theta_n + p_{n+1}$$

- $K = 0$: the map is linear, and only periodic and quasi-periodic orbits are possible.
- $K > 0$: the map is nonlinear, and certain initial conditions give chaotic dynamics. The larger K, the more chaotic.
- Used to model what can happen in certain plasma driven fusion experiments.

Diffusion Embedding of the Standard Map

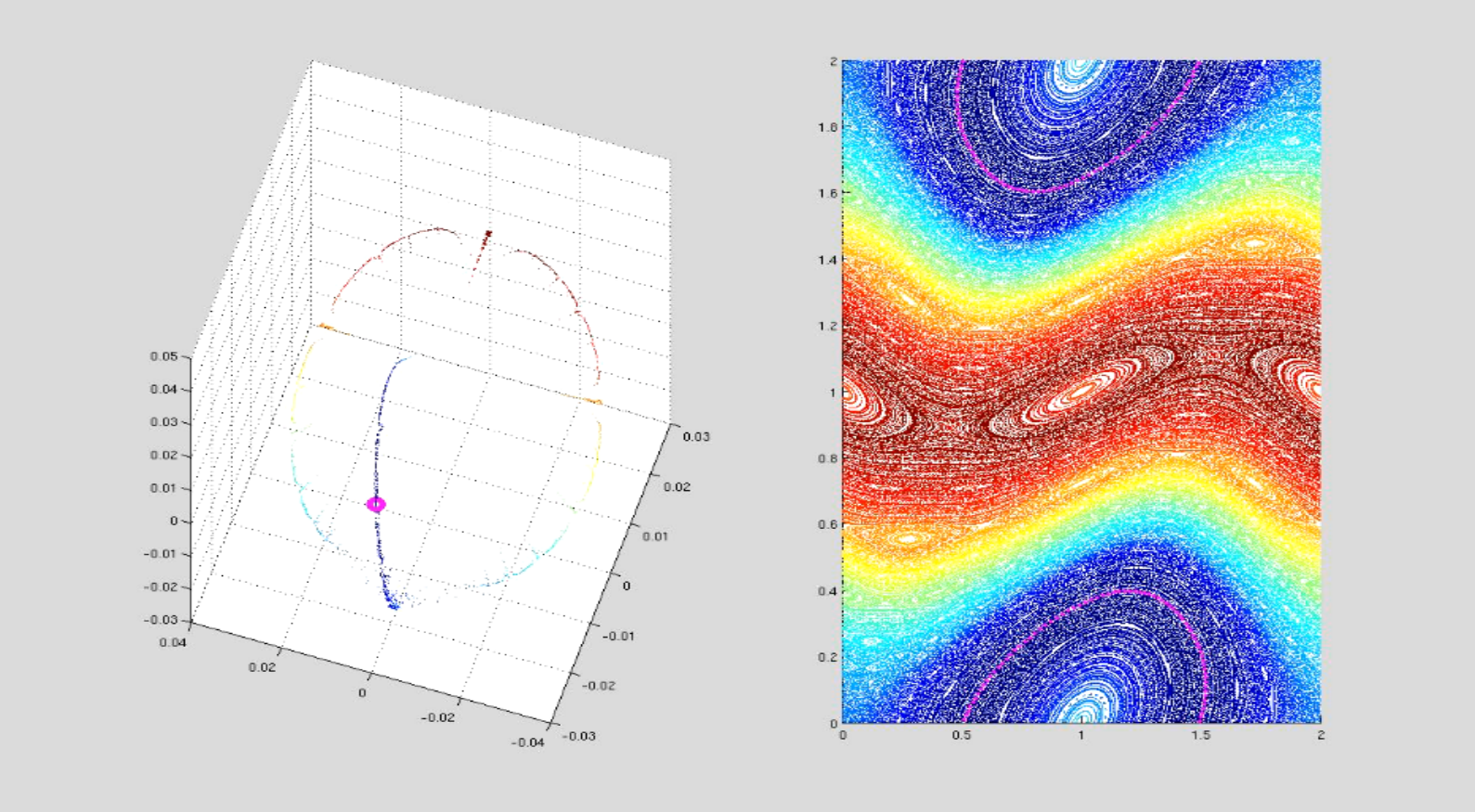


Figure: Standard map on right; diffusion embedding on left. The orbit of a particular color on the right corresponds to the embedded point of the same color on the left.

Diffusion Embedding as K Changes

Figure: Standard map on right; diffusion embedding on left.

