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# Local Spectral Clustering of Density Upper Level Sets

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## Abstract

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

## 8 1 Introduction

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

15 When applied to geometric graphs built from a large number of samples, global spectral clustering  
16 methods can be computationally cumbersome and insensitive to the local geometry of the underlying  
17 distribution [Leskovec et al., 2010, Mahoney et al., 2012]. This has led to increased interest in local  
18 spectral clustering algorithms, which leverage locally-biased spectra computed using random walks  
19 around some user-specified seed node. A popular local clustering algorithm is Personalized PageRank  
20 (PPR), first introduced by Haveliwala [2003], then further developed by [Spielman and Teng, 2011,  
21 2014, Andersen et al., 2006, Mahoney et al., 2012, Zhu et al., 2013], among others.

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

31 **PPR on a neighborhood graph.** We now describe the clustering algorithm that will be our focus  
32 for the rest of the paper. Let  $X = \{x_1, \dots, x_n\}$  be a sample drawn i.i.d. from a distribution  $\mathbb{P}$  on  
33  $\mathbb{R}^d$ , with density  $f$ . For a radius  $r > 0$ , we define  $G_{n,r} = (V, E)$  to be the  $r$ -neighborhood graph  
34 of  $X$ , an unweighted, undirected graph with vertices  $V = X$ , and an edge  $(x_i, x_j) \in E$  if and only  
35 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  
36 entries  $A_{uv} = 1$  if  $(u, v) \in E$  and 0 otherwise. We also denote by  $D$  the diagonal degree matrix,  
37 with  $D_{uu} = \sum_{v \in V} A_{uv}$ , and by  $I$  the  $n \times n$  identity matrix.

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

$$p = \alpha e_v + (1 - \alpha)pW, \quad (1)$$

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

$$S_\beta := \left\{ u \in V : \frac{p_u}{D_{uu}} > \frac{\beta}{\text{vol}_0} \right\}. \quad (2)$$

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

$$\Phi(S; G_{n,r}) := \frac{\text{cut}(S; G_{n,r})}{\min \{ \text{vol}(S; G_{n,r}), \text{vol}(S^c; G_{n,r}) \}}. \quad (3)$$

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

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**Algorithm 1** PPR on a neighborhood graph

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**Input:** data  $X = \{x_1, \dots, x_n\}$ , radius  $r > 0$ , teleportation parameter  $\alpha \in [0, 1]$ , seed  $v \in X$ , target  
 stationary volume  $\text{vol}_0 > 0$ .

**Output:** cluster  $\hat{C} \subseteq V$ .

- 1: Form the neighborhood graph  $G_{n,r}$ .
- 2: Compute the PPR vector  $p = p(v, \alpha; G_{n,r})$  as in (1).
- 3: For  $\beta \in (\frac{1}{40}, \frac{1}{11})$  compute sweep cuts  $S_\beta$  as in (2).
- 4: Return as a cluster  $\hat{C} = S_{\beta^*}$ , where

$$\beta^* = \arg \min_{\beta \in (\frac{1}{40}, \frac{1}{11})} \Phi(S_\beta; G_{n,r}).$$


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48 **Estimation of density clusters.** Let  $\mathbb{C}_f(\lambda)$  denote the connected components of the density upper  
 49 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  
 50 *empirical density cluster*. The size of the symmetric set difference between estimated and empirical  
 51 clusters is a commonly used metric to quantify cluster estimation error [Korostelev and Tsybakov,  
 52 1993, Polonik, 1995, Rigollet and Vert, 2009].

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

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

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

55 However, the symmetric set difference does not measure whether  $\hat{C}$  can distinguish any two distinct  
 56 clusters  $\mathcal{C}, \mathcal{C}' \in \mathbb{C}_f(\lambda)$ . We therefore also study a second notion of cluster estimation, first introduced  
 57 by Hartigan [1981], and defined asymptotically.

58 **Definition 2** (Consistent density cluster estimation). For an estimator  $\hat{C} \subseteq X$  and cluster  $\mathcal{C} \in \mathbb{C}_f(\lambda)$ ,  
 59 we say  $\hat{C}$  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  
 60  $n \rightarrow \infty$ :

$$\mathcal{C}[X] \subseteq \hat{C} \quad \text{and} \quad \hat{C} \cap \mathcal{C}'[X] = \emptyset, \quad (5)$$

61 with probability tending to 1.

