# Parametrizations of Manifolds with Laplacian Eigenfunctions and Heat Kernels

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In collaboration with P.W. Jones, R. Schul
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# Goals

- Motivations: graphs, spectral embeddings, data sets
- Parametrizations via Eigenfunctions
- Parametrizations via Heat Kernels

# Random walks and heat kernels on the data

We are interested in *weighted undirected graphs* $(G, E, W)$: vertices represent data points, edges connect $x_i, x_j$ with weight $W_{ij} := W(x_i, x_j)$, when positive. Let $D_{ii} = \sum_j W_{ij}$ and

$$\underbrace{P = D^{-1}W}_{random\ walk},\ \underbrace{T = D^{-\frac{1}{2}}WD^{-\frac{1}{2}}}_{symm.\ ``random\ walk''},\ \underbrace{H = e^{-tL}}_{Heat\ kernel}$$

Here $L = I - T$ is the normalized Laplacian.

# Basic properties

- $P^t(x, y)$ is the probability of jumping from $x$ to $y$ in $t$ steps
- $P^t(x, \cdot)$ is a "probability bump" on the graph
- $P$ and $T$ are similar, therefore share the same eigenvalues $\{\lambda_i\}$ and the eigenfunctions are related by a simple transformation. Let $T\varphi_i = \lambda_i \varphi_i$, with $1 = \lambda_1 \geq \lambda_2 \geq \dots$.
- $\lambda_i \in [-1, 1]$
- "typically" $P$ (or $T$) is large and sparse, but its high powers are full and low-rank

# Eigenfunctions and spectral mappings

How do these eigenfunctions look like?
We know a lot when: $G$=regular lattice in $\mathbb{R}^n$!
We know quite a bit also when $G$ has group structures or symmetries..., but in general these eigenfunctions may be quite complicated!
They have been studied by many people in many communities: physicists (e.g. resonances...), computer scientists (graph layouts/cuts/flows...), mathematicians (analysis on manifolds, group theory, representation theory...).
Spectral graph layout: map $G \to \mathbb{R}^d$ by

$$\Phi(x) = (\varphi_1(x), \ldots, \varphi_d(x)) .$$

Maps a graph to $\mathbb{R}^d$. In general properties of this map are far from being well understood.

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# Structured data in high-dimensional spaces

A deluge of data: documents, web searching, customer databases, hyper-spectral imagery (satellite, biomedical, etc...), social networks, gene arrays, proteomics data, neurobiological signals, sensor networks, financial transactions, traffic statistics (automobilistic, computer networks)...
Common feature/assumption: data is given in a high dimensional space, however it has a much lower dimensional intrinsic geometry.

(i) physical constraints. For example the effective state-space of at least some proteins seems low-dimensional, at least when viewed at the time scale when important processes (e.g. folding) take place.

(ii) statistical constraints. For example many dependencies among word frequencies in a document corpus force the distribution of word frequency to low-dimensional, compared to the dimensionality of the whole space.

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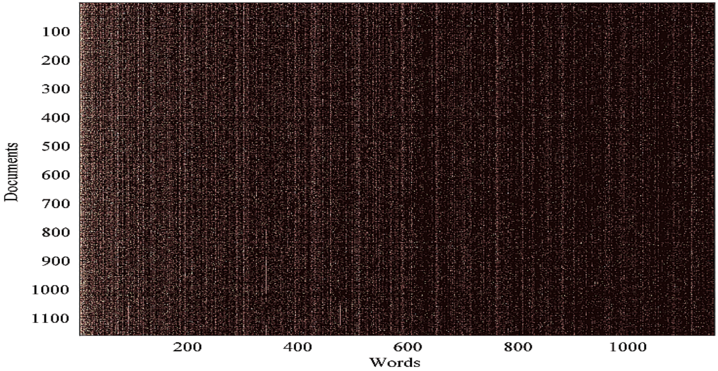
# Text documents

About 1100 Science News articles, from 8 different categories. We compute about 1000 coordinates, $i$-th coordinate of document $d$ represents frequency in document $d$ of the $i$-th word in a fixed dictionary.