Common Embedding

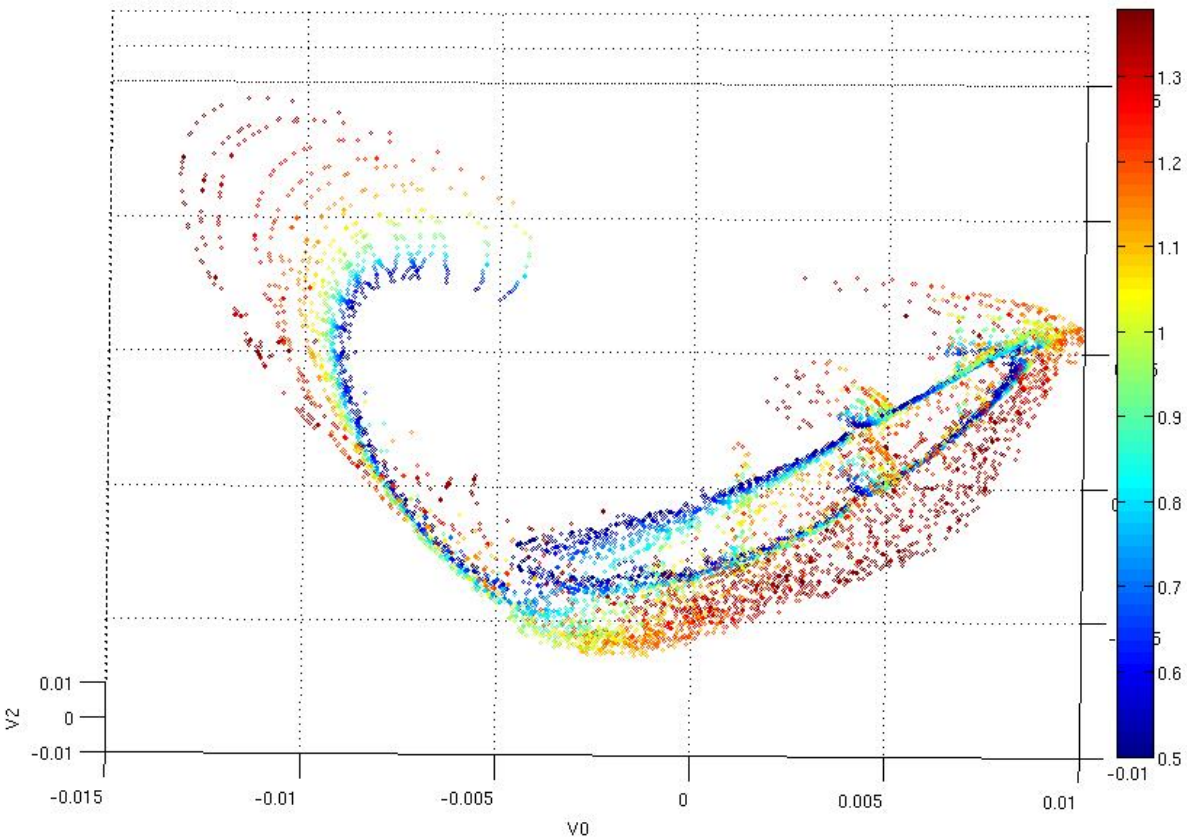


Figure: Diffusion embeddings of the standard map for various K all mapped into the same ℓ^2 space. The color of the points corresponds to the value of K (see color bar on right).

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Motivation

- In practice, one may only have samples $X_n = \{x^{(1)}, \ldots, x^{(n)}\}$ from the continuous data set X.
- Alternatively, one may wish to sample data on hand in order to reduce computational complexity.
- In either case, can we be sure that the results we get on the samples are accurate when compared to the ideal case?

Random Sampling and Empirical Operators

- Suppose μ is a probability measure.
- Let $X_n = \{x^{(1)}, \ldots, x^{(n)}\} \subset X$ be sampled i.i.d. according to μ.
- Set the following $n \times n$ matrices:

$$\mathbf{K}_\alpha[i,j] \triangleq \frac{1}{n} \cdot k_\alpha(x^{(i)}, x^{(j)}),$$

$$\mathbf{D}_\alpha[i,i] \triangleq \sum_{j=1}^{n} \mathbf{K}_\alpha[i,j],$$

$$\mathbf{A}_\alpha \triangleq \mathbf{D}_\alpha^{-\frac{1}{2}} \mathbf{K}_\alpha \mathbf{D}_\alpha^{-\frac{1}{2}}.$$

Empirical Diffusion Distance

Definition

For each positive integer t, let $D_n^{(t)} : (X_n \times \mathcal{I}) \times (X_n \times \mathcal{I}) \to \mathbb{R}$ denote the **empirical diffusion distance** at time t, where

$$D_n^{(t)}(x_\alpha^{(i)}, x_\beta^{(j)})^2 \triangleq n^2 \cdot \sum_{\ell=1}^{n} \left(\mathbf{A}_\alpha^t[i,\ell] - \mathbf{A}_\beta^t[j,\ell]\right)^2 .$$

- Recall that, even when evaluated just on X_n, the original diffusion distance was defined as:

$$D^{(t)}(x_\alpha^{(i)}, x_\beta^{(j)})^2 \triangleq \int_X \left(a_\alpha^{(t)}(x^{(i)}, s) - a_\beta^{(t)}(x^{(j)}, s)\right)^2 d\mu(s).$$

Approximation Theorem

Theorem Coifman and H.
Let $\tau > 0$. Then, with probability $1 - 2e^{-\tau}$,

$$D_n^{(t)}(x_\alpha^{(i)}, x_\beta^{(j)}) \approx D^{(t)}(x_\alpha^{(i)}, x_\beta^{(j)}),$$

to within accuracy $C \cdot \frac{\sqrt{\tau}}{\sqrt{n}}$.

Thank you

www.math.yale.edu/~mh644