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<sup>1</sup>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].

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

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

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

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

83 More broadly, density clustering and level set estimation is a well-studied problem. Polonik [1995],  
 84 Rigollet and Vert [2009] study density clustering under the symmetric set difference metric, Tsybakov  
 85 [1997], Singh et al. [2009] describe minimax optimal level set estimators under Hausdorff loss and  
 86 Hartigan [1981], Chaudhuri and Dasgupta [2010] consider consistent estimation of the cluster tree, to  
 87 note but a few works. Our goal is not to improve on these results, nor to offer a better algorithm for  
 88 level set estimation; indeed, seen as a density clustering algorithm, PPR has none of the optimality  
 89 guarantees found in the aforementioned works. Instead, our motivation is to start with a widely-used  
 90 local spectral method, PPR, and to better understand and characterize the distinctions between those  
 91 density clusters which are well-conditioned for PPR, and those which are not.

## 92 2 Estimation of well-conditioned density clusters

93 We formalize some geometric conditions, and use these to define a condition number  $\kappa(\mathcal{C})$ , which  
 94 measures the difficulty PPR will have in estimating  $\mathcal{C}$ . (Our theoretical guarantees for PPR will be  
 95 framed in terms of  $\kappa(\mathcal{C})$ .)

96 **Geometric conditions on density clusters.** At a high level, for PPR to be successful, the underly-  
 97 ing density cluster must be geometrically well-conditioned. At a minimum, we want to avoid sets that  
 98 contain arbitrarily thin bridges or spikes. Hence, as in Chaudhuri and Dasgupta [2010], we consider  
 99 a thickened version of  $\mathcal{C} \in \mathbb{C}_f(\lambda)$  defined as  $\mathcal{C}_\sigma := \{x \in \mathbb{R}^d : \text{dist}(x, \mathcal{C}) \leq \sigma\}$ , which we call the  
 100  $\sigma$ -expansion of  $\mathcal{C}$ . Here  $\text{dist}(x, \mathcal{C}) := \inf_{y \in \mathcal{C}} \|y - x\|$ . We now list our conditions on  $\mathcal{C}_\sigma$ .

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

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

105 (A3) *Low noise density:* There exist  $\gamma, c_0 > 0$  such that for  $x \in \mathbb{R}^d$  with  $0 < \text{dist}(x, \mathcal{C}_\sigma) \leq \sigma$ ,  
 106  $\inf_{x' \in \mathcal{C}_\sigma} f(x') - f(x) \geq c_0 \text{dist}(x, \mathcal{C}_\sigma)^\gamma$ .

107 (A4) *Lipschitz embedding:* There exists  $g : \mathbb{R}^d \rightarrow \mathbb{R}^d$  with the following properties: i) we have  
 108  $\mathcal{C}_\sigma = g(\mathcal{K})$ , for a convex set  $\mathcal{K} \subseteq \mathbb{R}^d$  with  $\text{diam}(\mathcal{K}) = \sup_{x, y \in \mathcal{K}} \|x - y\| =: \rho < \infty$ ; ii)

109  $\det(\nabla g(x)) = 1$  for all  $x \in \mathcal{C}_\sigma$ , where  $\nabla g(x)$  is the Jacobian of  $g$  evaluated at  $x$ ; and iii)  
 110 for some  $L \geq 1$ ,

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

111 Succinctly,  $\mathcal{C}_\sigma$  is the image of a convex set with finite diameter under a measure preserving,  
 112 bi-Lipschitz transformation.

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

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

114 where  $B(x, r)$  is the closed ball of radius  $r$  at  $x$ .

115 To motivate these conditions, Zhu et al. [2013] show for arbitrary graph  $G = (V, E)$  and subset of  
 116 vertices  $S \subseteq V$ , the PPR estimate  $\hat{C}$  of subset  $S$  satisfies, for a constant  $c > 0$ ,

$$\text{vol}(\hat{C} \setminus S; G) + \text{vol}(S \setminus \hat{C}; G) \leq c(\Phi(S, G) \cdot \tau_\infty(G[S])) \text{vol}(S; G), \quad (6)$$