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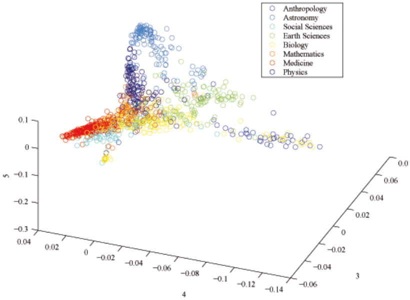
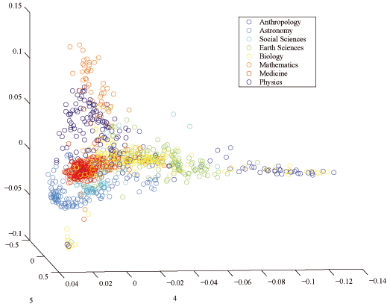
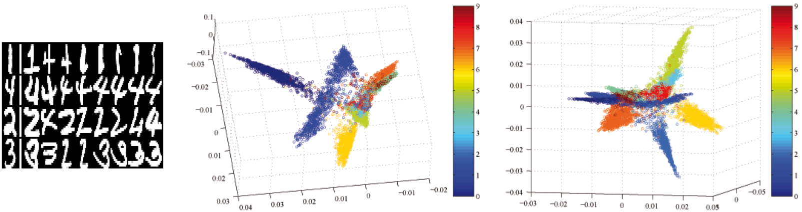


# Handwritten Digits

Data base of about $60,000$ $28 \times 28$ gray-scale pictures of handwritten digits, collected by USPS. Point cloud in $R^{28^2}$. Goal: automatic recognition.

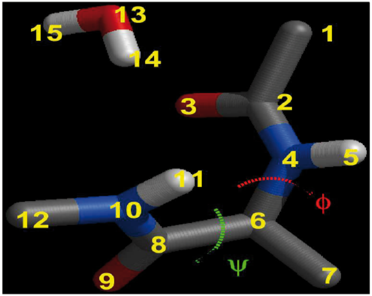


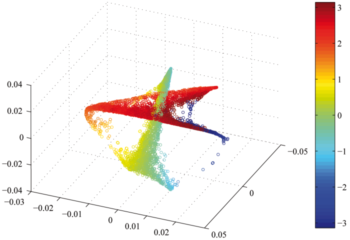
Set of $10,000$ picture (28 by 28 pixels) of 10 handwritten digits. Color represents the label (digit) of each point.

# A simple example from Molecular Dynamics

[Joint with C. Clementi]

The dynamics of a small protein (12 atoms, $H$ atoms removed) in a bath of water molecules is approximated by a Langevin system of stochastic equations $\dot{x} = -\nabla U(x) + \dot{w}$ . The set of states of the protein is a noisy ($\dot{w}$) set of points in $\mathbb{R}^{36}$.




Left: representation of an alanine dipeptide molecule. Right: embedding of the set of configurations.

# From data to weighted graphs

In all of the above: we assumed the data $X = \{x_i\}_{i=1}^{N} \subset \mathbb{R}^D$.
Define local similarities via a kernel function $W(x_i, x_j) \geq 0$.
Simplest example: $W_\sigma(x_i, x_j) = e^{-||x_i - x_j||^2/\sigma}$.
We obtained a *weighted graph* $(G, E, W)$:
We mapped the data via the spectral embedding:
$x \mapsto (\varphi_1(x), \ldots, \varphi_d(x))$, where $\varphi_i$ is the $i$-th lowest frequency eigenfunction of the Laplacian.
Note 1: $W$ depends on the type of data.
Note 2: $W$ should be "local", i.e. close to 0 for points not sufficiently close.

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# From graphs to manifolds

Spectral embeddings "seem to work quite well", very popular. Very few results on guarantees on any good property (e.g. Tutte's theorem for planar graphs, 1963).

More and more data may be acquired, and larger and larger graphs constructed: we model the limit as a continuous manifold, from which the points are sampled and the graph constructed.

Several results guarantee that natural operators on the graph (e.g. heat kernel, Laplacian, etc...) approximate in a suitable sense those on the underlying manifold.

