
Shortest path distance in random k -nearest neighbor graphs

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Abstract

Consider a weighted or unweighted k -nearest neighbor graph that has been built on n data points drawn randomly according to some density p on \mathbb{R}^d . We study the convergence of the shortest path distance in such graphs as the sample size tends to infinity. We prove that for unweighted kNN graphs, this distance converges to an unpleasant distance function on the underlying space whose properties are detrimental to machine learning. We also study the behavior of the shortest path distance in weighted kNN graphs.

1. Introduction

The shortest path distance is the most fundamental distance function between vertices in a graph, and it is widely used in computer science and machine learning. In this paper we want to understand the geometry induced by the shortest path distance in randomly generated geometric graphs like k -nearest neighbor graphs.

Consider a neighborhood graph G built from an i.i.d. sample X_1, \dots, X_n drawn according to some density p on $\mathcal{X} \subset \mathbb{R}^d$ (for exact definitions see Section 2). Assume that the sample size n goes to infinity. Two questions arise about the behavior of the shortest path distance between fixed points in this graph:

1. **Weight assignment:** Given a distance measure D on \mathcal{X} , how can we assign edge weights such that the shortest path distance in the graph converges to D ?

2. **Limit distance:** Given a function h that assigns weights of the form $h(\|X_i - X_j\|)$ to edges in G , what is the limit of the shortest path distance in this weighted graph as $n \rightarrow \infty$?

The first question has already been studied in some special cases. Tenenbaum et al. (2000) discuss the case of ε - and kNN graphs when p is *uniform* and D is the geodesic distance. Sajama & Orlitsky (2005) extend these results to ε -graphs from a general density p by introducing edge weights that depend on an explicit estimate of the underlying density. In a recent preprint, Hwang et al. (2012) consider completely connected graphs whose vertices come from a general density p and whose edge weights are powers of distances.

There is little work regarding the second question. Tenenbaum et al. (2000) answer the question for a very special case with $h(x) = x$ and uniform p . Hwang et al. (2012) study the case $h(x) = x^a$, $a > 1$ for arbitrary density p .

We have a more general point of view. In Section 4 we show that depending on properties of the function $h(x)$, the shortest path distance operates in different regimes, and we find the limit of the shortest path distance for particular function classes of $h(x)$. Our method also reveals a direct way to answer the first question without explicit density estimation.

An interesting special case is the unweighted kNN graph, which corresponds to the constant weight function $h(x) = 1$. We show that the shortest path distance on unweighted kNN-graphs converges to a limit distance on \mathcal{X} that does *not* conform to the natural intuition and induces a geometry on \mathcal{X} that can be detrimental for machine learning applications.

Our results have implications for many machine learning algorithms, see Section 5 for more discussion. (1) The shortest paths based on unweighted kNN graphs prefer to go through low density regions, and they even accept large detours if this avoids passing through high density regions (see Figure 1 for an illustration). This is exactly the opposite of what we would like to achieve in most applications. (2) For manifold learning algorithms like Isomap, unweighted kNN graphs introduce a fundamental bias that leads to huge distortions in the estimated manifold structure (see Figure 2 for an

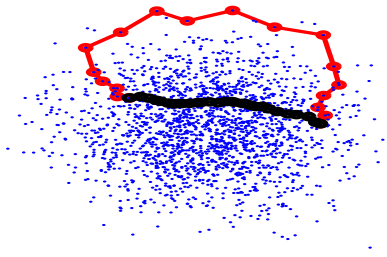


Figure 1. The shortest path based on an unweighted (red) and Euclidean weighted (black) kNN graph.

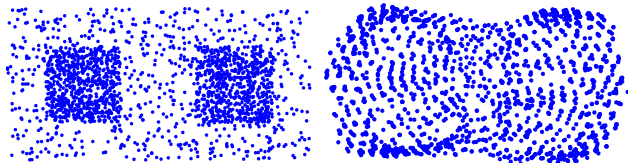


Figure 2. Original data (left) and its Isomap reconstruction based on an unweighted kNN graph (right).

illustration). (3) In the area of semi-supervised learning, a standard approach is to construct a graph on the sample points, then compute a distance between vertices of the graph, and finally use a standard distance-based classifier to label the unlabeled points (e.g., Sajama & Orlitsky, 2005 and Bijral et al., 2011). The crucial property exploited in this approach is that distances between points should be small if they are in the same high-density region. Shortest path distances in unweighted kNN graphs and their limit distances do exactly the opposite, so they can be misleading for this approach.

2. Basic definitions

Consider a closed, connected subset $\mathcal{X} \subseteq \mathbb{R}^d$ that is endowed with a density function p with respect to the Lebesgue measure. For the ease of presentation we assume for the rest of the paper that the density p is Lipschitz continuous with Lipschitz constant L and bounded away from 0 by $p_{\min} > 0$. To simplify notation later on, we define the shorthand $q(x) := (p(x))^{1/d}$.

We will consider different metrics on \mathcal{X} . A ball with respect to a particular metric D in \mathcal{X} will be written as $B(x, r, D) := \{y \in \mathcal{X} \mid D(x, y) \leq r\}$. We denote the Euclidean volume of the unit ball in \mathbb{R}^d by η_d .

