# Local Spectral Clustering of Density Upper Level Sets

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## Abstract

We analyze Personalized PageRank (PPR), a local spectral method for clustering, which extract clusters using locally-biased random walks around a user-specified seed node. In constrast to pervious work, we adopt a traditional statistical learning setup, where we obtain samples from an unknown distribution, and aim to identify connected regions of high-density (density clusters). We prove that PPR, run on a neighborhood graph, extracts sufficiently salient density clusters. We also provide empirical support for our theory.

## 1 Introduction

In this paper, we study the problem of clustering: splitting a given data set into groups that satisfy some notion of within-group similarity and between-group difference. We focus on spectral clustering, a family of powerful nonparametric clustering algorithms. Generally speaking, a spectral algorithm first constructs a geometric graph $G$, where vertices correspond to samples, and edges correspond to proximities between samples. It then learns a feature embedding based on the Laplacian of $G$, and applies a simple clustering technique (like k-means clustering) in the embedded feature space.

When applied to geometric graphs built from a large number of samples, global spectral clustering methods can be computationally cumbersome and insensitive to the local geometry of the underlying distribution [Leskovec et al., 2010, Mahoney et al., 2012]. This has led to recent increased interest in local spectral algorithms, which leverage locally-biased spectra computed using random walks around a user-specified seed node. A popular local clustering algorithm is Personalized PageRank (PPR), first introduced by Haveliwala [2003], and then further developed by [Spielman and Teng, 2011, 2014, Andersen et al., 2006, Mahoney et al., 2012, Zhu et al., 2013], among others.

Local spectral clustering techniques have been practically very successful [Leskovec et al., 2010, Andersen et al., 2012, Gleich and Seshadhri, 2012, Mahoney et al., 2012, Wu et al., 2012], leading many authors to develop supporting theory [Spielman and Teng, 2013, Andersen and Peres, 2009, Gharan and Trevisan, 2012, Zhu et al., 2013] that gives worst-case guarantees on traditional graph-theoretic notions of cluster quality (such as conductance). In this paper, we adopt a more traditional statistical viewpoint, and examine what the output of local clustering on a data set reveals about the underlying density $f$. In particular, we examine the ability of PPR to recover *density clusters* of $f$, defined as the connected components of the upper level set $\{x \in \mathbb{R}^d : f(x) \geq \lambda\}$ for some $\lambda > 0$ (a central object of interest in the statistical clustering literature, dating back to Hartigan [1981]).

**PPR on a neighborhood graph.** We now describe the clustering algorithm that will be our focus for the rest of the paper. Let $X = \{x_1, \ldots, x_n\}$ be a sample drawn i.i.d. from a distribution $\mathbb{P}$ on $\mathbb{R}^d$, with density $f$. For a radius $r > 0$, we define $G_{n,r} = (V, E)$ to be the *r-neighborhood graph* of $X$, an unweighted, undirected graph with vertices $V = X$, and an edge $(x_i, x_j) \in E$ if and only if $\|x_i - x_j\| \leq r$, where $\|\cdot\|$ is the $\ell_2$ norm. We denote by $A \in \mathbb{R}^{n \times n}$ the adjacency matrix, with entries $A_{uv} = 1$ if $(u, v) \in E$ and 0 otherwise. We also denote by $D$ the diagonal degree matrix, with $D_{uu} = \sum_{v \in V} A_{uv}$, and by $I$ the $n \times n$ identity matrix.

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Next, we define the PPR vector $p = p(v, \alpha; G_{n,r})$, based on a seed node $v \in V$ and a teleportation parameter $\alpha \in [0, 1]$, to be the solution of the following linear system:

$$p = \alpha e_v + (1 - \alpha) p W, \tag{1}$$

where $W = (I + D^{-1} A)/2$ is the lazy random walk matrix over $G_{n,r}$ and $e_v$ is the indicator vector for node $v$ (that has a 1 in the $v$th position and 0 elsewhere). For a level $\beta > 0$ and a target volume $\mathrm{vol}_0 > 0$, we define a *$\beta$-sweep cut* of $p = (p_u)_{u \in V}$ as

$$S_\beta := \left\{ u \in V : \frac{p_u}{D_{uu}} > \frac{\beta}{\mathrm{vol}_0} \right\}. \tag{2}$$

We will use the normalized cut metric to determine which sweep cut $S_\beta$ is the best cluster estimate. For a set $S \subseteq V$ with complement $S^c = V \setminus S$, we define $\mathrm{cut}(S; G_{n,r}) := \sum_{u \in S, v \in S^c} A_{uv}$, and $\mathrm{vol}(S; G_{n,r}) := \sum_{u \in S} D_{uu}$. We define the *normalized cut* of $S$ as

$$\Phi(S; G_{n,r}) := \frac{\mathrm{cut}(S; G_{n,r})}{\min\left\{\mathrm{vol}(S; G_{n,r}), \mathrm{vol}(S^c; G_{n,r})\right\}}. \tag{3}$$

Having computed sweep cuts $S_\beta$ over a range $\beta \in (\frac{1}{40}, \frac{1}{11})$[1], we output the cluster estimate $\widehat{C} = S_{\beta^*}$ that has minimum normalized cut. For concreteness, this is summarized in Algorithm 1.

