Semi-supervised regression on unknown manifolds

Yale Applied Math

Amit Moscovich
Joint with Ariel Jaffe and Boaz Nadler

January 10, 2018

Outline

- Introduction to semi-supervised regression
- Geodesic knn regression
- Efficient computation
- Applications

Introduction to semi-supervised regression

Supervised regression

Input:

- n labeled pairs $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n) \in \mathbb{R}^D \times \mathbb{R}$

Supervised regression

Input:

- n labeled pairs $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n) \in \mathbb{R}^D \times \mathbb{R}$

Assumptions:

- $(\mathbf{x}_i, y_i) \overset{i.i.d.}{\sim} \mu$
- $y_i = f(\mathbf{x}_i) + \text{noise}$

Supervised regression

Input:

- n labeled pairs $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n) \in \mathbb{R}^D \times \mathbb{R}$

Assumptions:

- $(\mathbf{x}_i, y_i) \overset{i.i.d.}{\sim} \mu$
- $y_i = f(\mathbf{x}_i) + \text{noise}$

Output:

- Regression estimator $\hat{f} : \mathbb{R}^D \to \mathbb{R}$

Semi-supervised regression

Input:

- n labeled instances $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)$

Semi-supervised regression

Input:

- n labeled instances $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)$
- m unlabeled instances $\mathbf{x}_{n+1}, \ldots \mathbf{x}_{n+m}$

Semi-supervised regression

Input:

- n labeled instances $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)$
- m unlabeled instances $\mathbf{x}_{n+1}, \ldots \mathbf{x}_{n+m}$

Output: (transductive) regression estimates

$$\hat{f}(\mathbf{x}_{n+1}), \ldots, \hat{f}(\mathbf{x}_{n+m})$$

Semi-supervised regression

Input:

- n labeled instances $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)$
- m unlabeled instances $\mathbf{x}_{n+1}, \ldots \mathbf{x}_{n+m}$

Output: (transductive) regression estimates

$$\hat{f}(\mathbf{x}_{n+1}), \ldots, \hat{f}(\mathbf{x}_{n+m})$$

Output: (inductive) regression estimator

$$\hat{f} : \mathbb{R}^D \rightarrow \mathbb{R}$$

Method 1: Laplacian Regularization

[Zhu, Ghahramani, Lafferty 2003]

Given affinities $w_{i,j}$, find $\hat{f}$ that minimizes

$$\sum_{i,j} w_{i,j} \left(\hat{f}(\mathbf{x}_i) - \hat{f}(\mathbf{x}_j) \right)^2 = \hat{f}^T L \hat{f}$$

Subject to $\hat{f}(\mathbf{x}_i) = y_i$ for labeled points.

Method 1: Laplacian Regularization

[Zhu, Ghahramani, Lafferty 2003]

Given affinities $w_{i,j}$, find $\hat{f}$ that minimizes

$$\sum_{i,j} w_{i,j} \left(\hat{f}(\mathbf{x}_i) - \hat{f}(\mathbf{x}_j)\right)^2 = \hat{f}^T L \hat{f}$$

Subject to $\hat{f}(\mathbf{x}_i) = y_i$ for labeled points.

Reminder: the (unweighted) graph Laplacian is $L = W - D$ where W are the edge weights and D is the diagonal degree matrix $D_{ii} = \sum_j W_{ij}$.

Method 1: Laplacian Regularization

Disadvantage: pathological behavior when the number of unlabeled points $\rightarrow \infty$ [Nadler, Srebro, Zhou 2009]

Method 2: Laplacian eigenvector regression

[Belkin&Niyogi (2004)]

Method 2: Laplacian eigenvector regression

[Belkin&Niyogi (2004)]

(i) Construct (weighted) graph Laplacian

Method 2: Laplacian eigenvector regression

[Belkin&Niyogi (2004)]

(i) Construct (weighted) graph Laplacian
(ii) Compute p Laplacian eigenvectors with smallest eigenvalues

Method 2: Laplacian eigenvector regression

[Belkin&Niyogi (2004)]

(i) Construct (weighted) graph Laplacian
(ii) Compute p Laplacian eigenvectors with smallest eigenvalues
(iii) Find a linear combination of the eigenvectors that approximates the labeled points

Laplacian eigenvectors

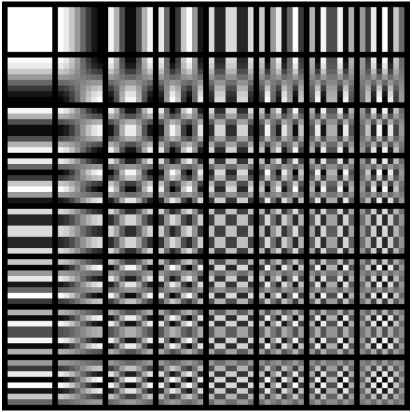


Figure: All 64 Laplacian eigenvectors of an 8x8 grid (image by Devcore)

Laplacian eigenvectors

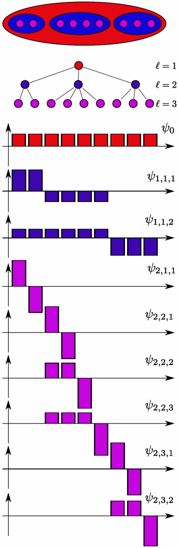
Figure: First 5 Laplacian eigenvectors for points on a 2D man-shaped manifold surface (image by Franck Hétroy)

Method 3: Multiscale wavelets

[Gavish, Nadler, Coifman 2010]

(i) Construct a tree of point sets by hierarchical partitioning.
(ii) Take Haar-like wavelet basis on tree.
(iii) Perform regression using this basis.