Assume the finite dataset X_1, \dots, X_n has been drawn i.i.d according to p . We build a geometric graph $G = (V, E)$ that has the data points as vertices and connects vertices that are close. Specifically, for the kNN graph we connect X_i with X_j if X_i is among the k nearest neighbors of X_j or vice versa. For the ε -graph, we connect X_i and X_j whenever their Euclidean distance

satisfies $\|X_i - X_j\| \leq \varepsilon$. In this paper, all graphs are undirected, but might carry edge weights $w_{ij} \geq 0$. In unweighted graphs, we define the length of a path by its number of edges, in weighted graphs we define the length of a path by the sum of the edge weights along the path. In both cases, the shortest path (\mathcal{SP}) distance $D_{sp}(x, y)$ between two vertices $x, y \in V$ is the length of the shortest path connecting them.

Let f be a positive continuous scalar function defined on \mathcal{X} . For a given path γ in \mathcal{X} that connects x with y and is parameterized by t , we define the f -length of the path as

$$D_{f,\gamma} = \int_{\gamma} f(\gamma(t)) |\gamma'(t)| dt.$$

This expression is also known as the *line integral* along γ with respect to f . The f -geodesic path between x and y is the path with minimum f -length.

The f -length of the geodesic path is called the f -distance between x and y . We denote it by $D_f(x, y)$. If $f(x)$ is a function of the density p at x , then the f -distance is sometimes called a density based distance (Sajama & Orlitsky, 2005).

The f -distance on \mathcal{X} is a metric, and in particular it satisfies the triangle inequality. Another useful property is that for a point u on the f -geodesic path between x and y we have $D_f(x, y) = D_f(x, u) + D_f(u, y)$.

The function f determines the behavior of the f -distance. When $f(x)$ is a monotonically decreasing function of density $p(x)$, passing through a high density region will cost less than passing through a low density region. It works the other way round when f is a monotonically increasing function of density. A constant function does not impose any preference between low and high density regions.

The main purpose of this paper is to study the relationship between the \mathcal{SP} distance in various geometric graphs and particular f -distances on \mathcal{X} . For example, in Section 3 we show that the \mathcal{SP} distance in unweighted kNN graphs converges to the f -distance with $f(x) = p(x)^{1/d}$.

In the rest of the paper, all statements refer to points x and y in the interior of \mathcal{X} such that their f -geodesic path is bounded away from the boundary of \mathcal{X} .

3. Shortest paths in unweighted graphs

In this section we study the behavior of the shortest path distance in the family of *unweighted* kNN graphs. We show that the rescaled graph \mathcal{SP} distance converges to the q -distance in the original space \mathcal{X} .

Theorem 1 (\mathcal{SP} limit in unweighted k NN graphs)

Consider the unweighted k NN graph G_n based on the i.i.d. sample $X_1, \dots, X_n \in \mathcal{X}$ from the density p . Choose λ and a such that

$$\lambda \geq \frac{4L}{\eta_d^{1/d} p_{\min}^{1+1/d}} \left(\frac{k}{n}\right)^{1/d}, \quad a < 1 - \log_k \left(4^d(1 + \lambda)^2\right).$$

Fix two points $x = X_i$ and $y = X_j$. Then there exist $e_1(\lambda, k), e_2(\lambda, k, n), e_3(\lambda)$ (see below for explicit definitions) such that with probability at least $1 - 3e_3 n \exp(-\lambda^2 k^a / 6)$ we have

$$e_1 D_q(x, y) \leq e_2 D_{sp}(x, y) \leq D_q(x, y) - e_2.$$

Moreover if $n \rightarrow \infty, k \rightarrow \infty, k/n \rightarrow 0, \lambda \rightarrow 0$ and $\lambda^2 k^a / \log(n) \rightarrow \infty$, then the probability converges to 1 and $(k/(\eta_d n))^{1/d} D_{sp}(x, y)$ converges to $D_q(x, y)$ in probability.

The convergence conditions on n and k are the ones to be expected for random geometric graphs. The condition $\lambda^2 k^a / \log(n) \rightarrow \infty$ is slightly stronger than the usual $k / \log(n) \rightarrow \infty$ condition. This condition is satisfied as soon as k is of the order a bit larger than $\log(n)$. For example $k \approx \log(n)^{1+\alpha}$ with a small α will work. For k smaller than $\log(n)$, the graphs are not connected anyway (see e.g. Penrose, 1999) and are unsuitable for machine learning applications.

Before proving Theorem 1, we need to state a couple of propositions and lemmas. We start by introducing some ad-hoc notation:

Definition 2 (Connectivity parameters) Consider a geometric graph based on a fixed set of points $X_1, \dots, X_n \in \mathbb{R}^d$. Let r_{low} be a real number such that $D_f(X_i, X_j) \leq r_{low}$ implies that X_i is connected to X_j in the graph. Analogously, consider r_{up} to be a real number such that $D_f(X_i, X_j) \geq r_{up}$ implies that X_i is not connected to X_j in the graph.