**Algorithm 1** PPR on a neighborhood graph

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Input: data $X = \{x_1, \ldots, x_n\}$, radius $r > 0$, teleportation parameter $\alpha \in [0,1]$, seed $v \in X$, target stationary volume $\mathrm{vol}_0 > 0$.
Output: cluster $\widehat{C} \subseteq V$.
Form the neighborhood graph $G_{n,r}$.
Compute the PPR vector $p = p(v, \alpha; G_{n,r})$ as in (1).
For $\beta \in (\frac{1}{40}, \frac{1}{11})$ compute sweep cuts $S_\beta$ as in (2).
Return as a cluster $\widehat{C} = S_{\beta^*}$, where
    $\beta^* = \operatorname*{arg\,min}_{\beta \in (\frac{1}{40}, \frac{1}{11})} \Phi(S_\beta; G_{n,r})$.
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**Estimation of density clusters** Let $\mathbb{C}_f(\lambda)$ denote the connected components of the density upper level set $\{x \in \mathbb{R}^d : f(x) > \lambda\}$. For a given density cluster $\mathcal{C} \in \mathbb{C}_f(\lambda)$, we call $\mathcal{C}[X] = \mathcal{C} \cap X$ the *empirical density cluster*. The size of the symmetric set difference between estimated and empirical clusters is a commonly used metric to quantify cluster estimation error [Korostelev and Tsybakov, 1993, Polonik, 1995, Rigollet and Vert, 2009].

**Definition 1** (Symmetric set difference)**.** *For an estimator $\widehat{C} \subseteq X$ and set $\mathcal{S} \subseteq \mathbb{R}^d$, we define*

$$\Delta(\widehat{C}, \mathcal{S}) := |\widehat{C} \setminus \mathcal{S}[X] \cup \mathcal{S}[X] \setminus \widehat{C}|, \tag{4}$$

*the cardinality of the symmetric set difference between $\widehat{C}$ and $\mathcal{S} \cap X = \mathcal{S}[X]$.*

Note that this symmetric set difference metric does not account for the distance points in $\widehat{C} \setminus \mathcal{S}[X]$ may be from $\mathcal{S}$ [Singh et al., 2009]. Hence in this paper, in addition to the symmetric set difference metric, we also study a second asymptotic notion for the quality of a cluster estimator introduced by Hartigan [1981].

**Definition 2** (Consistent density cluster estimation)**.** *For an estimator $\widehat{C} \subseteq X$ and cluster $\mathcal{C} \in \mathbb{C}_f(\lambda)$, we say $\widehat{C}$ is a consistent estimator of $\mathcal{C}$ if for all $\mathcal{C}' \in \mathbb{C}_f(\lambda)$ with $\mathcal{C} \neq \mathcal{C}'$, the following holds as $n \to \infty$:*

$$\mathcal{C}[X] \subseteq \widehat{C} \quad \textit{and} \quad \widehat{C} \cap \mathcal{C}'[X] = \emptyset, \tag{5}$$

*with probability tending to 1.*

[1] The choice of a specific range such as $(\frac{1}{40}, \frac{1}{11})$ is standard in the analysis of PPR algorithms, see, e.g., [Zhu et al., 2013].

**Summary of results.** A summary of our results (and outline for this paper) is as follows.

1. In Section 2, we introduce a set of natural geometric conditions on the density cluster $\mathcal{C}$ and show that when Algorithm 1 is properly initialized, the size of the symmetric set difference of $\widehat{C}$ and a thickened version of the density cluster $\mathcal{C}_\sigma$ can be bounded in a meaningful way.
2. We further show in Section 2 that if the density cluster $\mathcal{C}$ is particularly well-conditioned, Algorithm 1 will consistently estimate a density cluster in the sense of (5).
3. In Section 3, we detail some of the analysis required to prove our main results, and expose the parts various geometric quantities play in the difficulty of the clustering problem.
4. In Section 4, we empirically investigate the tightness of our analysis, and provide examples showing how violations of our geometric conditions impact density cluster recovery by PPR.

Our main takeaway: PPR, run on a neighborhood graph, recovers geometrically compact high-density clusters.

**Related work.** In addition to the background on local spectral clustering given previously, a few related lines of work are worth highlighting. [Shi et al., 2009, Schiebinger et al., 2015] examine the consistency of spectral algorithms in recovering the latent labels in certain nonparametric mixture models. Their results focus on global rather than local methods, and thus impose global rather than local conditions on the nature of the density. Moreover, they do not in general guarantee recovery of density clusters, which is the focus in our work. Perhaps most importantly, these works rely on general cluster saliency conditions, which implicitly depend on many distinct geometric aspects of the cluster $\mathcal{C}$ under consideration. We make this dependence more explicit, and in doing so expose the role each geometric condition plays in the clustering problem.

More broadly, density clustering and level set estimation is a well-studied problem. Polonik [1995], Rigollet and Vert [2009] study density clustering under symmetric set difference, Tsybakov [1997], Singh et al. [2009] exhibit minimax optimal level set estimators under Hausdorff loss and Hartigan [1981], Chaudhuri and Dasgupta [2010] consider consistent estimation of the cluster tree, to note but a few works in the area. Our goal is not to improve on these results, nor to offer a new algorithm for level set estimation; indeed, seen as a density clustering algorithm, PPR has none of the optimality guarantees of the methods in the aforementioned works. Rather, our motivation is start with a popular and flexible local spectral algorithm, PPR, and to better understand and characterize the distinctions between those density clusters which are well-conditioned for PPR, and those which are not.