Method 3: Multiscale wavelets



Semi-supervised regression

Many other methods have been proposed

Semi-supervised regression

Many other methods have been proposed

Empirically, unlabeled data helpful only on some data sets

Semi-supervised regression

Many other methods have been proposed

Empirically, unlabeled data helpful only on some data sets

Better theoretical understanding needed

Why should unlabeled data help?

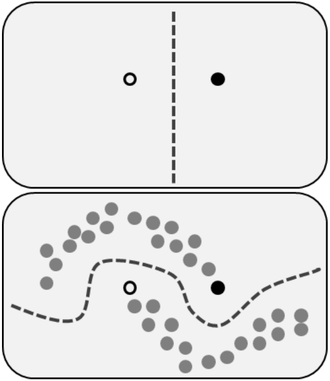
The cluster assumption:

- Points belong to distinct clusters.
- Points in same cluster have similar responses

Why should unlabeled data help?

The cluster assumption:

- Points belong to distinct clusters.
- Points in same cluster have similar responses



Why should unlabeled data help?

A direct solution for clustered data: [Rigollet (2007), Lafferty & Wasserman (2009)]:

- Estimate clusters.
- Compute the cluster-average response

Why should unlabeled data help?

A direct solution for clustered data: [Rigollet (2007), Lafferty & Wasserman (2009)]:

- Estimate clusters.
- Compute the cluster-average response

Singh, Nowak & Zhu (2009) analyzed the potential benefit of SSL in this setting.

Why should unlabeled data help?

A direct solution for clustered data: [Rigollet (2007), Lafferty & Wasserman (2009)]:

- Estimate clusters.
- Compute the cluster-average response

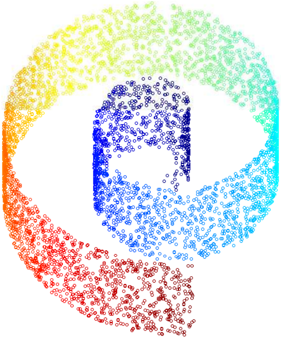
Singh, Nowak & Zhu (2009) analyzed the potential benefit of SSL in this setting.

Their key insight: unlabeled data can help estimate cluster boundaries

Why should unlabeled data help?

The manifold assumption:

- Points lie close to a low-dimensional manifold.
- Responses vary slowly w.r.t. the geodesic distance.



Why should unlabeled data help?

Main idea

Given enough data points, we can:

(i) Estimate the manifold geometry

(ii) Perform regression in dimension d instead of D

Why should unlabeled data help?

Main idea

Given enough data points, we can:

(i) Estimate the manifold geometry

(ii) Perform regression in dimension d instead of D

Unlabeled data may be key to (i).

How can unlabeled data help?

A naïve approach:

(i) Estimate the intrinsic dimension d

How can unlabeled data help?

A naïve approach:

(i) Estimate the intrinsic dimension d

(ii) Embed $\mathbf{x}_1, \ldots \mathbf{x}_{n+m} \hookrightarrow \mathbb{R}^d$ somehow

How can unlabeled data help?

A naïve approach:

(i) Estimate the intrinsic dimension d

(ii) Embed $\mathbf{x}_1, \ldots \mathbf{x}_{n+m} \hookrightarrow \mathbb{R}^d$ somehow

(iii) Apply classical methods in $\mathbb{R}^{\mathbf{d}}$

How can unlabeled data help?

A naïve approach:

(i) Estimate the intrinsic dimension d

(ii) Embed $\mathbf{x}_1, \ldots \mathbf{x}_{n+m} \hookrightarrow \mathbb{R}^d$ somehow

(iii) Apply classical methods in $\mathbb{R}^{\mathbf{d}}$

Problem: It is not always possible to faithfully embed to dimension d.

Lower bounds of nonparametric regression

Minimax lower-bound for the MSE:
Let $L > 0$ be a constant and let $\mathbf{x} \in \mathbb{R}^D$ be some point. For any regression estimator $\hat{f} : \mathbb{R}^D \to \mathbb{R}$ there exists an L-Lipschitz function f and an input distribution such that

$$\mathbb{E}(\hat{f}(\mathbf{x}) - f(\mathbf{x}))^2 \geq cn^{-\frac{2}{2+D}}$$

Lower bound of nonparametric regression

Any estimator that satisfies for all f

$$\mathbb{E}(\hat{f}(\mathbf{x}) - f(\mathbf{x}))^2 \leq c' n^{-\frac{2}{2+D}}$$

is called **minimax optimal.** (e.g. knn regression)

Nonparametric regression on manifolds

Theorem: [Kpotufe (2011)]
If the points $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^D$ are sampled from a d-dimensional manifold and if f is Lipschitz then classic knn regression satisfies

$$\sup_{\mathbf{x} \in \mathcal{M}} \left(\hat{f}_{knn}(\mathbf{x}_i) - f(\mathbf{x}_i) \right)^2 = \tilde{O}_P(n^{-\frac{2}{2+d}})$$

Caveat: $\mathbf{x}_1, \ldots, \mathbf{x}_n$ must form a dense cover of $\mathcal{M}$

Nonparametric regression on manifolds

Theorem: [Niyogi (2013)]
There are manifolds for which semi-supervised learning is provably better than supervised

Our results

Our results

We prove that if the number of **unlabeled** points is sufficiently large then semi-supervised regression can achieve the **finite-sample** minimax bound $n^{-\frac{2}{2+d}}$

Our results

We prove that if the number of **unlabeled** points is sufficiently large then semi-supervised regression can achieve the **finite-sample** minimax bound $n^{-\frac{2}{2+d}}$

This settles a conjecture by Goldberg, Zhu, Singh, Xu & Nowak (2009).