Definition 3 (Dense sampling assumption) Consider a graph G with connectivity parameters r_{low} and r_{up} . We say that it satisfies the dense sampling assumption if there exists an $\varsigma < r_{low}/4$ such that for all $x \in \mathcal{X}$ there exists a vertex y in the graph with $D_f(x, y) \leq \varsigma$.

Proposition 4 (Bounding D_{sp} by D_f) Consider any unweighted geometric graph based on a fixed set $X_1, \dots, X_n \in \mathcal{X} \subset \mathbb{R}^d$ that satisfies the dense sampling assumption. Fix two vertices x and y of the graph and set

$$e_1 = (r_{low} - 2\varsigma)/r_{up}, \quad e_2 = r_{low} - 2\varsigma.$$

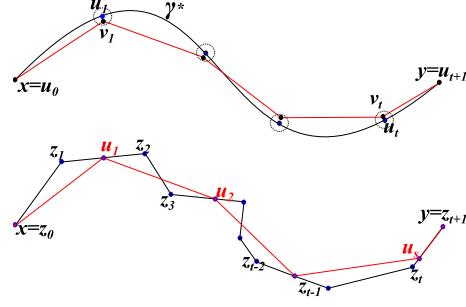


Figure 3. Path constructions in the proofs of Proposition 4 (top) and Theorem 9 (bottom).

Then the following statement holds:

$$e_1 D_f(x, y) \leq e_2 D_{sp}(x, y) \leq D_f(x, y) - e_2.$$

Proof. Right hand side. Consider the f -geodesic path $\gamma_{x,y}^*$ connecting x to y . Divide $\gamma_{x,y}^*$ to segments by $u_0 = x, u_1, \dots, u_t, u_{t+1} = y$ such that $D_f(u_i, u_{i+1}) = r_{low} - 2\varsigma$ for $i = 0, \dots, t-1$ and $D_f(u_t, u_{t+1}) \leq r_{low} - 2\varsigma$ (see Figure 3). Because of the dense sampling assumption, for all $i = 1, \dots, t$ there exists a vertex v_i in the ball $B(u_i, \varsigma; D_f)$ and we have

$$\begin{aligned} D_f(v_i, u_i) &\leq \varsigma \\ D_f(u_i, u_{i+1}) &\leq r_{low} - 2\varsigma \\ D_f(u_{i+1}, v_{i+1}) &\leq \varsigma. \end{aligned}$$

Applying the triangle inequality gives $D_f(v_i, v_{i+1}) \leq r_{low}$, which shows that v_i and v_{i+1} are connected. By summing up along the path we get

$$\begin{aligned} (r_{low} - 2\varsigma)(D_{sp}(x, y) - 1) &\leq (r_{low} - 2\varsigma)t \\ &= \sum_{i=0}^{t-1} D_f(u_i, u_{i+1}) \stackrel{(a)}{\leq} D_f(x, y). \end{aligned}$$

In step (a) we use the simple fact that if u is on the f -geodesic path from x to y , then

$$D_f(x, y) = D_f(x, u) + D_f(u, y).$$

Left hand side. Assume that the graph \mathcal{SP} between x and y consists of vertices $z_0 = x, z_1, \dots, z_s = y$. By $D_f(z_i, z_{i+1}) \leq r_{up}$ we can write

$$\begin{aligned} (r_{low} - 2\varsigma)D_{sp}(x, y) &\geq \frac{r_{low} - 2\varsigma}{r_{up}} \sum_{i=0}^{s-1} D_f(z_i, z_{i+1}) \\ &\geq \frac{r_{low} - 2\varsigma}{r_{up}} D_f(x, y). \end{aligned}$$

□

The next lemma uses the Lipschitz continuity and boundedness of p to show that $q(x)\|x - y\|$ is a good approximation of $D_q(x, y)$ in small intervals.

Lemma 5 (Approximating D_q in small balls)

Consider any given $\lambda < 1$. If $\|x - y\| \leq p_{\min} \lambda / L$ then the following statements hold:

1. We can approximate $p(y)$ by the density at x :

$$p(y)(1 - \lambda) \leq p(x) \leq p(y)(1 + \lambda).$$

2. We can approximate $D_q(x, y)$ by $q(x)\|x - y\|$:

$$(1 - \lambda)^{1/d} q(x)\|x - y\| \leq D_q(x, y) \leq (1 + \lambda)^{1/d} q(x)\|x - y\|.$$

Proof. Part (1). By the Lipschitz continuity of p for $\|x - y\| \leq \delta$ we have

$$|p(x) - p(y)| \leq L\|x - y\| \leq L\delta.$$

Setting $\delta = \lambda p_{\min} / L$ leads to the result.