## 2 Estimation of well-conditioned density clusters

We formalize some geometric conditions, before using these to define a condition number $\kappa(\mathcal{C})$ which measures the difficulty PPR will have in estimating $\mathcal{C}$. We motivate this measure, and the underlying geometric conditions, by giving density cluster estimation guarantees for Algorithm 1 in terms of $\kappa(\mathcal{C})$.

**Geometric conditions on density clusters** As mentioned previously, successful recovery of a density cluster by PPR requires the density cluster to be geometrically well-conditioned. At a minimum, we wish to avoid sets $\mathcal{C}$ which contain arbitrarily thin bridges or spikes, and therefore as in Chaudhuri and Dasgupta [2010] we introduce a buffer zone around $\mathcal{C}$. Let $B(x, r)$ be the closed ball of radius $r > 0$ centered at $x \in \mathbb{R}^d$. For $\lambda > 0$, consider a given cluster $\mathcal{C} \in \mathbb{C}_f(\lambda)$. We denote the distance between $x$ and $\mathcal{C}$ as $\mathrm{dist}(x, \mathcal{C}) := \inf_{y \in \mathcal{C}} \|y - x\|$, and for a given $\sigma > 0$, we refer to $\mathcal{C}_\sigma := \left\{x \in \mathbb{R}^d : \mathrm{dist}(x, \mathcal{C}) \leq \sigma\right\}$ as the $\sigma$-expansion of $\mathcal{C}$. We now state our conditions with respect to $\mathcal{C}_\sigma$.

(A1) *Bounded density within cluster:* There exist constants $\lambda_\sigma, \Lambda_\sigma$ such that $0 < \lambda_\sigma = \inf_{x \in \mathcal{C}_\sigma} f(x) \leq \sup_{x \in \mathcal{C}_\sigma} f(x) \leq \Lambda_\sigma < \infty$.

(A2) *Cluster separation:* For all $\mathcal{C}' \in \mathbb{C}_f(\lambda)$ with $\mathcal{C}' \neq \mathcal{C}$, $\mathrm{dist}(\mathcal{C}_\sigma, \mathcal{C}'_\sigma) > \sigma$, where $\mathrm{dist}(\mathcal{C}_\sigma, \mathcal{C}'_\sigma) := \inf_{x \in \mathcal{C}_\sigma} \mathrm{dist}(x, \mathcal{C}'_\sigma)$.

(A3) *Low noise density:* There exists $\gamma, c_0 > 0$ such that for all $x \in \mathbb{R}^d$ with $0 < \mathrm{dist}(x, \mathcal{C}_\sigma) \leq \sigma$,

$$\inf_{x' \in \mathcal{C}_\sigma} f(x') - f(x) \geq c_0 \mathrm{dist}(x, \mathcal{C}_\sigma)^\gamma.$$

(A4) *Lipschitz embedding:* There exists $g : \mathbb{R}^d \to \mathbb{R}^d$ which has the following properties: i) there exists a convex set $\mathcal{K} \subseteq \mathbb{R}^d$ with $\mathrm{diam}(\mathcal{K}) = \sup_{x,y \in \mathcal{K}} \|x - y\| =: \rho < \infty$, such that $\mathcal{C}_\sigma = g(\mathcal{K})$, ii) $\det(\nabla g(x)) = 1$ for all $x \in \mathcal{C}_\sigma$, where $\nabla g(x)$ is the Jacobian of $g$ evaluated at $x$, and iii) for some $L \geq 1$,

$$\frac{1}{L} \|x - y\| \leq \|g(x) - g(y)\| \leq L \|x - y\| \text{ for all } x, y \in \mathcal{K}.$$

Simply put, $\mathcal{C}_\sigma$ is the image of a convex set with finite diameter, under a measure preserving, biLipschitz transformation.

(A5) *Bounded volume:* Let the neighborhood graph radius $0 < r \leq \sigma/2d$ be such that

$$2 \int_{\mathcal{C}_\sigma} \mathbb{P}(B(x,r)) f(x) dx \leq \int_{\mathbb{R}^d} \mathbb{P}(B(x,r)) f(x) dx$$

To motivate these conditions, for an arbitrary graph $G = (V, E)$ and subset of vertices $S \subseteq V$, consider the normalized cut $\Phi(S; G)$ (defined as in (3)), as well as the mixing time of a random walk over the induced subgraph $G[S]$ (defined in Section 3 by (16), and denoted by $\tau_\infty(G[S])$). In Zhu et al. [2013], it is shown that for a constant $c > 0$, the PPR estimate $\widehat{C}$ of $S$ satisfies

$$\mathrm{vol}(\widehat{C} \setminus S; G) + \mathrm{vol}(S \setminus \widehat{C}; G) \leq c\big(\Phi(S, G) \cdot \tau_\infty(G[S])\big) \mathrm{vol}(S; G) \tag{6}$$

where the left hand side resembles a (degree-weighted) form of the symmetric set difference of (4).