117 where  $\Phi(S; G)$  is the normalized cut of  $S$  (as defined in (3)), and  $\tau_\infty(G[S])$  is called the *mixing*  
 118 *time* of a random walk over the induced subgraph  $G[S]$  (to be defined precisely later, in (16)). The  
 119 left-hand side in (6) resembles a (degree-weighted) form of the symmetric set difference metric in  
 120 (4). As we will show in Section 3, the conditions (A1)–(A5) allow us to upper bound the normalized  
 121 cut  $\Phi(\mathcal{C}_\sigma[X]; G_{n,r})$ , and the mixing time  $\tau_\infty(G_{n,r}[\mathcal{C}_\sigma[X]])$ .<sup>2</sup>

122 **Condition number.** Motivated by (6), we will define  $\kappa(\mathcal{C})$  to be an upper bound on the product  
 123  $\Phi(\mathcal{C}_\sigma[X]; G_{n,r}) \cdot \tau_\infty(G_{n,r}[\mathcal{C}_\sigma[X]])$ . The smaller  $\kappa(\mathcal{C})$  is, the more success PPR will have in recover-  
 124 ing  $\mathcal{C}$ . Let  $\theta := (r, \sigma, \lambda, \lambda_\sigma, \Lambda_\sigma, \gamma, \rho, L)$  contain the geometric parameters from (A1)–(A5).

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

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

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

128 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  $\tau_\infty(G_{n,r}[\mathcal{C}_\sigma[X]])$   
 129 that we derive in our analysis later, in Section 3.

130 **Well-initialized algorithm.** As is typical in the local clustering literature, our algorithmic results  
 131 will be stated with respect to specific ranges of each of the user-specified parameters. In particular,  
 132 for a well-conditioned density cluster  $\mathcal{C}$  (with respect to some  $\theta$ ), we require

$$0 < r \leq \frac{\sigma}{2d}, \quad \alpha \in [1/10, 1/9] \cdot \frac{1}{\tau_u(\theta)}, \quad (8)$$

$$v \in \mathcal{C}_\sigma[X]^g, \quad \text{vol}_0 \in [3/4, 5/4] \cdot n(n-1) \int_{\mathcal{C}_\sigma} \mathbb{P}(B(x, r)) f(x) dx,$$

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

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

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

<sup>2</sup>Informally, assumptions (A2), (A3) yield an upper bound on  $\text{cut}(\mathcal{C}_\sigma[X]; G_{n,r})$ , and (A1) yields a lower bound on  $\text{vol}(\mathcal{C}_\sigma[X]; G_{n,r})$ ; together with (A5), this gives an upper bound on the normalized cut. On the other hand, (A1), (A4) preclude bottlenecks in the induced subgraph  $G_{n,r}[\mathcal{C}_\sigma[X]]$ , and combined with the upper bound on diameter in (A4), this leads to an upper bound on the mixing time over this subgraph.

141 **Main theorems.** The results of Section 3, combined with (6), give an upper bound on the volume  
 142 of  $\widehat{C} \setminus \mathcal{C}_\sigma[X]$  and  $\mathcal{C}_\sigma[X] \setminus \widehat{C}$ ,

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

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

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

149 Note that the latter condition in (A6) will hold if the boundary  $\partial\mathcal{X}$  is sufficiently regular. Now we  
 150 present our main bound on the symmetric set difference metric.

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

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

154 The proof of Theorem 1, along with all other proofs in this paper, is deferred to the supplementary  
 155 material. Note that this result says the symmetric set difference metric  $\Delta(\mathcal{C}_\sigma[X], \widehat{C})$  is proportional  
 156 to the difficulty of the clustering problem, as measured by the condition number  $\kappa(\mathcal{C})$ .

157 Neither (9) nor (10) imply consistent density cluster estimation in the sense of (5). This notion of  
 158 consistency requires a uniform bound over  $p$ : for all  $\mathcal{C}' \in \mathbb{C}_f(\lambda)$ ,  $\mathcal{C}' \neq \mathcal{C}$ , and each  $u \in \mathcal{C}$ ,  $w \in \mathcal{C}'$ ,  
 159

$$\frac{p_w}{D_{ww}} \leq \frac{1}{40\text{vol}_0} < \frac{1}{11\text{vol}_0} \leq \frac{p_u}{D_{uu}}, \quad (11)$$