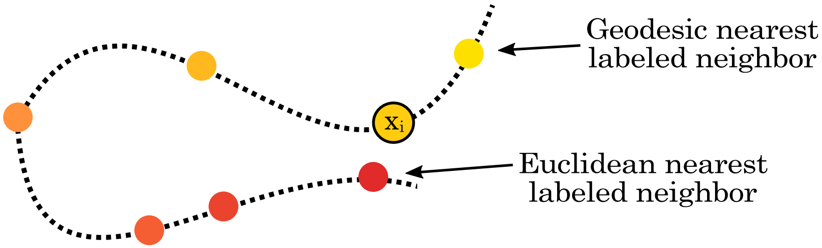
Our results

We prove that if the number of **unlabeled** points is sufficiently large then semi-supervised regression can achieve the **finite-sample** minimax bound $n^{-\frac{2}{2+d}}$

This settles a conjecture by Goldberg, Zhu, Singh, Xu & Nowak (2009).

Furthermore, we do this using a simple and fast method that demonstrates good empirical performance.

Geodesic knn regression - intuition



Geodesic knn regression

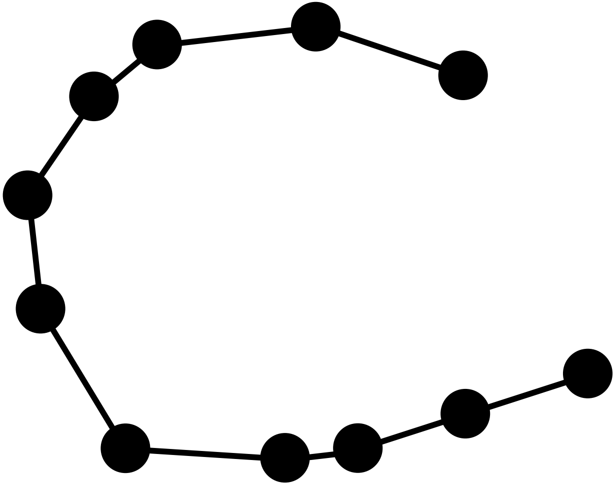
Step 1
Estimate the manifold geodesic distance $d_{\mathcal{M}}(\mathbf{x}_i, \mathbf{x}_j)$ for every pair $\{(\mathbf{x}_i, \mathbf{x}_j) : \mathbf{x}_i \in \mathcal{L},\, \mathbf{x}_j \in \mathcal{L} \cup \mathcal{U}\}$.

Geodesic knn regression

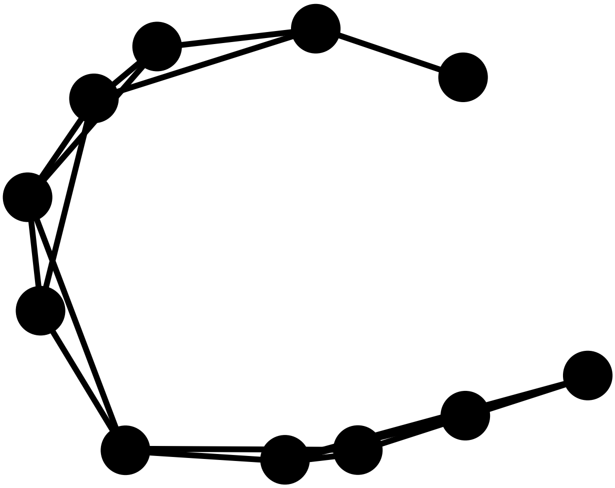
Step 1
Estimate the manifold geodesic distance $d_{\mathcal{M}}(\mathbf{x}_i, \mathbf{x}_j)$ for every pair $\{(\mathbf{x}_i, \mathbf{x}_j) : \mathbf{x}_i \in \mathcal{L},\ \mathbf{x}_j \in \mathcal{L} \cup \mathcal{U}\}$.

Step 2
Apply knn regression using the estimated distances

Step 1: estimate geodesic distances



Step 1: estimate geodesic distances



Step 2: geodesic knn regression

Step 2
Let $\mathrm{knn}_G(\mathbf{x}_i) \subseteq \mathcal{L}$ denote the set of k nearest **labeled** neighbors to $\mathbf{x}_i$

The **geodesic knn regressor** at $\mathbf{x}_i \in \mathcal{L} \cup \mathcal{U}$ is

$$\hat{f}(\mathbf{x}_i) := \frac{1}{|\mathrm{knn}_G(\mathbf{x}_i)|} \sum_{(\mathbf{x}_j, y_j) \in \mathrm{knn}_G(\mathbf{x}_i)} y_j \tag{1}$$

Geodesic knn regression - inductive case

What about new instances $\mathbf{x} \notin \mathcal{L} \cup \mathcal{U}$?