Part (2). The previous part can be written as

$$(1 - \lambda)^{1/d} q(x) \leq q(y) \leq (1 + \lambda)^{1/d} q(x).$$

Denote the q -geodesic path between x and y by γ^* and the line segment connecting x to y by l . Using the definition of a q -geodesic path, we can write

$$\begin{aligned} \int_{\gamma^*} q(\gamma^*(t)) |\gamma^*(t)'| dt &\leq \int_l q(l(t)) |l(t)'| dt \leq \\ (1 + \lambda)^{1/d} \int_l q(x) |l(t)'| dt &= (1 + \lambda)^{1/d} q(x) \|x - y\|. \end{aligned}$$

Also,

$$\begin{aligned} \int_{\gamma^*} q(\gamma^*(t)) |\gamma^*(t)'| dt &\geq (1 - \lambda)^{1/d} \int_{\gamma^*} q(x) |\gamma^*(t)'| dt \\ &\geq (1 - \lambda)^{1/d} q(x) \|x - y\|. \end{aligned}$$

□

Now we are going to show how the quantities r_{low} and r_{up} introduced in Definition 2 can be bounded in random unweighted kNN graphs and how they are related to the metric D_q .

To this end, we define the kNN q -radii at vertex x as $R_{q,k}(x) = D_q(x, y)$ and the approximated kNN q -radii at vertex x as $\hat{R}_{q,k}(x) = q(x)\|x - y\|$, where y is the k -nearest neighbor of x . The minimum and maximum values of kNN q -radii are defined as

$$R_{q,k}^{min} = \min_u R_{q,k}(u), \quad R_{q,k}^{max} = \max_u R_{q,k}(u).$$

Accordingly we define $\hat{R}_{q,k}^{min}$ and $\hat{R}_{q,k}^{max}$ for the approximated q -radii.

The following proposition is a direct adaptation of Proposition 31 from von Luxburg et al. (2010).

Proposition 6 (Bounding $R_{p,k}^{min}$ and $R_{p,k}^{max}$)

Given $\lambda < 1/2$ define r_{low} and r_{up} as

$$r_{low} := \left(\frac{k}{(1 + \lambda)n\eta_d} \right)^{1/d}, \quad r_{up} := \left(\frac{k}{(1 - \lambda)n\eta_d} \right)^{1/d}$$

and radius \hat{r}_{low} and \hat{r}_{up} as

$$\hat{r}_{low} = \frac{r_{low}}{(1 + \lambda)^{1/d}}, \quad \hat{r}_{up} = \frac{r_{up}}{(1 - \lambda)^{1/d}}.$$

Assume that $\hat{r}_{up} \leq \lambda p_{\min}^{1+1/d} / L$. Then

$$P\left(R_{p,k}^{min} \leq r_{low}\right) \leq n \exp(-\lambda^2 k / 6)$$

$$P\left(R_{p,k}^{max} \geq r_{up}\right) \leq n \exp(-\lambda^2 k / 6).$$

Proof. Consider a ball B_x with radius $\hat{r}_{low}/q(x)$ around x . Note that $\hat{r}_{low}/q(x) \leq p_{\min} \lambda / L$, so we can bound the density of points in B_x by $(1 + \lambda)p(x)$ using Lemma 5. Denote the probability mass of the ball by $\mu(x)$, which is bounded by

$$\begin{aligned} \mu(x) = \int_{B_x} p(s) ds &\leq (1 + \lambda)p(x) \int_{B_x} ds \\ &= (1 + \lambda) \hat{r}_{low}^d \eta_d =: \mu_{\max}. \end{aligned}$$

Observe that $\hat{R}_{q,k}(x) \leq \hat{r}_{low}$ if and only if there are at least k data points in B_x . Let $Q \sim \text{Binomial}(n, \mu(x))$ and $S \sim \text{Binomial}(n, \mu_{\max})$. By the choice of \hat{r}_{low} we have $E(S) = k/(1 + \lambda)$. It follows that

$$\begin{aligned} P\left(\hat{R}_{q,k}(x) \leq \hat{r}_{low}\right) &= P(Q \geq k) \leq P(S \geq k) \\ &= P\left(S \geq (1 + \lambda)E(S)\right). \end{aligned}$$

Now we apply a concentration inequality for binomial random variables (see Prop. 28 in von Luxburg et al., 2010) and a union bound to get

$$\begin{aligned} P\left(\hat{R}_{q,k}^{min} \leq \hat{r}_{low}\right) &\leq P\left(\exists i : \hat{R}_{q,k}(X_i) \leq \hat{r}_{low}\right) \\ &\leq n \exp\left(\frac{-\lambda^2 k}{3(1 + \lambda)}\right) \\ &\leq n \exp(-\lambda^2 k / 6). \end{aligned}$$

By a similar argument we can prove the analogous statement for $R_{p,k}^{max}$. Finally, Lemma 5 gives

$$\hat{R}_{q,k}^{min} \geq \frac{R_{q,k}^{min}}{(1 + \lambda)^{1/d}}, \quad \hat{R}_{q,k}^{max} \leq \frac{R_{q,k}^{max}}{(1 - \lambda)^{1/d}}.$$

□

The following proposition shows how the sampling parameter ς can be chosen to satisfy the dense sampling

assumption. Note that we decided to choose ς in a form that keeps the statements in Theorem 1 simple, rather than optimizing over the parameter ς to maximize the probability of success.