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

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

167 Next we give our main result on consistent cluster recovery by PPR.

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

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

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

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

176 *Remark 2.* While taking the radius of the neighborhood graph  $r \rightarrow 0$  as  $n \rightarrow \infty$  (thereby ensuring  
 177  $G_{n,r}$  is sparse) is computationally attractive, the presence of a factor of  $\log^2(1/r)/r$  in  $\kappa(\mathcal{C})$  unfor-  
 178 tunately prevents us from making claims about the behavior of PPR in this regime. Although the  
 179 restriction to a kernel function fixed in  $n$  is standard for spectral clustering theory [Schiebinger et al.,  
 180 2015, von Luxburg et al., 2008], it is an interesting question whether PPR exhibits some degeneracy  
 181 over  $r$ -neighborhood graphs as  $r \rightarrow 0$ , or if this is merely looseness in our upper bounds.

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

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

188 Application of (13) within the proofs of Theorems 1 and 2 leads to analogous results which hold for  
 189  $p^{(\epsilon)}$ . We formally state and prove this in the supplement.

### 190 3 Analysis

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

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

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

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

199 then

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

200 with probability at least  $1 - \delta$ , where  $c_1 > 0$  is a universal constant.

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

**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

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

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

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

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

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

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

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

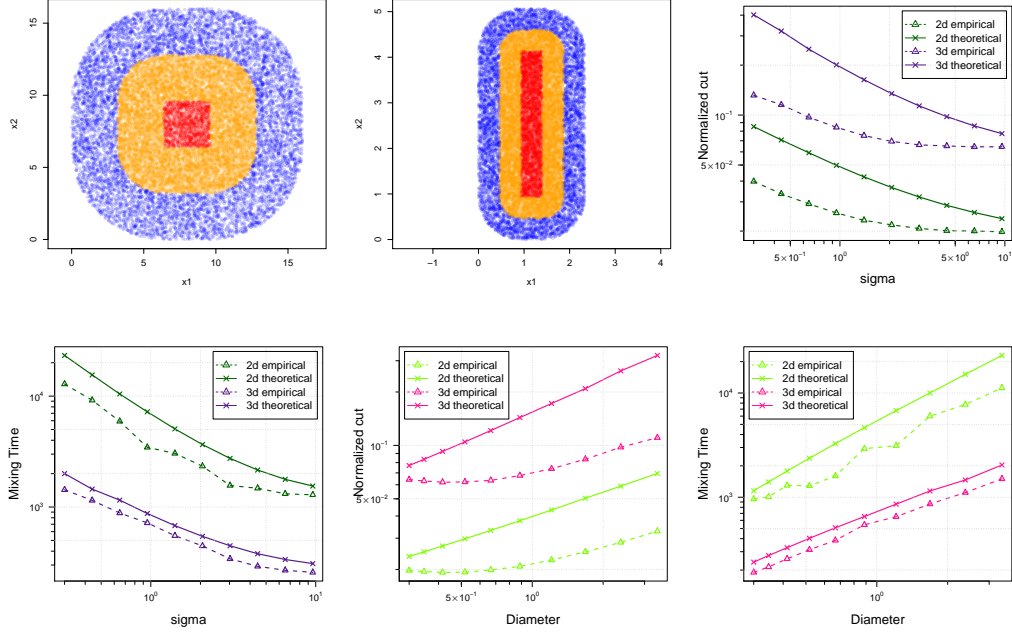


Figure 1: Top left and top middle: samples from a geometrically well- and poor-conditioned cluster. The points in  $C$  are colored in red, points in  $C_\sigma \setminus C$  are colored in yellow, and the remaining points in blue. Other panels: empirical normalized cut and mixing time, as a function of  $\sigma$  or  $\rho$ , versus their theoretical upper bounds.

216 The proof of Theorem 4 relies heavily on analogous mixing time bounds developed for the mixing  
 217 time of a continuous-space “ball walk” over convex sets. To the best of our knowledge, our result is  
 218 the first bound, albeit asymptotic, on the mixing time of random walks over neighborhood graphs  
 219 that is independent of  $n$ , the number of vertices.

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

## 228 4 Experiments

229 We provide numerical experiments to investigate the tightness of our bounds on the normalized cut  
 230 and mixing time of  $C_\sigma[X]$ , and examine the performance of PPR on the “two moons” dataset. For  
 231 space reasons, we defer details of the experimental settings to the supplement.