As we will formally show in Section 3, the conditions (A1)-(A5) allow us to upper bound the normalized cut $\Phi(\mathcal{C}_\sigma[X]; G_{n,r})$, and the mixing time $\tau_\infty(G_{n,r}[\mathcal{C}_\sigma[X]])$. Intuitively, the low noise (A2) and cluster separation (A3) assumptions yield an upper bound on $\mathrm{cut}(\mathcal{C}_\sigma[X]; G_{n,r})$, the lower bound on density in (A1) yields a lower bound on $\mathrm{vol}(\mathcal{C}_\sigma[X]; G_{n,r})$, and along with (A5), which ensures $\mathrm{vol}(\mathcal{C}_\sigma[X]; G_{n,r}) \leq \mathrm{vol}(\mathcal{C}_\sigma[X]^c; G_{n,r})$, these imply an upper bound on the normalized cut. (A1) and (A4) preclude bottlenecks in the induced subgraph $G_{n,r}[\mathcal{C}_\sigma[X]]$, and combined with the upper bound on diameter in (A4), they yield an upper bound on the mixing time over this subgraph.

**Condition number** We will return to the topic of conditions in Section 3. Now, we define the condition number, $\kappa(\mathcal{C})$, which reflects the difficulty of the local spectral clustering task. Motivated by (6), we will set $\kappa(\mathcal{C})$ to be an upper bound on $\Phi(\mathcal{C}_\sigma[X]; G_{n,r}) \cdot \tau_\infty(G_{n,r}[\mathcal{C}_\sigma[X]])$. The smaller $\kappa(\mathcal{C})$ is, the more success PPR will have in recovering $\mathcal{C}$. Let $\theta := (r, \sigma, \lambda, \lambda_\sigma, \Lambda_\sigma, \gamma, \rho, L)$ contain those geometric parameters detailed in (A1) - (A5).

**Definition 3** (Well-conditioned density clusters)**.** *For $\lambda > 0$ and $\mathcal{C} \in \mathbb{C}_f(\lambda)$, let $\mathcal{C}$ satisfy (A1) - (A5) for some $\theta$. Then, for universal constants $c_1, c_2, c_3 > 0$ to be specified later, we set*

$$\Phi_u(\theta) := c_1 r \frac{d}{\sigma} \frac{\lambda}{\lambda_\sigma} \frac{(\lambda_\sigma - c_0 \frac{r^\gamma}{\gamma+1})}{\lambda_\sigma}, \ \tau_u(\theta) := c_2 \frac{\Lambda_\sigma^4 d^3 \rho^2 L^2}{\lambda_\sigma^4 r^2} \log^2\left(\frac{1}{r}\right) + c_3 \tag{7}$$

*and letting $\kappa(\mathcal{C}) := \Phi_u(\theta) \cdot \tau_u(\theta)$, we call $\mathcal{C}$ a $\kappa$-well-conditioned density cluster.*

We note that $\Phi_u(\theta)$ and $\tau_u(\theta)$ are exactly the upper bounds on $\Phi(\mathcal{C}_\sigma[X]; G_{n,r})$ and $\tau_\infty(G_{n,r}[\mathcal{C}_\sigma[X]])$ that we derive in Section 3.

**Well-initialized algorithm** As is typical in the local clustering literature, our algorithmic results will be stated with respect to specific ranges of each of the user-specified parameters.

In particular, for a well-conditioned density cluster $\mathcal{C}$ (with respect to some $\theta$), we require

$$\begin{aligned} &0 < r \leq \frac{\sigma}{2d}, \alpha \in [1/10, 1/9] \cdot \frac{1}{\tau_u(\theta)}, \\ &v \in \mathcal{C}_\sigma[X]^g, \mathrm{vol}_0 \in [3/4, 5/4] \cdot n(n-1) \int_{\mathcal{C}_\sigma} \mathbb{P}(B(x,r)) f(x) dx \end{aligned} \tag{8}$$

where $\mathcal{C}_\sigma[X]^g \subseteq \mathcal{C}_\sigma[X]$ will be some large subset of $\mathcal{C}_\sigma[X]$. In particular, letting $\mathrm{vol}_{n,r}(S) := \mathrm{vol}(S; G_{n,r})$ for $S \subseteq X$, we have $\mathrm{vol}_{n,r}(\mathcal{C}_\sigma[X]^g) \geq \mathrm{vol}_{n,r}(\mathcal{C}_\sigma[X])/2$.

**Definition 4.** *If the input parameters to Algorithm 1 satisfy* (8) *for some well-conditioned density cluster $\mathcal{C}$, we say the algorithm is* well-initialized.

In practice it is clearly not feasible to set hyperparameters based on the underlying (unknown) density $f$. Typically, one tunes PPR over a range of hyperparameters and optimizes for some criterion such as minimum normalized cut; it is not obvious how this scheme would affect the performance of PPR in the density clustering context.