Lemma 7 (Sampling lemma) *Assume X_1, \dots, X_n are sampled i.i.d. from a probability distribution p and a constant $a < 1$ is given. Set λ as in Theorem 1,*

$$\varsigma := (1 + \lambda)^{1/d} \left(\frac{k^a}{\eta d n} \right)^{1/d},$$

and $e_3(\lambda) := 2^d / (1 - \lambda)^2$. Then with probability at least $1 - e_3 n \exp(-k^a/6)$, for every $x \in \mathcal{X}$ exists a $y \in X_1, \dots, X_n$ such that $D_q(x, y) \leq \varsigma$.

Proof. Define $\varsigma_0 = (1 + \lambda)^{-1/d} \varsigma$. We prove that for every $x \in \mathcal{X}$, there exist a vertex y such that $q(x) \|x - y\| \leq \varsigma_0$. Then using Lemma 5 will give the result.

The proof idea is a generalization of the covering argument in the proof of the sampling lemma in Tenenbaum et al. (2000). We first construct a covering of \mathcal{X} that consists of balls with approximately the same probability mass. The centers of the balls are chosen by an iterative procedure that ensures that no center is contained in any of the balls we have so far. We choose the radius $\varsigma_0/q(x)$ for the ball at point x and call it $B_q(x, \varsigma_0)$. The probability mass of this ball can be bounded by

$$\mathcal{V}(B_q(x, \varsigma_0)) \geq (1 - \lambda) \varsigma_0^d \eta d$$

Note that smaller balls $B_q(u, (1 - \lambda)^{1/d} \varsigma_0/2)$ are all disjoint. To see this, consider two balls $B_q(x, (1 - \lambda)^{1/d} \varsigma_0/2), B_q(y, (1 - \lambda)^{1/d} \varsigma_0/2)$. Observe that

$$\frac{(1 - \lambda)^{1/d} \varsigma_0}{2q(x)} + \frac{(1 - \lambda)^{1/d} \varsigma_0}{2q(y)} \leq \frac{\varsigma_0}{q(x)}.$$

We can bound the total number of balls by

$$S \leq \frac{1}{\mathcal{V}(B_q(x, (1 - \lambda)^{1/d} \varsigma_0/2))} \leq \frac{2^d}{\eta d (1 - \lambda)^2 \varsigma_0^d}.$$

Now we sample points from the underlying space and apply the same concentration inequality as above. We bound the probability that a ball $B_q(u, \varsigma_0)$ does not contain any sample point (“is empty”) by

$$\Pr(\text{Ball } i \text{ is empty}) \leq \exp(-n \varsigma_0^d \eta d / 6).$$

Rewriting and Substituting the value of ς_0 gives

$$\begin{aligned} \Pr(\text{no ball is empty}) &\geq 1 - \sum_i \Pr(B_i \text{ is empty}) \\ &\geq 1 - S \cdot e^{-n \varsigma_0^d \eta d / 6} \geq 1 - \frac{2^d n e^{-k^a/6}}{(1 - \lambda)^2 k^a} \\ &\geq 1 - \frac{2^d n e^{-k^a/6}}{(1 - \lambda)^2} = 1 - e_3 n e^{-k^a/6}. \end{aligned}$$

□

Proof of Theorem 1. Set r_{low} and r_{up} as in Proposition 6. The assumption on λ ensures that $\hat{r}_{up} \leq \lambda p_{\min}^{1+1/d} / L$. It follows from Proposition 6 that the statements about r_{low} and r_{up} in Definition 2 both hold for G_n with probability at least $\mu_1 = 1 - 2n \exp(-\lambda^2 k/6)$. Set ς as in Lemma 7 and define the constant $a < 1 - \log_k(4^d(1 + \lambda)^2)$. By this choice we have $r_{low} > 4\varsigma$. Lemma 7 shows that the sampling assumption holds in G_n for the selected ς with probability at least $\mu_2 = 1 - e_3 n \exp(-k^a/6)$. Together, all these statements about G_n hold with probability at least $\mu := 1 - 3e_3 n \exp(-\lambda^2 k^a/6)$.

Using Proposition 4 completes the first part of the theorem. For the convergence we have

$$e_1 = \frac{r_{low} - 2\varsigma}{r_{up}} = \left(\frac{1 - \lambda}{1 + \lambda} \right)^{1/d} - 2 \left(\frac{1 - \lambda^2}{k^{1-a}} \right)^{1/d}.$$

This shows that $e_1 \rightarrow 1$ as $\lambda \rightarrow 0$ and $k \rightarrow \infty$. For $\lambda \rightarrow 0$ and $k \rightarrow \infty$ we can set a to any constant smaller than 1. Finally it is easy to check that $e_2 \rightarrow 0$ and $\varsigma/r_{low} \rightarrow 0$. □

4. Shortest paths in weighted graphs

In this section we discuss both questions from the Introduction. We also extend our results from the previous section to weighted kNN graphs and ε -graphs.