232 **Validating theoretical bounds.** We investigate the tightness of Theorems 3 and 4 via simulation.  
 233 Figure 1 compares our upper bounds with the actual empirically-computed quantities (3) and (16), as  
 234 we vary the diameter  $\rho$  and thickness  $\sigma$  of a cluster  $C$ . The top left and top middle panels display the  
 235 resulting empirical clusters for two different values of  $\rho, \sigma$ .

236 The bottom left and bottom right panels assure that our mixing time upper bounds track closely the  
 237 empirical mixing time, in both 2 and 3 dimensions.<sup>3</sup> This provides empirical evidence that Theorem 4  
 238 has the right dependency on both expansion parameter  $\sigma$  and diameter  $\rho$ . The story for the normalized

<sup>3</sup>We rescaled all values of theoretical upper bounds by a constant, to mask the effect of large universal constants in these bounds. Therefore only the comparison of slopes, rather than intercepts, is meaningful.

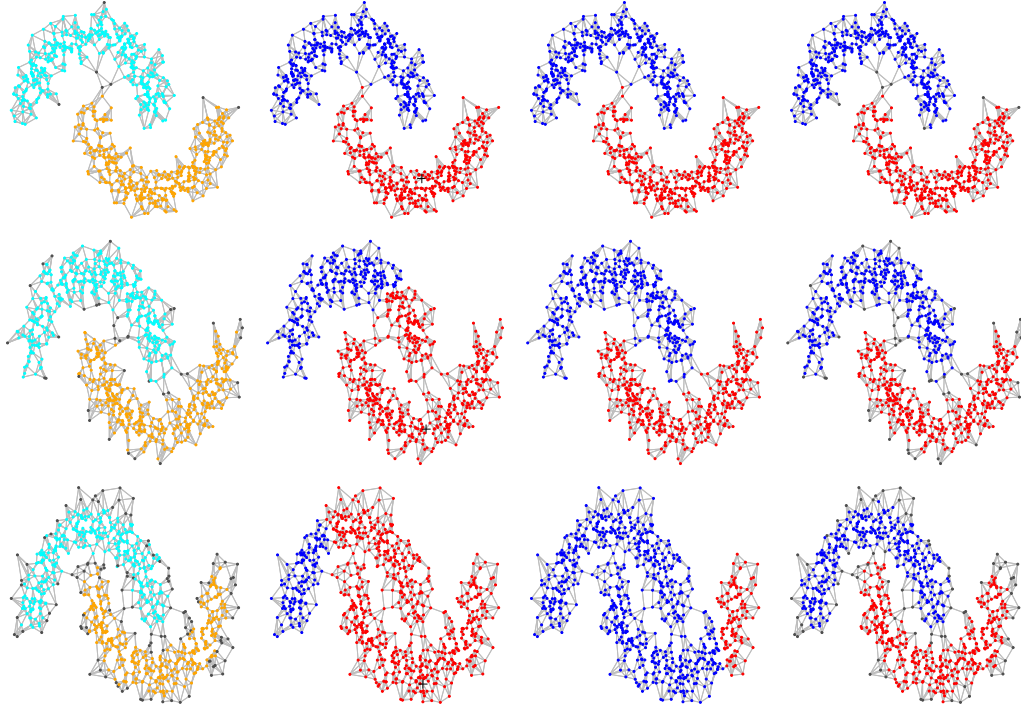


Figure 2: True density (column 1), PPR (column 2), normalized cut (column 3) and estimated density (column 4) clusters for 3 different simulated data sets. Seed node for PPR denoted by a black cross.

cut panels is less obvious. We remark 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, the slopes of empirical and theoretical curves become more similar.

**Empirical behavior of PPR.** In Figure 2, to drive home the main implications of Theorems 1 and 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 shows the empirical density clusters  $\mathcal{C}[X]$  and  $\mathcal{C}'[X]$  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]. We can see 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 the Chaudhuri-Dasgupta algorithm succeeds even when both PPR and normalized cut fail. While our main message was that PPR recovers geometrically well-conditioned density clusters, it would be interesting to establish that it *only* recovers such clusters, a direction for future work.

## 5 Discussion

There are an almost limitless number of ways to define what the “right” clustering is. In this paper, 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 theory to show that our geometric conditions are required for successful recovery of a density level set. This seems to be supported by our empirical work, and it remains a direction for future work.



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