Geodesic knn regression - inductive case

What about new instances $\mathbf{x} \notin \mathcal{L} \cup \mathcal{U}$?

- Find its **Euclidean** nearest neighbor $\mathbf{x}^* \in \mathcal{L} \cup \mathcal{U}$
- The geodesic knn regression estimate at $\mathbf{x}$ is

$$\hat{f}(\mathbf{x}) := \hat{f}(\mathbf{x}^*) = \hat{f}\left(\underset{\mathbf{x}' \in \mathcal{L} \cup \mathcal{U}}{\operatorname{argmin}} \|\mathbf{x} - \mathbf{x}'\|\right) \quad (2)$$

Geodesic knn regression

Minimax optimality under the manifold assumption

Suppose we are given

(i) A labeled sample $\left\{ \left(\mathbf{x}_i, f(\mathbf{x}_i) + \mathcal{N}(0, \sigma^2)\right) \right\}_{i=1}^{n}$ where $\mathbf{x}_i \in \mathcal{M}$ and $f : \mathcal{M} \to \mathbb{R}$ is Lipschitz.

Geodesic knn regression

Minimax optimality under the manifold assumption

Suppose we are given

(i) A labeled sample $\left\{\left(\mathbf{x}_i, f(\mathbf{x}_i) + \mathcal{N}(0, \sigma^2)\right)\right\}_{i=1}^{n}$ where $\mathbf{x}_i \in \mathcal{M}$ and $f : \mathcal{M} \to \mathbb{R}$ is Lipschitz.

(ii) An unlabeled sample of m points.

Geodesic knn regression

Minimax optimality under the manifold assumption

Suppose we are given

(i) A labeled sample $\left\{ \left(\mathbf{x}_i, f(\mathbf{x}_i) + \mathcal{N}(0, \sigma^2) \right) \right\}_{i=1}^{n}$ where $\mathbf{x}_i \in \mathcal{M}$ and $f : \mathcal{M} \to \mathbb{R}$ is Lipschitz.

(ii) An unlabeled sample of m points.

(iii) A test point $\mathbf{x}$.

Geodesic knn regression

Minimax optimality under the manifold assumption

Suppose we are given

(i) A labeled sample $\left\{ \left(\mathbf{x}_i, f(\mathbf{x}_i) + \mathcal{N}(0, \sigma^2)\right) \right\}_{i=1}^{n}$ where $\mathbf{x}_i \in \mathcal{M}$ and $f : \mathcal{M} \to \mathbb{R}$ is Lipschitz.

(ii) An unlabeled sample of m points.

(iii) A test point $\mathbf{x}$.

Then we prove that geodesic knn regression obtains the **finite-sample** minimax bound on the MSE.

Definitions of manifold complexity

Definition: minimum radius of curvature

$$r_0(\mathcal{M}) := 1/\max_{\gamma,t} \|\ddot{\gamma}(t)\|$$

Definitions of manifold complexity

Definition: minimum radius of curvature

$$r_0(\mathcal{M}) := 1/\max_{\gamma,t} \|\ddot{\gamma}(t)\|$$

Definition: minimum branch separation
Largest s_0 such that for every pair $\forall \mathbf{x}, \mathbf{x}' \in \mathcal{M}$

$$\|\mathbf{x} - \mathbf{x}'\| < s_0 \quad \Longrightarrow \quad d_{\mathcal{M}}(\mathbf{x}, \mathbf{x}') \leq \pi r_0$$

Geodesic kNN regression

Minimax optimality under the manifold assumption

We assume that:

- $\mathcal{M}$ has bounded radius of curvature and branch separation.
- $\forall \mathbf{x} \in \mathcal{M}, r < R$ we have $\mu(B_{\mathbf{x}}(r)) \geq Qr^d$.

Geodesic kNN regression

Minimax optimality under the manifold assumption

We assume that:

- $\mathcal{M}$ has bounded radius of curvature and branch separation.
- $\forall \mathbf{x} \in \mathcal{M}, r < R$ we have $\mu(B_{\mathbf{x}}(r)) \geq Qr^d$.

Theorem 1 (simplified)
The geodesic knn regressor $\hat{f}$ satisfies

$$\mathbb{E}\left[\left(\hat{f}(\mathbf{x}) - f(\mathbf{x})\right)^2\right] \leq cn^{-\frac{2}{2+d}} + c'e^{-c''\cdot(n+m)}f_D^2.$$

where $f_D := f_{\max} - f_{\min}$.

Proof sketch

Since $\hat{f}(\mathbf{x}) := \hat{f}(\mathbf{x}^*)$ we have,

$$\mathbb{E}\left[(\hat{f}(\mathbf{x}) - f(\mathbf{x}))^2\right] = \mathbb{E}\left[(\hat{f}(\mathbf{x}^*) - f(\mathbf{x}))^2\right]$$

$$= \mathbb{E}\left[\Big((\hat{f}(\mathbf{x}^*) - f(\mathbf{x}^*)) + (f(\mathbf{x}^*) - f(\mathbf{x}))\Big)^2\right]$$

$$\leq 2\underbrace{\mathbb{E}\left[(\hat{f}(\mathbf{x}^*) - f(\mathbf{x}^*))^2\right]}_{(*)} + 2\underbrace{\mathbb{E}\left[(f(\mathbf{x}^*) - f(\mathbf{x}))^2\right]}_{(**)}.$$

Proof sketch (bound on (**))

Recall that $\forall r \leq R : \mu(B_{\mathbf{x}}(r)) \geq Q r^d$.