Gallot et al. considered an infinite-dimensional spectral mapping of a manifold in $\ell^2$, and showed that it is indeed an embedding.

# A Theorem, heuristics

Let $\mathcal{M}$ be a Riemannian manifold. Coordinate chart: $\mathcal{M} \supset B \mapsto \tilde{B} \subset \mathbb{R}^d$, one-to-one, $F(x) = (f_1(x), \ldots, f_d(x))$. Distortion of $F$ (on $B$), $||F||_{Lip} \cdot ||F^{-1}||_{Lip}$, where

$$||F||_{Lip} = \sup_{x,y \in B, x \neq y} \frac{||F(x) - F(y)||}{d_{\mathcal{M}}(x,y)} .$$

Prime example: coordinate chart of a simply connected planar domain $\mathcal{D}$, $|\mathcal{D}| = 1$, given by a Riemann mapping $F : \mathcal{D} \to \mathbb{D}$ (the unit disk), centered at $z_0$, i.e. normalized so that $F(z_0) = 0$. For $z_0 \in \mathcal{D}$, let $r = \mathrm{dist}(z_0, \partial\mathcal{D})$. Then

$$B(0, \kappa^{-1}) \subset F(B(z_0, \frac{r}{2})) \subset B(0, 1 - \kappa^{-1}) ,$$

with distortion less than $\kappa$. Think of $F$ on $B(z_0, \frac{r}{2})$ as a perturbation of the linear map $z \to F'(z_0)(z - z_0)$ and $|F'(z_0)| \sim \frac{1}{r}$.

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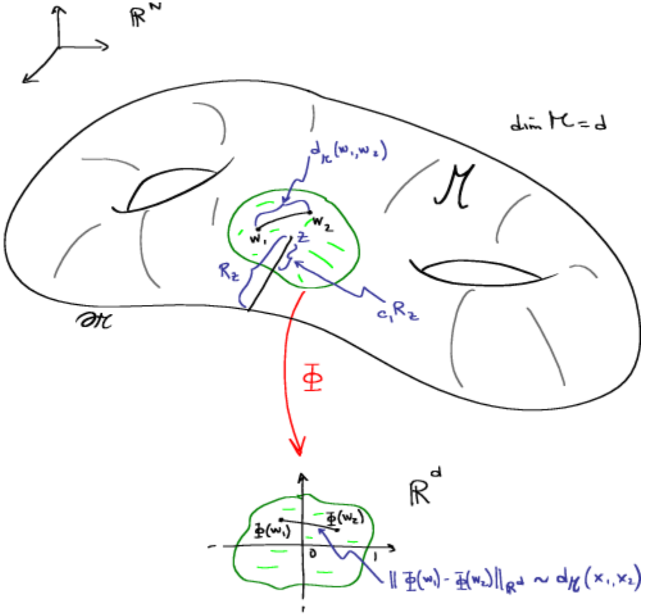
# Charts and local parametrizations



# A Theorem, heuristics

We look for an analogue of the above, on Riemannian manifolds of finite unit volume. Back to $\mathcal{D}, z_0, r, F$ as above. Classical formula, known to Riemann:

$$F(z) = exp\{-G(z, z_0) - iG^*(z, z_0)\},$$

$G(\cdot, z_0)$ is the Green's function for $\mathcal{D}$, and $G^*$ its (multi-valued) conjugate. But $G(z, z_0) = \int_0^{+\infty} K(z, z_0, t)dt$, $K$ the (Dirichlet) heat kernel for $\mathcal{D}$. Since

$$K(z, z_0, t) = \sum_{j=1}^{+\infty} \varphi_j(z)\varphi_j(z_0)e^{\lambda_j t}$$

where $\{\varphi_j\}$ are the global Dirichlet eigenfunctions, and $|F'(z)| = |\nabla G(z, z_0)|e^{-G(z,z_0)} \sim \frac{1}{r}$ on $B(z_0, \frac{r}{2})$, one may guess that there are eigenfunctions $\varphi_j$ such that