**Density cluster estimation by** PPR The results of Section 3, along with (6), give an upper bound on the volume of $\widehat{C} \setminus \mathcal{C}_\sigma[X]$ and $\mathcal{C}_\sigma[X] \setminus \widehat{C}$,

$$\mathrm{vol}_{n,r}(\widehat{C} \setminus \mathcal{C}_\sigma[X]) + \mathrm{vol}_{n,r}(\mathcal{C}_\sigma[X] \setminus \widehat{C}) \leq c\kappa(\mathcal{C})\mathrm{vol}_{n,r}(\mathcal{C}_\sigma[X]). \tag{9}$$

To translate (9) into meaningful bounds on the symmetric set difference $\Delta(\mathcal{C}_\sigma[X], \widehat{C})$, we wish to preclude vertices $x \in X$ from having arbitrarily small degree, and so we make some regularity assumptions on $\mathcal{X} := \mathrm{supp}(f)$. Let $\nu$ denote the Lebesgue measure on $\mathbb{R}^d$, and $\nu_d := \nu(B)$ be the measure of the unit ball $B = B(0,1)$.

(A6) *Regular support:* There exists some number $\lambda_{\min} > 0$ such that $\lambda_{\min} < f(x)$ for all $x \in \mathcal{X}$. Additionally, there exists some $c > 0$ such that for each $x \in \partial\mathcal{X}$, $\nu(B(x,r) \cap \mathcal{X}) \geq c\nu_d r^d$.

Note that the latter condition in (A6) will be satisfied if, for instance, the support $\mathcal{X}$ is a $\sigma$-expanded set.

**Theorem 1.** *Fix $\lambda > 0$, let $\mathcal{C} \in \mathbb{C}_f(\lambda)$ be a $\kappa$-well-conditioned density cluster (with respect to some $\theta$), and additionally assume $f$ satisfies (A6). Then, there exists a universal constant $c_4 > 0$ such that with probability tending to* 1 *as $n \to \infty$,*

$$\Delta(\mathcal{C}_\sigma[X], \widehat{C}) \leq c_4 \kappa(\mathcal{C}) \frac{\Lambda_\sigma}{\lambda_{\min}}. \tag{10}$$

The proof of Theorem 1, along with all other proofs in this paper, can be found in the supplementary material. We observe that the symmetric set difference $\Delta(\mathcal{C}_\sigma[X], \widehat{C})$ is proportional to the difficulty of the clustering problem, as measured by the condition number $\kappa(\mathcal{C})$.

Neither (9) nor Theorem 1 imply consistent density cluster estimation in the sense of (5). This notion of consistency requires a uniform bound over $p$: namely, for all $\mathcal{C}' \in \mathbb{C}_f(\lambda), \mathcal{C}' \neq \mathcal{C}$, and each $u \in \mathcal{C}, w \in \mathcal{C}'$,

$$\frac{p_w}{D_{ww}} \leq \frac{1}{40\mathrm{vol}_0} < \frac{1}{11\mathrm{vol}_0} \leq \frac{p_u}{D_{uu}}, \tag{11}$$

so that any sweep cut $S_\beta$ for $\beta\mathrm{vol}_0 \in [1/40, 1/11]$ (i.e. any sweep cut considered by Algorithm 1) will fulfill both conditions laid out in (5). In Theorem 2, we show that a sufficiently small upper bound on $\kappa(\mathcal{C})$ ensures such a gap exists with probability one as $n \to \infty$, and therefore guarantees $\widehat{C}$ will be a consistent estimator. As was the case before, we wish to preclude arbitrarily low degree vertices, this time for points $x \in \mathcal{C}'[X]$.

(A7) *Bounded density:* Letting $\sigma, \lambda_\sigma$ be as in (A1), for each $\mathcal{C}' \in \mathbb{C}_f(\lambda)$ and for all $x \in \mathcal{C}'_\sigma$, $\lambda_\sigma \leq f(x)$.

**Theorem 2.** *Fix $\lambda > 0$, let $\mathcal{C} \in \mathbb{C}_f(\lambda)$ be a $\kappa$-well-conditioned cluster (with respect to some $\theta$), and additionally assume $f$ satisfies (A7). If Algorithm 1 is well-initialized, there exists a universal constant $c_5 > 0$ such that if*

$$\kappa(\mathcal{C}) \leq c_5 \frac{\lambda_\sigma^2 r^d \nu_d}{\Lambda_\sigma \mathbb{P}(\mathcal{C}_\sigma)}, \tag{12}$$

*then the output set $\widehat{C} \subseteq X$ is a consistent estimator for $\mathcal{C}$, in the sense of Definition 2.*

*Remark* 1. We note that the restriction on $\kappa(\mathcal{C})$ imposed by (12) results in a symmetric set difference $\Delta(\mathcal{C}_\sigma[X], \widehat{C})$ on the order of $r^d$. In plain terms, we are able to recover a density cluster $\mathcal{C}$ in the sense of (5) only when we can guarantee a very small fraction of points will be misclassified. This strong condition is the price we pay in order to obtain the uniform bound of (11).

*Remark* 2. While taking the radius of the neighborhood graph $r \to 0$ as $n \to \infty$—and thereby ensuring $G_{n,r}$ is sparse—is computationally attractive, the presence of a factor of $\frac{\log^2(1/r)}{r}$ in $\kappa(\mathcal{C})$ unfortunately prevents us from making claims about the behavior of PPR in this regime. Although the restriction to a kernel function fixed in $n$ is standard for theoretical analysis of spectral clustering Schiebinger et al. [2015], von Luxburg et al. [2008], it is an interesting question whether PPR exhibits some degeneracy over $r$-neighborhood graphs as $r \to 0$, or if this is merely looseness in our upper bounds.