Proof sketch (bound on (**))

Recall that $\forall r \leq R : \mu(B_{\mathbf{x}}(r)) \geq Q r^d$.

Using this and some calculus, we obtain,

$$\begin{aligned}(**) &= \mathbb{E}\left[(f(\mathbf{x}^*) - f(\mathbf{x}))^2\right] \\ &\leq c(n+m)^{-\frac{2}{d}} + e^{-QR^d(n+m)} f_D^2.\end{aligned}$$

Proof sketch (bound on (*))

Let $(X_G^{(i,n)}(\mathbf{x}^*), Y_G^{(i,n)}(\mathbf{x}^*))$ denote the i-th closest labeled sample to $\mathbf{x}^*$ in terms of the graph distance.

Proof sketch (bound on (*))

Let $(X_G^{(i,n)}(\mathbf{x}^*), Y_G^{(i,n)}(\mathbf{x}^*))$ denote the i-th closest labeled sample to $\mathbf{x}^*$ in terms of the graph distance.

In this notation

$$\begin{aligned}\hat{f}(\mathbf{x}^*) &= \frac{1}{k}\sum_{i=1}^{k} Y_G^{(i,n)}(\mathbf{x}^*) \\ &= \frac{1}{k}\sum_{i=1}^{k} f(X_G^{(i,n)}(\mathbf{x}^*)) + \eta_G^{(i,n)}(\mathbf{x}^*)\end{aligned}$$

Proof sketch (bound on (*))

Consider the (easier) noiseless case.

$$\mathbb{E}\left[(\hat{f}(\mathbf{x}^*) - f(\mathbf{x}^*))^2\right]$$
$$= \mathbb{E}\left[\left(\frac{1}{k}\sum_{i=1}^{k} f(X_G^{(i,n)}(\mathbf{x}^*)) - f(\mathbf{x}^*)\right)^2\right]$$

How can we bound $f(X_G^{(i,n)}(\mathbf{x}^*)) - f(\mathbf{x}^*)$?

Proof sketch (bound on (*))

We can use the Lipschitz-continuity of f to bound

$$f(X_G^{(i,n)}(\mathbf{x}^*)) - f(\mathbf{x}^*) \leq L d_{\mathcal{M}}(X_G^{(i,n)}(\mathbf{x}^*), \mathbf{x}^*)$$

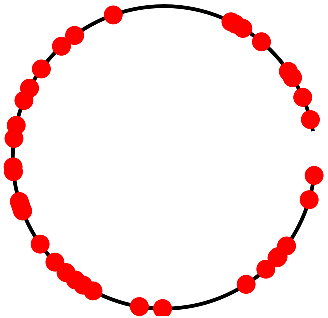
Proof sketch (bound on (*))

We can use the Lipschitz-continuity of f to bound

$$f(X_G^{(i,n)}(\mathbf{x}^*)) - f(\mathbf{x}^*) \leq L d_{\mathcal{M}}(X_G^{(i,n)}(\mathbf{x}^*), \mathbf{x}^*)$$

Problem: $X_G^{(i,n)}(\mathbf{x}^*)$ is close to $\mathbf{x}^*$ in terms of the graph distance but may be very far in terms of the manifold distance!

Proof sketch (bound on (*))



Proof sketch (bound on (*))

Solution: Theorems B and C of [Tenenbaum, de Silva, Langford (2000)] guarantee that

$$1 - \delta \leq \frac{d_G(X_i, X_j)}{d_{\mathcal{M}}(X_i, X_j)} \leq 1 + \delta \qquad (3)$$

hold for all i, j with probability $\geq 1 - c_a e^{-c_b(n+m)}$.

Proof sketch (bound on (*))

Conditioned on these inequalities, we can prove that

$$d_{\mathcal{M}}\left(X_G^{(i,n)}(\mathbf{x}^*), \mathbf{x}^*\right) \leq \tfrac{1+\delta}{1-\delta} d_{\mathcal{M}}\left(X_{\mathcal{M}}^{(i,n)}(\mathbf{x}^*), \mathbf{x}^*\right).$$

Proof sketch (bound on (*))

Conditioned on these inequalities, we can prove that

$$d_{\mathcal{M}}\left(X_G^{(i,n)}(\mathbf{x}^*), \mathbf{x}^*\right) \leq \tfrac{1+\delta}{1-\delta} d_{\mathcal{M}}\left(X_{\mathcal{M}}^{(i,n)}(\mathbf{x}^*), \mathbf{x}^*\right).$$

We obtain a bound on (*) using an extension of the classical knn proof [Györfi et. al, 2002] to the manifold setting.

Efficient computation of geodesic nearest neighbors

Efficient computation

Problem:

How to compute $\text{knn}_G(\mathbf{x}_i)$ for all $x_i \in \mathcal{L} \cup \mathcal{U}$?

Efficient computation

Problem:

How to compute $\mathrm{knn}_G(\mathbf{x}_i)$ for all $x_i \in \mathcal{L} \cup \mathcal{U}$?