4.1. Weight assignment problem

Consider a graph based on the i.i.d. sample $X_1, \dots, X_n \in \mathcal{X}$ from the density p . We are given a positive scalar function f which is only a function of the density: $f(x) = \tilde{f}(p(x))$. We want to assign edge weights such that the graph \mathcal{SP} distance converges to the f -distance in \mathcal{X} .

It is well known that the f -length of a curve $\gamma : [a, b] \rightarrow \mathcal{X}$ can be approximated by a Riemann sum over a partition of $[a, b]$ to subintervals $[x_i, x_{i+1}]$:

$$\hat{D}_{f,\gamma} = \sum_i f\left(\frac{\gamma(x_i) + \gamma(x_{i+1})}{2}\right) \|\gamma(x_i) - \gamma(x_{i+1})\|.$$

As the partition gets finer, the approximation $\hat{D}_{f,\gamma}$ converges to $D_{f,\gamma}$ (cf. Chapter 3 of Gamelin, 2007). This suggests using edge weights

$$w_{ij} = \tilde{f}\left(p\left(\frac{X_i + X_j}{2}\right)\right) \|X_i - X_j\|.$$

However the underlying density $p(x)$ is not known in many machine learning applications. Sajama & Orłitsky (2005) already proved that the plug-in approach

using a kernel density estimator $\hat{p}(x)$ for $p(x)$ will lead to the convergence of the \mathcal{SP} distance to f -distance in ε -graphs. Our next result shows how to choose edge weights in kNN graphs without estimating the density. It is a corollary from a theorem that will be presented in Section 4.2.

We use a notational convention to simplify our arguments and hide approximation factors that will eventually go to 1 as the sample size goes to infinity. We say that f is approximately larger than g ($f \succ_{\lambda} g$) if there exists a function $e(\lambda)$ such that $f \geq e(\lambda)g$ and $e(\lambda) \rightarrow 1$ as $n \rightarrow \infty$ and $\lambda \rightarrow 0$. The symbol \preccurlyeq_{λ} is defined similarly. We use the notation $f \approx_{\lambda} g$ if $f \preccurlyeq_{\lambda} g$ and $f \succ_{\lambda} g$.

Corollary 8 (Weight assignment) *Consider the kNN graph based on the i.i.d. sample $X_1, \dots, X_n \in \mathcal{X}$ from the density p . Let f be of the form $f(x) = \tilde{f}(p(x))$ with \tilde{f} increasing. We assume that \tilde{f} is Lipschitz continuous and f is bounded away from 0. Define $r = (k/(n\eta_d))^{1/d}$ and set the edge weights*

$$w_{ij} = \|X_i - X_j\| \tilde{f}\left(\frac{r^d}{\|X_i - X_j\|^d}\right). \quad (1)$$

Fix two points $x = X_i$ and $y = X_j$. Choose λ and a as in Theorem 9. Then with probability at least $1 - 3e_3 n \exp(-\lambda^2 k^a/6)$ we have $D_{sp}(x, y) \approx_{\lambda} D_f(x, y)$.

4.2. Limit distance problem

Consider a weighted graph based on the i.i.d. sample $X_1, \dots, X_n \in \mathcal{X}$ from the density p . We are given an increasing edge weight function $h : \mathbb{R}^+ \rightarrow \mathbb{R}^+$ which assigns weight $h(\|x - y\|)$ to the edge (x, y) . We are interested in finding the limit of the graph \mathcal{SP} distance with respect to edge weight function h as the sample size goes to infinity. In particular we are looking for a distance function f such that the \mathcal{SP} distance converges to the f -distance.

Assume we knew the solution $f^* = \tilde{f}^*(p(x))$ of this problem. To guarantee the convergence of the distances, f^* should assign weights of the form of $w_{ij} \approx \tilde{f}^*(p(X_i))\|X_i - X_j\|$. This would mean

$$\tilde{f}^*(p(X_i)) \approx \frac{h(\|X_i - X_j\|)}{\|X_i - X_j\|},$$

which shows that determining \tilde{f}^* is closely related to finding a density based estimation for $\|X_i - X_j\|$.

Depending on h , we distinguish two regimes for this problem: subadditive and superadditive.

4.2.1. SUBADDITIVE WEIGHTS

A function $h(x)$ is called subadditive if $\forall x, y \geq 0 : h(x) + h(y) \geq h(x+y)$. Common examples of subadditive functions are $f(x) = x^a$, $a < 1$ and $f(x) = xe^{-x}$. For a subadditive h , the \mathcal{SP} in the graph will satisfy the triangle inequality and it will prefer jumping along distant vertices. Based on this intuition, we come up with the following guess for vertices along the \mathcal{SP} : For ε -graphs we have the approximation $\|X_i - X_j\| \approx \varepsilon$ and $f(x) = h(\varepsilon)/\varepsilon$. For kNN-graphs we have $\|X_i - X_j\| \approx r/q(X_i)$ with $r = (k/(n\eta_d))^{1/d}$ and

$$f(x) = h\left(\frac{r}{q(x)}\right) \frac{q(x)}{r}, \quad \tilde{f}(x) = h\left(\frac{r}{x^{1/d}}\right) \frac{x^{1/d}}{r}.$$

We formally prove this statement for kNN graphs in the next theorem. In contrast to Theorem 1, the scaling factor is moved into f . The proof for ε -graphs is much simpler and can be adapted by setting $r = \varepsilon$, $q(x) = 1$, and $r_{low} = r_{up} = \varepsilon$.