**Approximate** PPR **vector** In practice, exactly solving (1) may be too computationally expensive. To address this limitation, Andersen et al. [2006] introduced the *$\epsilon$-approximate* PPR *vector* (aPPR), which we will denote $p^{(\epsilon)}$. We refer the curious reader to Andersen et al. [2006] for a formal algorithmic definition of the aPPR vector, and limit ourselves to highlighting a few salient points. Namely, the aPPR vector can be computed in order $\mathcal{O}\left(\frac{1}{\epsilon\alpha}\right)$ time, while satisfying the following uniform error bound:

$$\text{for all } u \in V, \quad p(u) - \epsilon D_{uu} \le p^{(\epsilon)}(u) \le p(u). \tag{13}$$

Application of (13) within the proofs of Theorems 1 and 2 leads to analogous results which hold with respect to $p^{(\epsilon)}$. We formally state and prove this fact in the supplementary material.

## 3 Analysis

The primary technical contribution of our work is showing that the geometric conditions (A1) - (A5) translate to meaningful bounds on the normalized cut and mixing time of $\mathcal{C}_\sigma[X]$ in $G_{n,r}$. In doing so, we elaborate on how some of the geometric conditions introduced in Section 2 contribute to the difficulty of the clustering problem.

**Normalized cut** We start with a finite sample upper bound on the normalized cut (3) of $\mathcal{C}_\sigma[X]$. For simplicity, we write $\Phi_{n,r}(\mathcal{C}_\sigma[X]) := \Phi(\mathcal{C}_\sigma[X]; G_{n,r})$.

**Theorem 3.** *Fix $\lambda > 0$, and let $\mathcal{C} \in \mathbb{C}_f(\lambda)$ satisfy Assumptions (A1)-(A3), and (A5) for some $r, \sigma, \lambda_\sigma, c_0, \gamma > 0$ (no bound on maximum density is needed). Then for any $0 < \delta < 1$, $\epsilon > 0$, if*

$$n \ge \frac{(2+\epsilon)^2 \log(3/\delta)}{\epsilon^2} \left(\frac{25}{6\lambda_\sigma^2 \nu(\mathcal{C}_\sigma)\nu_d r^d}\right)^2, \tag{14}$$

*then*

$$\frac{\Phi_{n,r}(\mathcal{C}_\sigma[X])}{r} \le c_1 \frac{d}{\sigma} \frac{\lambda}{\lambda_\sigma} \frac{(\lambda_\sigma - c_0 \frac{r^\gamma}{\gamma+1})}{\lambda_\sigma} + \epsilon, \tag{15}$$

*with probability at least $1 - \delta$ (where $c_1 > 0$ is a universal constant).*

*Remark* 3. Observe that the diameter $\rho$ is absent from Theorem 3, in contrast to the difficulty function $\kappa(\mathcal{C})$, which worsens (increases) as $\rho$ increases. This phenomenon reflects established wisdom regarding spectral partitioning algorithms more generally Guattery and Miller [1995], Hein and Bühler [2010], albeit newly applied to the density clustering setting. It suggests that if the diameter $\rho$ is large, PPR may fail to recover $\mathcal{C}_\sigma[X]$ even when $\mathcal{C}$ is sufficiently well-conditioned to ensure $\mathcal{C}_\sigma[X]$ has a small normalized cut in $G_{n,r}$. This intuition will be supported by simulations in Section 4.

**Inverse mixing time** For $S \subseteq V$, denote by $G[S] = (S, E_S)$ the subgraph induced by $S$ (where the edges are $E_S = E \cap (S \times S)$). Let $W_S$ be the (lazy) random walk matrix over $G[S]$, and write

$$q_v^{(t)}(u) = e_v W_S^t e_u$$

for the $t$-step transition probability of the lazy random walk over $G[S]$ originating at $v \in V$. Also write $\pi = (\pi(u))_{u \in S}$ for the stationary distribution of this random walk. (As $W_S$ is the transition matrix of a lazy random walk, it is well-known that a unique stationary distribution exists and is given by $\pi(u) = (D_S)_{uu}/\mathrm{vol}(S; G[S])$, where $D_S$ is the degree matrix of $G[S]$.)

Then, the *relative pointwise mixing time* of $G[S]$ is

$$\tau_\infty(G[S]) = \min\left\{t : \frac{\pi(u) - q_v^{(t)}(u)}{\pi(u)} \le \frac{1}{4}, \text{ for } u, v \in V\right\}. \tag{16}$$

In the following theorem, we give an asymptotic (in the number of vertices $n$) upper bound on $\tau_\infty(G_{n,r}[\mathcal{C}_\sigma[X]])$.