Solution 1: Floyd-Warshall all-pairs shortest paths

- $O(N^3)$ where $N = n + m$

Efficient computation

Problem:

How to compute $\mathrm{knn}_G(\mathbf{x}_i)$ for all $x_i \in \mathcal{L} \cup \mathcal{U}$?

Solution 1: Floyd-Warshall all-pairs shortest paths

- $O(N^3)$ where $N = n + m$

Solution 2: Run Dijkstra from all labeled nodes:

Efficient computation

Problem:

How to compute $\text{knn}_G(\mathbf{x}_i)$ for all $x_i \in \mathcal{L} \cup \mathcal{U}$?

Solution 1: Floyd-Warshall all-pairs shortest paths

- $O(N^3)$ where $N = n + m$

Solution 2: Run Dijkstra from all labeled nodes:

- $O(n(N \log N + |E|))$
- Dense graph: $O(nN^2)$
- Sparse graph: $O(nN \log N)$

Efficient computation

Problem:
How to compute $\mathrm{knn}_G(\mathbf{x}_i)$ for all $x_i \in \mathcal{L} \cup \mathcal{U}$?

Solution 1: Floyd-Warshall all-pairs shortest paths

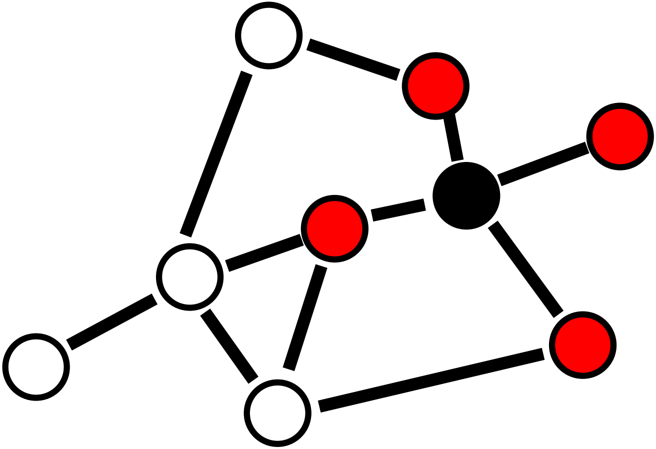
- $O(N^3)$ where $N = n + m$

Solution 2: Run Dijkstra from all labeled nodes:

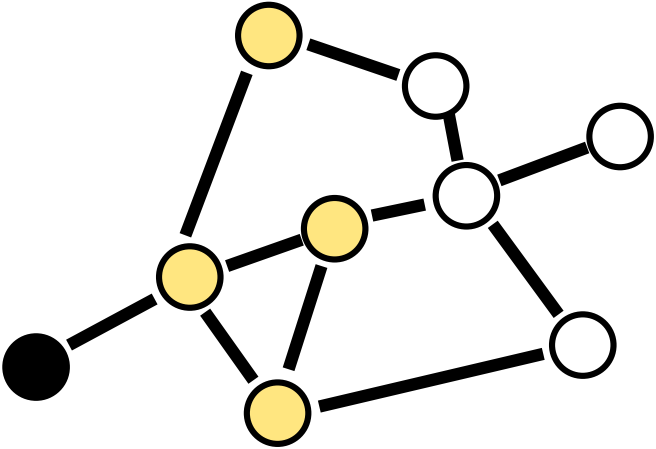
- $O(n(N \log N + |E|))$
- Dense graph: $O(nN^2)$
- Sparse graph: $O(nN \log N)$