$$|\nabla\varphi_j| \gtrsim \frac{1}{r}$$

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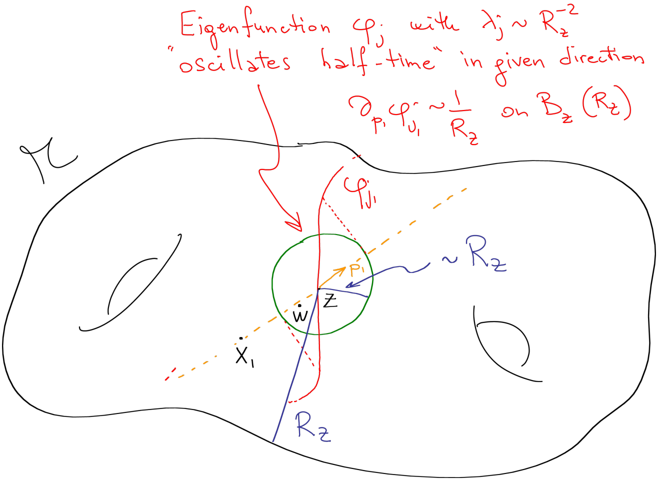
# A Theorem on eigenfunction parametrizations

We prove that there is a **locally** defined $F$ that has these properties, and that this choice of $F$ will come from **globally** defined Laplacian eigenfunctions. On a metric embedded ball $B \subset \mathcal{M}$ of radius $r$, we will choose **global** Laplacian eigenfunctions $\varphi_{i_1}, \dots, \varphi_{i_d}$ and constants $\gamma_1, \dots, \gamma_d \leq \kappa$ (for a universal constant $\kappa$) and define

$$\Phi(x) := (\gamma_1 \varphi_{i_1}, \dots, \gamma_d \varphi_{i_d}) .$$

This choice of $\Phi$, depending heavily on $z_0$ and $r$, is globally defined, and on $B(z_0, \kappa^{-1} r)$ enjoys the same properties as the Riemann map. In other words, $\Phi$ maps $B(z_0, \kappa^{-1} r)$ to, roughly, an Euclidean ball of unit size, with low distortion.

# Charts and local parametrizations



$\mathcal{M}$ smooth, $d$-dimensional compact manifold, possibly with boundary. Metric tensor $g \in \mathcal{C}^\alpha$. Fix $z_0 \in \mathcal{M}$, let $(U, F)$ be a coordinate chart s.t. $z_0 \in U$ and normalized so that $g^{il}(F(z_0)) = \delta^{il}$. Assume that for any $x \in U, \xi, \nu \in \mathbb{R}^d$,

$$c_{\min}(g)||\xi||^2_{\mathbb{R}^d} \leq \sum_{i,j=1}^{d} g^{ij}(F(x))\xi_i\xi_j \,, \sum_{i,j=1}^{d} g^{ij}(F(x))\xi_i\nu_j \leq c_{\max}(g)||\xi||_{\mathbb{R}^d}||\nu||_{\mathbb{R}^d}$$

Let $r_U(z_0) = \sup\{r > 0 : B_r(F(z_0)) \subseteq F(U)\}$.
Recall Weyl's estimate: let $C_{count}$ be s.t. for any $T > 0$

$$\#\{j : 0 < \lambda_j \leq T\} \leq C_{count} T^{\frac{d}{2}} |\Omega| \,.$$

[In the Dirichlet case $C_{count}$ does not depend on $\Omega$. Neumann case is more delicate.]

# Embedding with Eigenfunctions, for Manifolds

**Theorem (P.W. Jones, MM, R. Schul)**

*Let $(\mathcal{M}, g)$, $z \in \mathcal{M}$ be a $d$ dimensional manifold and $(U, F)$ be a chart as above. Assume $|\mathcal{M}| = 1$. There is a constant $\kappa > 1$, depending on $d$, $c_{\min}$, $c_{\max}$, $||g||_\alpha$, $\alpha$, such that the following hold.*
*Let $\rho \leq r_U(z)$, then $\exists i_1, \ldots, i_d$ : if $\gamma_l = (\fint_{B(z,\kappa^{-1}\rho)} \varphi_{i_l}^2)^{-\frac{1}{2}}$ , $l = 1, \ldots, d$:*