Theorem 9 (Limit of \mathcal{SP} in weighted graphs)

Consider the kNN graph based on the i.i.d. sample $X_1, \dots, X_n \in \mathcal{X}$ from the density p . Let h be an increasing, Lipschitz continuous and subadditive function, and define the edge weights $w_{ij} = h(\|X_i - X_j\|)$. Fix two points $x = X_i$ and $y = X_j$. Define $r = (k/(n\eta_d))^{1/d}$ and set

$$f(x) = h\left(\frac{r}{q(x)}\right) \frac{q(x)}{r}.$$

Choose λ and a such that

$$\lambda \geq \frac{4L}{\eta_d^{1/d} p_{\min}^{1+1/d}} \left(\frac{k}{n}\right)^{1/d}, \quad a < 1 - \log_k \left(4^d(1+\lambda)^2\right).$$

Then with probability at least $1 - 3e_3 n \exp(-\lambda^2 k^a/6)$ we have $D_{sp}(x, y) \approx_{\lambda} D_f(x, y)$.

Proof. The essence of the proof is similar to the one in Theorem 1, we present a sketch only. The main step is to adapt Proposition 4 to weighted graphs with weight function h . Adapting Lemma 5 for general f is straightforward. The lemma states that $D_f(x, y) \approx_{\lambda} f(x)\|x - y\|$ for nearby points. We set r_{low} and ς as in the sampling lemma and Proposition 6 (these are properties of kNN graphs and hold for any f). Proposition 6 says that in kNN graphs, x is connected to y with high probability iff $\|x - y\| \preccurlyeq_{\lambda} r/q(x)$. The probabilistic argument and the criteria on choosing λ are similar to Theorem 1.

First we show that $D_{sp}(x, y) \preccurlyeq_{\lambda} D_f(x, y)$. Consider the f -geodesic path $\gamma_{x,y}^*$ connecting x to y . Divide $\gamma_{x,y}^*$ into segments $u_0 = x, u_1, \dots, u_t, u_{t+1} = y$ such that $D_q(u_i, u_{i+1}) = r_{low} - 2\varsigma$ for $i = 0, \dots, t-1$

and $D_q(u_t, u_{t+1}) \leq r_{low} - 2\zeta$ (see Figure 3). There exists a vertex v_i near to u_i such that v_i and v_{i+1} are connected. We show that the length of the path x, v_1, \dots, v_t, y is approximately smaller than $D_f(x, y)$. From the path construction we have

$$\|v_i - v_{i+1}\| \approx_\lambda \|u_i - u_{i+1}\| \approx_\lambda r/q(u_i).$$

By summing up along the path we get

$$\begin{aligned} D_{sp}(x, y) &\leq \sum_i h(\|v_i - v_{i+1}\|) \\ &\approx_\lambda \sum_i h(\|u_i - u_{i+1}\|) \approx_\lambda \sum_i h\left(\frac{r}{q(u_i)}\right) \\ &= \sum_i f(u_i) \frac{r}{q(u_i)} \approx_\lambda \sum_i f(u_i) \|u_i - u_{i+1}\| \end{aligned}$$

From the adaptation of Lemma 5 we have $D_f(u_i, u_{i+1}) \approx_\lambda f(u_i) \|u_i - u_{i+1}\|$, which gives

$$\sum_i f(u_i) \|u_i - u_{i+1}\| \approx_\lambda \sum_i D_f(u_i, u_{i+1}) = D_f(x, y).$$

This shows that $D_{sp}(x, y) \preccurlyeq_\lambda D_f(x, y)$.

For the other way round, we use a technique different from Proposition 4. Denote the graph shortest path between x and y by $\pi : z_0 = x, z_1, \dots, z_s, z_{s+1} = y$. Consider π' as a continuous path in \mathcal{X} corresponding to π . As in the previous part, divide π' into segments $u_0 = x, u_1, \dots, u_t, u_{t+1} = y$ (see Figure 3). From $D_q(z_i, z_{i+1}) \preccurlyeq_\lambda r$ and $D_q(u_i, u_{i+1}) \approx_\lambda r$ we have $s \succcurlyeq_\lambda t$. Using this and the subadditivity of h we get

$$D_{sp}(x, y) = \sum_i h(\|z_i - z_{i+1}\|) \succcurlyeq_\lambda \sum_i h(\|u_i - u_{i+1}\|).$$

To prove $D_{sp}(x, y) \succcurlyeq_\lambda D_f(x, y)$, we can write

$$\begin{aligned} \sum_i h(\|u_i - u_{i+1}\|) &\approx_\lambda \sum_i h\left(\frac{r}{q(u_i)}\right) = \sum_i \frac{f(u_i)r}{q(u_i)} \\ &\approx_\lambda \sum_i f(u_i) \|u_i - u_{i+1}\| \\ &\approx_\lambda \sum_i D_f(u_i, u_{i+1}) \geq D_f(x, y). \end{aligned}$$

□

The **proof of Theorem 8** is a direct consequence of this theorem. It follows by choosing $h(t) = t\tilde{f}(r^d/t^d)$ (which is subadditive if \tilde{f} is increasing) and setting $w_{ij} = h(\|X_i - X_j\|)$.