We can do better! $O(kN \log N)$

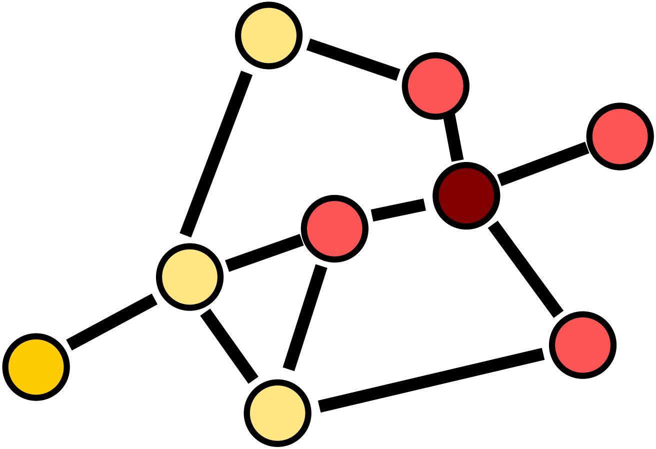
Dijkstra's algorithm

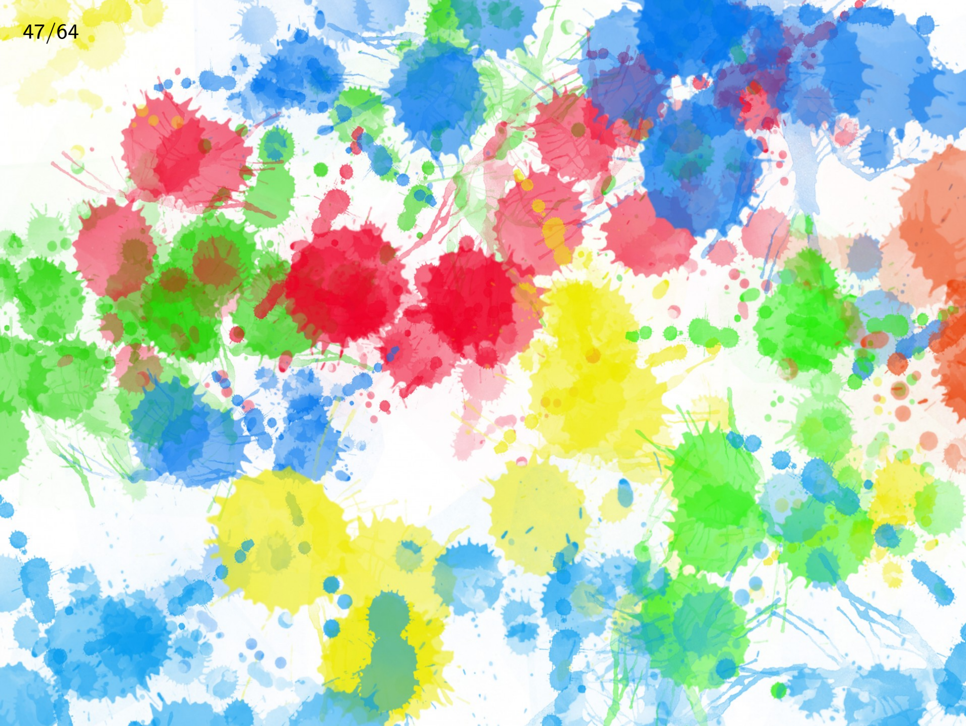


Dijkstra's algorithm



Simultaneous Dijkstra (k=1)





Simultaneous Dijkstra - correctness

Let NLV(u, j) be the set of j nearest labeled vertices to the vertex u

Simultaneous Dijkstra - correctness

Let $\mathrm{NLV}(u, j)$ be the set of j nearest labeled vertices to the vertex u

Lemma

Let $v \in V$ be a vertex and let s be its j-th nearest labeled vertex. If $s \rightsquigarrow u \rightsquigarrow v$ is a shortest path then $s \in NLV(u, j)$.

Algorithm 1

$Q \leftarrow \text{PriorityQueue}()$
for $v \in V$ **do**
  $\text{kNN}[v] \leftarrow \text{Empty-List}()$
  $S_v \leftarrow \phi$
  if $v \in \mathcal{L}$ **then**
    $\text{insert}(Q, (v, v), \text{priority} = 0)$

Algorithm 1 - continued

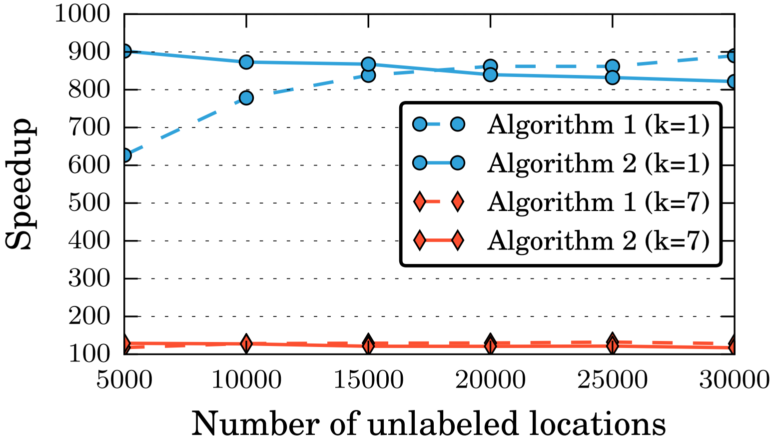
while $Q \neq \phi$ **do**
    (seed, v_0, dist) $\leftarrow$ pop-minimum(Q)
    $S_{v_0} \leftarrow S_{v_0} \cup \{\text{seed}\}$
    if length(kNN[v_0]) $< k$ **then**
        append (dist, seed) **to** kNN[v_0]
        for all $v \in$ neighbors(v_0) **do**
            if len(kNN[v]) $< k$ and seed $\notin S_v$ **then**
                decrease-or-insert(Q, (seed, v),
                priority $=$ dist $+w(v_0, v)$)

Efficient computation

Related works:

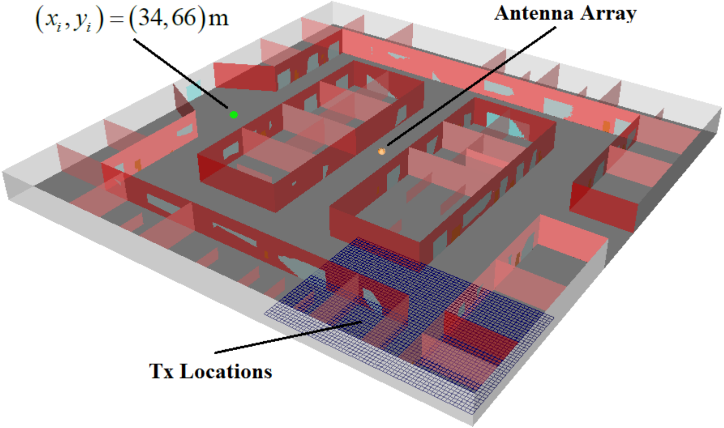
- Algorithm 1 extends the $k = 1$ algorithm of Erwig (2000)
- Independently, Har-Peled (2016) proposed Algorithm 1 and also described a variant (Algorithm 2) which gives tighter guarantees on the running time