**Theorem 4.** *Fix $\lambda > 0$, and let $\mathcal{C} \in \mathbb{C}_f(\lambda)$ satisfy Assumptions (A1) and (A4) for some $\sigma, \lambda_\sigma, \Lambda_\sigma, \rho, L > 0$. Then, for any $0 < r < \sigma/2\sqrt{d}$, with probability* 1

$$\limsup_{n \to \infty} \tau_\infty(G_{n,r}[\mathcal{C}_\sigma[X]]) \leq c_2 \frac{\Lambda_\sigma^4 d^3 \rho^2 L^2}{\lambda_\sigma^4 r^2} \log^2\left(\frac{1}{r}\right) + c_3 \tag{17}$$

*for $c_2, c_3 > 0$ universal constants.*

To the best of our knowledge, Theorem 4 is the first bound, albeit asymptotic, on the mixing time of random walks over neighborhood graphs which is independent of $n$, the number of vertices.

*Remark* 4. The embedding assumption (A4) and Lipschitz parameter $L$ play an important role in proving the upper bound of Theorem 4. There is some interdependence between $L$ and other geometric parameters $\sigma$ and $\rho$, which might lead one to hope that (A4) is non-essential. However, it is not possible to eliminate this condition without incurring an additional factor of at least $(\rho/\sigma)^d$ in (17), achieved, for instance, when $\mathcal{C}_\sigma$ is a dumbbell-like set consisting of two balls of diameter $\rho$ linked by a cylinder of radius $\sigma$. [Abbasi-Yadkori et al., 2017, Abbasi-Yadkori, 2016] develop theory regarding biLipschitz deformations of convex sets, wherein it is observed that star-shaped sets as well as half-moon shapes of the type we consider in Section 4 both satisfy (A4) for reasonably small values of $L$.

# 4 Experiments

We provide numerical experiments to investigate the tightness of our bounds on normalized cut and mixing time of $\mathcal{C}_\sigma[X]$, and examine the performance of PPR on the "two moons" dataset. For space reasons, we defer details of the experimental settings to the supplement.

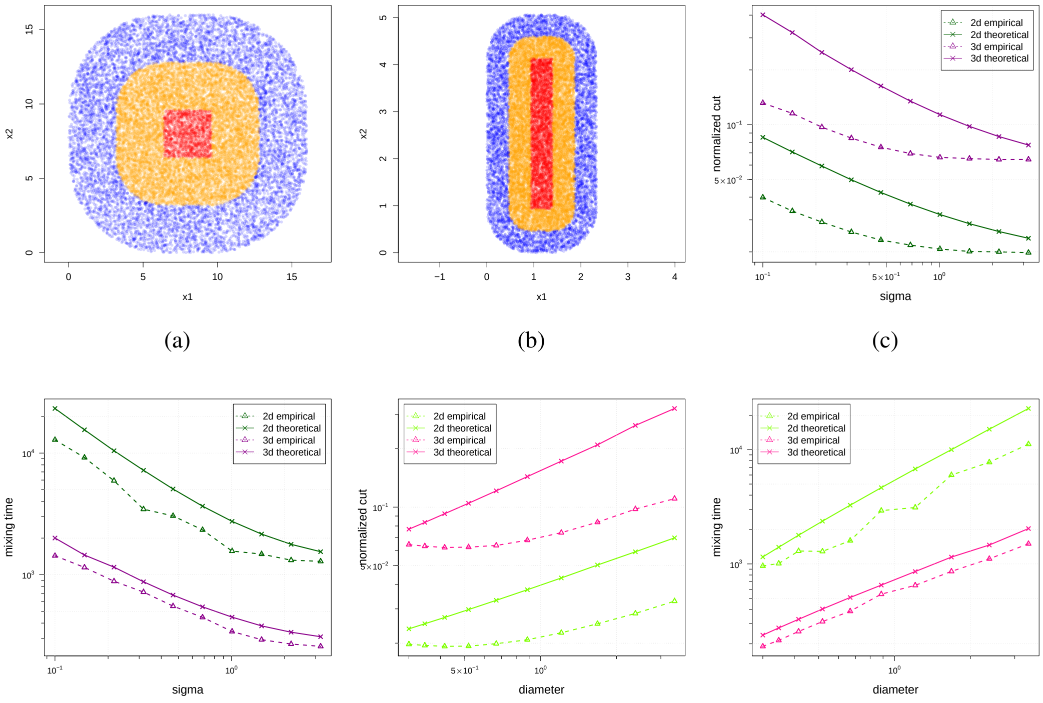
**Validating theoretical bounds** As we do not provide any theoretical lower bounds, we investigate the tightness of Theorems 3 and 4 via simulation. Figure 1 compares these theoretical bounds with the empirical quantities (3) and (16), as we vary the diameter $\rho$ and thickness $\sigma$ of a cluster $\mathcal{C}$. Panels $(a)$ and $(b)$ show the resulting empirical clusters for two different values of $\rho$ and $\sigma$.

Panels $(d)$ and $(f)$ show our theoretical bounds on mixing time tracking closely with empirical mixing time, in both 2 and 3 dimensions.[2] This provides empirical evidence that the upper bound on mixing time given by Theorem 4 has the right dependency on both expansion parameter $\sigma$ and diameter $\rho$. The story in panels $(c)$ and $(e)$ is less obvious. We note that while, broadly speaking, the trends do not appear to match, this gap between theory and empirical results seems largest when $\sigma$ and $\rho$ are approximately equal. As the ratio $\rho/\sigma$ grows, we see the slopes of the empirical curves become more similar to those predicted by theory.