(a) *the map $\Phi : B(z, \kappa^{-1}\rho) \to \mathbb{R}^d$*

$$x \mapsto (\gamma_1 \varphi_{i_1}(x), \ldots, \gamma_d \varphi_{i_d}(x))$$

*satisfies for any $x_1, x_2 \in B(z, \kappa^{-1}\rho)$*

$$\frac{\kappa^{-1}}{\rho} d_{\mathcal{M}}(x_1, x_2) \leq ||\Phi(x_1) - \Phi(x_2)|| \leq \frac{\kappa}{\rho} d_{\mathcal{M}}(x_1, x_2) \,.$$

(b) $\kappa^{-1}\rho^{-2} \leq \lambda_{i_1}, \ldots, \lambda_{i_d} \leq \kappa\rho^{-2}$ .

(c) $\gamma_1, \ldots, \gamma_d \leq \kappa C_{count}{}^{\frac{1}{2}}$ .

# An example

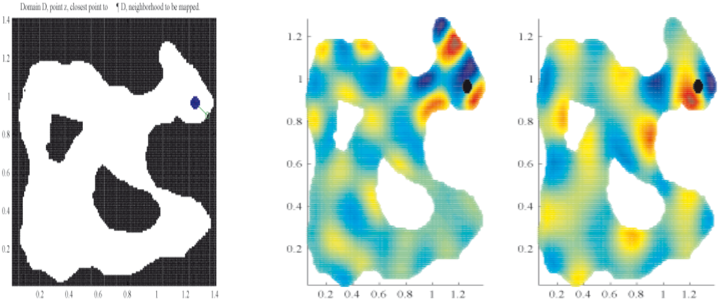



Figure: Top left: a non-simply connected domain in $\mathbb{R}^2$, and the point $z$ with its neighborhood to be mapped. Top right: the image of the neighborhood under the map. Bottom: Two eigenfunctions for mapping.

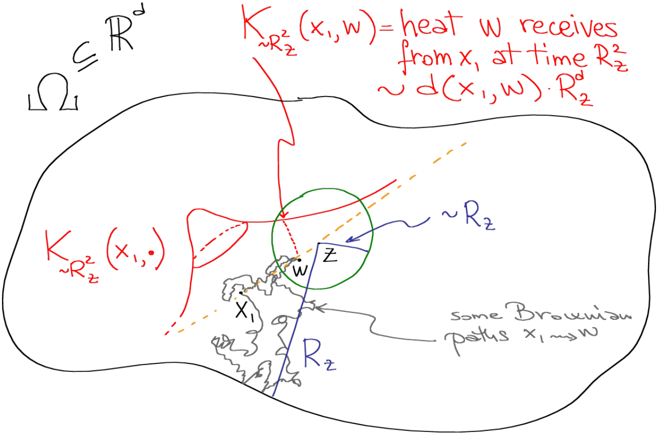
# A second Theorem, heuristics

Recall that $F(z) = exp\{-G(z, z_0) - iG^*(z, z_0)\}$, and

$$G(z, z_0) = \int_0^{+\infty} K(z, z_0, t)dt\,,$$

$K$ the (Dirichlet) heat kernel for $\mathcal{D}$, and from $K(z, z_0, t) = \sum_{j=1}^{+\infty} \varphi_j(z)\varphi_j(z_0)e^{\lambda_j t}$ we extracted eigenfunctions with large gradient, as suggested by $|F'(z)| = |\nabla G(z, z_0)|e^{-G(z,z_0)} \sim \frac{1}{r}$ on $B(z_0, \frac{r}{2})$.
In fact, this suggest that the heat kernel itself could be used to generate good coordinate char ts. Instead of d eigenfunctions we are able to pick $d$ heat kernels $\{K_t(x, y_i)\}_{i=1,\dots,d}$ , and obtain a coordinate chart with similar (in fact, stronger!) guarantees.