Efficient computation



Applications

Geodesic knn regression for indoor localization



Indoor localization using WiFi fingerprints

Feature vectors are 48×48 complex matrices computed by sampling the received signals at 6 antennas of a WiFi router. [Kupershtein, Wax & Cohen (2013)]

Indoor localization using WiFi fingerprints

Feature vectors are 48×48 complex matrices computed by sampling the received signals at 6 antennas of a WiFi router. [Kupershtein, Wax & Cohen (2013)]

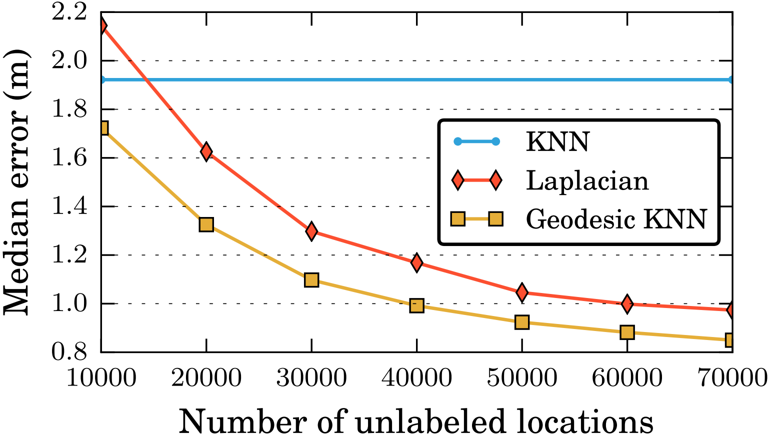
The labeled points were placed on a regular grid.

Indoor localization using WiFi fingerprints

Feature vectors are 48×48 complex matrices computed by sampling the received signals at 6 antennas of a WiFi router. [Kupershtein, Wax & Cohen (2013)]

The labeled points were placed on a regular grid. The unlabeled points were drawn at random.

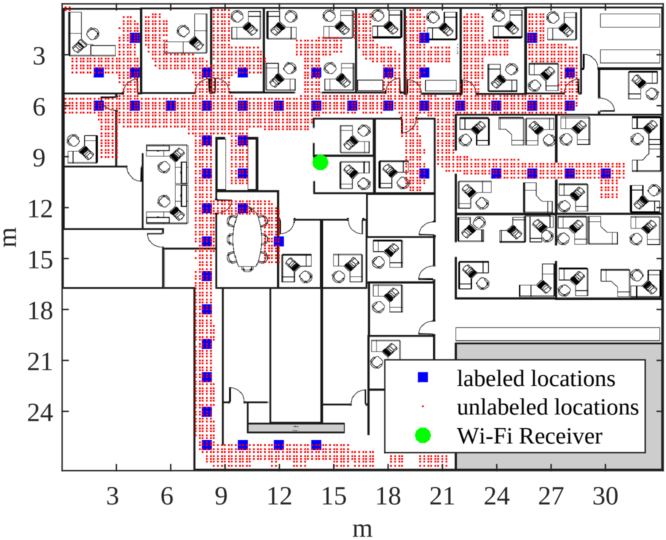
Indoor localization performance



Indoor localization runtime

#unlabeled	Laplacian	Geodesic 7NN	Graph build
1000	7.6s	2.3s	9s
10000	195s	7s	76s
100000	114min	56s	66min

Indoor localization performance: real data

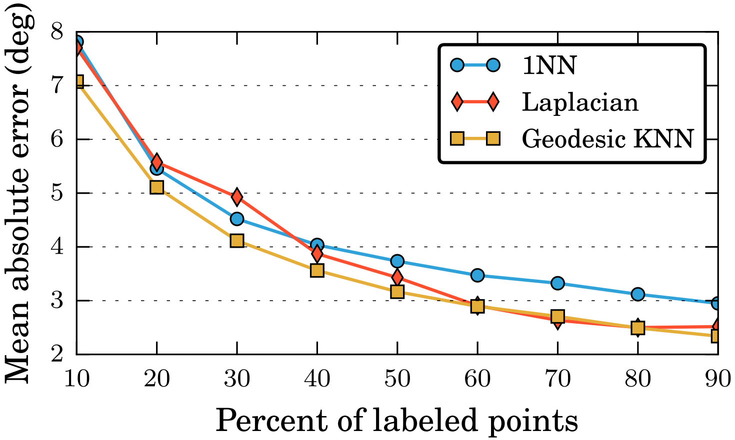


Indoor localization performance: real data

Labeled grid	n	knn	Laplacian	Geodesic knn
1.5m	73	1.49m	1.36m	**1.11**m
2.0m	48	2.27m	1.65m	**1.49**m
3m	23	3.41m	2.79m	**2.41**m

Facial pose estimation

Facial pose estimation



In summary

Geodesic knn regression is:

- The first semi-supervised method that is minimax optimal in the finite-sample sense
- Very fast to compute
- Obtains good empirical results on low-dimensional manifolds.

Graph semisupervised regression vs. classical nonparametric regression

Graph method	Classical analogue
Laplacian regularization	$\mathbb{R} \Rightarrow$ linear interpolation $\mathbb{R}^n \Rightarrow$???
Laplacian eigenvector regr.	Fourier regression
Multiscale wavelets	Haar wavelet regression
Geodesic regression	knn regression or Kernel smoothing

Paper&code: **http://moscovich.org**