

# Unsupervised Learning (2018 Fall)

## Homework #3

Xinyuan Cao - xc2461

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### Problem 1

#### 1. Nearest neighbor preserving embeddings by Indyk and Naor.

This paper introduces nearest neighbor preserving embeddings, which means randomized embeddings between two metric spaces that maintain the approximate nearest neighbors. This can be very time efficient when given a new data, and to quickly find an approximate neighbor. In the literature we know that this task is closely related to low-distortion embeddings. And more recently, we've found that the embedding must be oblivious to  $X$ , and that the embedding does not need to preserve all interpoint distances. Here we define a good NN preserving embedding as follows:

Let  $(Y, d_Y), (Z, d_Z)$  be metric spaces and  $X \subset Y$ . We say that a distribution over mappings  $f : Y \rightarrow Z$  is a nearest neighbor preserving embedding (NN-preserving) with distortion  $D \geq 1$  and probability of correctness  $P \in [0, 1]$  if for every  $c \geq 1$  and any  $q \in Y$ , with probability at least  $P$ , if  $x \in X$  is such that  $f(x)$  is a  $c$ -approximate nn of  $f(q)$  in  $f(X)$ , then  $x$  is a  $D \cdot c$  approximate nn of  $q$  in  $X$ . It is easy to see that JL lemma is an example of NN-preserving embedding. So here we focus on NN-preserving embeddings into low-dimensional spaces. And prove that such embedding exist for the following subset of  $l_x^d$ : doubling sets and sets with small aspect ratio and small  $\gamma$ -dimension. This algorithm has several applications to efficient approximate nearest neighbor problems. The first application combines NN-preserving embeddings with efficient  $(1 + \epsilon)$ -approximate nearest neighbor data structures in  $l_2^k$  using  $O(|x|/\epsilon^k)$  space and  $O(k \log(|X|/\epsilon))$  query time. The second application is approximating NN where the data set contains objects that are more complex than points. So the approach can have simplicity preservation and modularity.

So here we introduce some basic concepts. Let  $(X, d_X)$  be a metric space.  $B_X(x, r) = \{y \in X : d_X(x, y) < r\}$ . We define the **doubling constant** of  $X$  (denoted as  $\lambda_X$ ) is the least integer  $\lambda \geq 1$  s.t. for every  $x \in X$  and  $r > 0$  there is  $S \subset X$  with  $|S| \leq \lambda$  s.t.

$$B_X(x, 2r) \subset \bigcup_{s \in S} B_X(s, r)$$

Fix  $N \in \mathbb{Z}$ ,  $g = (g_1, \dots, g_N)$  is a standard Gaussian vector in  $\mathbb{R}^N$ . Given  $X \subset l_2^N$ , denote the **parameter**

$$E_X = \mathbb{E} \sup_{x \in X} | \langle x, g \rangle |$$

We observe that for every bounded  $X \subset l_2^N$ :

$$E_X = O(\text{diam}(X) \sqrt{\log \lambda_X})$$

Given a metric space  $(X, d_X)$  set  $\gamma_2(X) = \inf \sup_{x \in X} \sum_{s=0}^{\infty} 2^{s/2} d_X(x, A_s)$ , where  $\inf$  is taken over  $A_s \subset X$  with  $|A_s| < 2^{2^s}$ . Define  $\gamma$  **dimension** of  $X$  to be:

$$\gamma \dim(X) = \left\lceil \frac{\gamma_2(X)}{\text{diam}(X)} \right\rceil^2$$

Now we consider the case of Euclidean space with low  $\gamma$ -dimension. Let  $(X, d_X), (Y, d_Y)$  be metric spaces, and  $\delta, D > 0$ . A mapping  $f : X \rightarrow Y$  is said to be  $D$  **bi-Lipschitz with solution**  $\delta$  if there is a scaling factor  $C > 0$  s.t.

$$\forall a, b \in X, d_X(a, b) > \delta \Rightarrow C d_X(a, b) \leq d_Y(f(a), f(b)) \leq C D d_X(a, b)$$