# Charts and local parametrizations,II

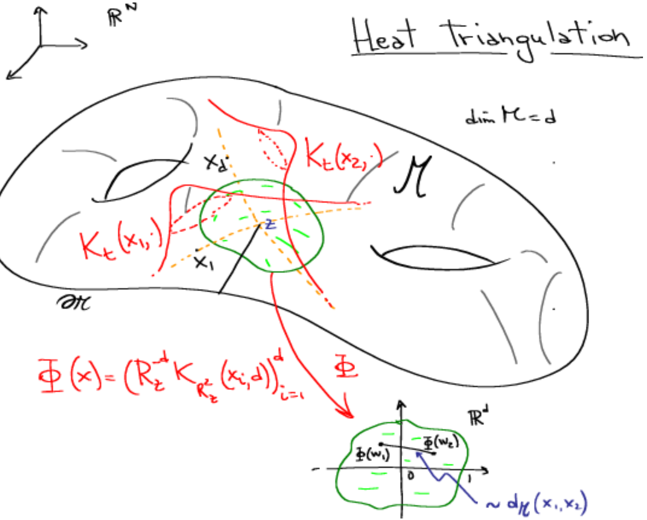



$$w \mapsto (R_z^{-d} K_{\sim R_z^2}(x_i, w))_{i=1,\ldots,d}$$

for $d$ reasonably chosen points $x_1, \ldots, x_d$.

The heat kernel computes distances by averaging along all paths, weighted by their probability of happening (Wiener measure for Brownian motion), with paths of length $\sim d(x_i, w)$ having the highest probability.

# Charts and local parametrizations,III




Note: this can be interpreted as a "kernel map" that linearizes the data to the "largest extent possible" under a distortion constraint.

# Heat Triangulation Theorem

**Theorem (P.W. Jones, MM, R. Schul)**

*Let $(\mathcal{M}, g)$, $z \in \mathcal{M}$ and $(U, F)$ be as above, with the exception we now make no assumptions on the finiteness of the volume of $\mathcal{M}$ and the existence of $C_{count}$. Let $\rho \le r_U(z)$. Let $p_1, ..., p_d$ be $d$ linearly independent directions. There are constants $c > 0$ and $c', \kappa > 1$, depending on $d$, $c_{\min}$, $c_{\max}$, $\rho^\alpha ||g||_\alpha$, $\alpha$, and the smallest and largest eigenvalues of the Gramian matrix $(\langle p_i, p_j \rangle)_{i,j=1,\ldots,d}$, such that the following holds. Let $y_i$ be so that $y_i - z$ is in the direction $p_i$, with $c\rho \le d_{\mathcal{M}}(y_i, z) \le 2c\rho$ for each $i = 1, \ldots, d$ and let $t = \kappa^{-1}\rho^2$. The map*

$$x \mapsto (\rho^d K_t(x, y_1)), \ldots, \rho^d K_t(x, y_d)) \tag{1}$$

*satisfies, for any $x_1, x_2 \in B(z, \kappa^{-1}\rho)$,*

$$\frac{\kappa^{-1}}{c'\rho} d_{\mathcal{M}}(x_1, x_2) \le ||\Phi(x_1) - \Phi(x_2)|| \le \frac{\kappa c'}{\rho} d_{\mathcal{M}}(x_1, x_2) \,. \tag{2}$$

# Applications

Applications of the above and related ideas:

(i) construct provably good charts (i.e. large, robust and with low-metric distortion) of manifolds [joint with P.W. Jones and R. Schul];

(ii) do semisupervised learning on manifolds and graphs [joint with A. Szlam and R. Coifman];

(iii) construct multiscale decompositions and multiscale bases on manifolds and graphs [joint with R. Coifman];

(iv) applied the above to various data sets, Markov Decision Processes, image denoising, hyperspectral images, etc...

# Some open questions and applications

Generalizations:

- Unions of manifolds, of possibly different dimensions
- Graphs
- Manifolds+noise

Implementation:

- Need to know intrinsic dimensionality - done: use multiscale geometric techniques.
- Need to know $\rho$ - done: use greedy algorithm with increasing choices of $\rho$.
- Need to know how to pick $x_i$'s in the heat kernel theorem - done: almost any random choice in the correct annulus will work

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Thank you!

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