**Empirical behavior of** PPR To drive home the main implications of Theorems 1 and 2, in Figure 2 we show the behavior of PPR, normalized cut, and the density clustering algorithm of [Chaudhuri and Dasgupta, 2010] on the well known "two moons" dataset (with added 2d Gaussian noise), considered a prototypical success story for spectral clustering algorithms. The first column consists of the empirical density clusters $C_n$ and $C_n'$ for a particular threshold $\lambda$ of the density function; the second column shows the cluster recovered by PPR; the third column shows the global minimum normalized cut, computed according to the algorithm of Szlam and Bresson [2010]; and the last column shows a cut of the density cluster tree estimator of [Chaudhuri and Dasgupta, 2010].

Figure 2 shows the degrading ability of PPR to recover density clusters as the two moons become less well-separated. Of particular interest is the fact that PPR fails to recover one of the moons even when normalized cut still succeeds in doing so, supporting our claim from Remark 3. Additionally, we note that a density clustering algorithm recovers a moon even when both PPR and normalized cut fail, lending empirical weight to our overall message that PPR recovers only geometrically well-conditioned density clusters.

[2] Note that we have rescaled all values of theoretical upper bounds by a constant, in order to mask the effect of large universal constants in these bounds. Therefore only comparison of slopes, rather than intercepts, is meaningful.



(a) (b) (c)

(d) (e) (f)

Figure 1: Samples, empirical results, and theoretical bounds for mixing time and normalized cut as diameter and thickness are varied. In (a) and (b), points in $\mathcal{C}$ are colored in red; points in $\mathcal{C}_\sigma \setminus \mathcal{C}$ are colored in yellow; and remaining points in blue.

# 5 Discussion

For given data, there are an almost limitless number of ways to define what the "right" clustering is. We have considered one such notion – density upper level sets – and have detailed a set of natural geometric criteria which, when appropriately satisfied, translate to provable bounds on estimation of the cluster by PPR. We do not, however, provide a theoretical lower bound showing that our geometric conditions are required for successful recovery on an upper level set. Although we investigate the matter empirically, this is a direction for future work.

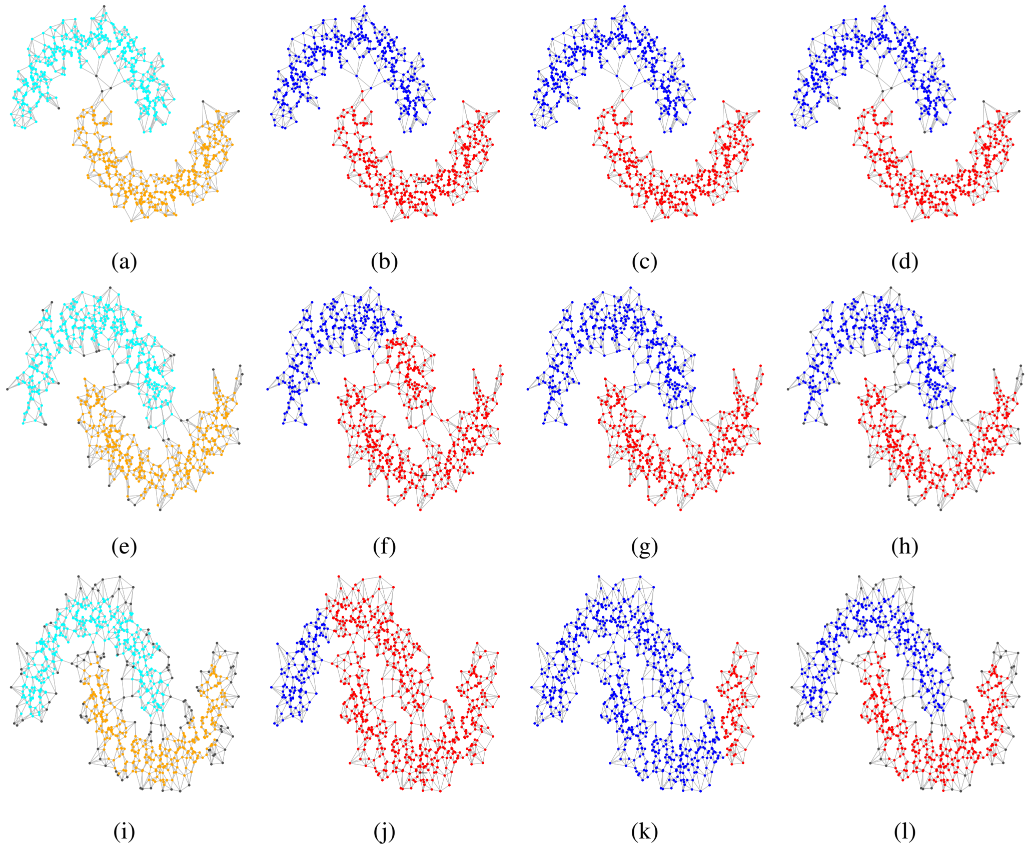


Figure 2: True density (column 1), PPR (column 2), normalized cut (column 3) and estimated density (column 4) clusters for 3 different simulated data sets. Seed node for PPR denoted by a black cross.

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