4.2.2. SUPERADDITIVE WEIGHTS

A function h is called superadditive if $\forall x, y \geq 0 : h(x) + h(y) \leq h(x+y)$. Examples are $f(x) = x^a; a > 1$ and $f(x) = xe^x$. To get an intuition on the behavior of the \mathcal{SP} for a superadditive h , take an example of three vertices x, y, z which are all connected in the graph and sit on a straight line such that $\|x - y\| + \|y - z\| = \|x - z\|$. By the superadditivity, the \mathcal{SP} between x and z will prefer going through y rather than directly jumping to z . More generally, the graph \mathcal{SP} will prefer taking many “small” edges

rather than fewer “long” edges. For this reason, we do not expect a big difference between superadditive weighted kNN graphs and ε -graphs: the long edges in the kNN graph will not be used anyway. However, due to technical problems we did not manage to prove a formal theorem to this effect.

The special case of the superadditive family $h(x) = x^a, a > 1$ is treated in Hwang et al. (2012) by completely different methods. Although their results are presented for complete graphs, we believe that it can be extended to ε and kNN graphs. We are not aware of any other result for the limit of \mathcal{SP} distance in the superadditive regime.

5. Consequences in applications

In this section we study the consequences of our results on manifold embedding using Isomap and on a particular semi-supervised learning method.

There are two cases where we do not expect a drastic difference between the \mathcal{SP} in weighted and unweighted kNN graph: (1) If the underlying density p is close to uniform. (2) If the intrinsic dimensionality of our data d is high. The latter is because in the q -distance, the underlying density arises in the form of $p(x)^{1/d}$, where the exponent flattens the distribution for large d .

5.1. Isomap

Isomap is a widely used method for low dimensional manifold embedding (Tenenbaum et al., 2000). The main idea is to use metric multidimensional scaling on the matrix of pairwise geodesic distances. Using the Euclidean length of edges as their weights will lead to the convergence of the \mathcal{SP} distance to the geodesic distance. But what would be the effect of applying Isomap to unweighted graphs?

Our results of the last section already hint that there is no big difference between unweighted and weighted ε -graphs for Isomap. However, the case of kNN graphs is different because weighted and unweighted shortest paths measure different quantities. The effect of applying Isomap to unweighted kNN graphs can easily be demonstrated by the following simulation. We sample 2000 points in \mathbb{R}^2 from a distribution that has two uniform high-density squares, surrounded by a uniform low density region. An unweighted kNN graph is constructed with $k = 10$, and we apply Isomap with target dimension 2. The result is depicted in Figure 2. We can see that the Isomap embedding heavily distorts the original data: it stretches high density regions and compacts low density regions to make the vertex distribution close to uniform.

5.2. Semi-supervised learning

Our work has close relationship to some of the literature on semi-supervised learning (SSL). In regularization based approaches, the underlying density is either exploited implicitly as attempted in Laplacian regularization (Zhu et al., 2003 but see Nadler et al., 2009; Alamgir & von Luxburg, 2011 and Zhou & Belkin, 2011), or more explicitly as in measure based regularization (Bousquet et al., 2004). Alternatively, one defines new distance functions on the data that take the density of the unlabeled points into account. Here, the papers by Sajama & Orlitsky (2005) and Bijral et al. (2011) are most related to our paper. Both papers suggest different ways to approximate the density based distance from the data. In Sajama & Orlitsky (2005) it is achieved by estimating the underlying density while in Bijral et al. (2011), the authors omit the density estimation and use an approximation.

Our work shows a simpler way to converge to a similar distance function for a specific family of f -distances, namely constructing a kNN graph and assigning edge weights as in Equation 1.

6. Conclusions and outlook

We have seen in this paper that the shortest path distance on unweighted kNN graphs has a very funny limit behavior: it prefers to go through regions of low density and even takes large detours in order to avoid the high density regions. In hindsight, this result seems obvious, but most people are surprised when they first hear about it. In particular, we believe that it is important to spread this insight among machine learning practitioners, who routinely use unweighted kNN-graphs as a simple, robust alternative to ε -graphs.

In some sense, unweighted ε -graphs and unweighted kNN graphs behave as “duals” of each other: while degrees in ε -graphs reflect the underlying density, they are independent of the density in kNN graphs. While the shortest path in ε -graphs is independent of the underlying density and converges to the Euclidean distance, the shortest paths in kNN graphs take the density into account.

Current practice is to use ε and kNN graphs more or less interchangeably in many applications, and the decision for one or the other graph is largely driven by robustness or convenience considerations. However, as our results show it is important to be aware of the implicit consequences of this choice. Each graph carries different information about the underlying density, and depending on how a particular machine learning

algorithm makes use of the graph structures, it might either miss out or benefit from this information.

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