$S^{d-1}$  denotes the unit Euclidean sphere centered at the origin. Using Gordon's theorem we know that fix  $X \subset S^{d-1}$  and  $\epsilon \in (0, 1)$ . There exists an integer  $k = O(\frac{E_X^2}{\epsilon^2})$  and a linear mapping  $T : \mathbb{R}^d \rightarrow \mathbb{R}^k$  s.t.  $\forall x \in X, 1 - \epsilon \leq \|Tx\|_2 \leq 1 + \epsilon$ . Now let  $X$  be a symmetric random variable s.t.  $\mathbb{E}X^2 = 1$ . Assume  $X$  is sub-Gaussian. Fix a unit vector  $a \in S^{n-1}$ . Let  $X_i$  be iid copies of  $X$  and denote  $U = \sum_{j=1}^n a_j X_j$ . Then  $\mathbb{E}U^2 = 1$ , and for every  $0 \leq t \leq \frac{1}{8c}$  we have

$$\begin{aligned} \mathbb{E}e^{tU^2} &= \mathbb{E}_U \mathbb{E}_g \exp(\sqrt{2t}gU) = \mathbb{E}_g \left( \prod_{j=1}^n \mathbb{E}_X \exp(\sqrt{2t}a_j g X) \right) \\ &\leq \mathbb{E}_g \left[ \prod_{j=1}^n \exp(2cta_j^2 g^2) \right] = \mathbb{E}_g e^{2ctg^2} = \frac{1}{\sqrt{1-4ct}} \leq \sqrt{2} \end{aligned}$$

So we can see that for every  $-\frac{1}{8c} \leq t \leq \frac{1}{8c}$  we have

$$\begin{aligned} \mathbb{E} \exp(tU^2) &= \sum_{m=0}^{\infty} \frac{t^m \mathbb{E}U^{2m}}{m!} \leq 1 + t + \sum_{m=2}^{\infty} \frac{(8c|t|)^m (1/8c)^m \mathbb{E}Y^{2m}}{m!} \\ &\leq 1 + t + (8ct)^2 \mathbb{E} \exp(U^2/8c) \leq 1 + t + 100c^2 t^2 \leq \exp(t + 100c^2 t^2) \end{aligned}$$

So we can prove that for every  $0 < \epsilon < 25c$  we have

$$\Pr \left[ \left| \frac{1}{k} \sum_{i=1}^k U_i^2 - 1 \right| \geq \epsilon \right] \leq 2 \exp(-k\epsilon^2/(400c^2))$$

And we can get a corollary that fix  $\epsilon, \delta > 0$ ,  $X \subset \mathbb{R}^d$ . There exists an integer  $k = O(\frac{E_X^2}{\delta^2 \epsilon^2})$  s.t.  $X$  embeds  $1 + \epsilon$  bi-Lipschitzly in  $\mathbb{R}^k$  with resolution  $\delta$ . The embedding extends to a linear mapping defined on all of  $\mathbb{R}^d$ . We can make this cor scale invariant by normalizing by  $\text{diam}(X)$ . Here we can get a  $1 + \epsilon$  bi-Lipschitz embedding with resolution  $\delta \text{diam}(X)$ , where  $k = O(\frac{\gamma \text{dim}(X)}{\delta^2 \epsilon^2})$ .

For the case of euclidean doubling spaces. We can prove the following theorem: For  $X \subset \mathbb{R}^d$ ,  $\epsilon \in (0, 1)$  and  $\delta \in (0, 0.5)$  there exists  $k = (O(\frac{\log(2/\epsilon)}{\epsilon^2} \log(1/\delta) \log \lambda_X))$  such that for every  $x_0 \in X$  with probability at least  $1 - \delta$ ,

$$d(Gx_0, G(X - \{x_0\})) \leq (1 + \epsilon)d(x_0, X - \{x_0\})$$

For every  $x \in X$  with  $\|x_0 - x\|_2 > (1 + 2\epsilon)d(x_0, X - \{x_0\})$  satisfies  $\|Gx_0 - Gx\| > (1 + \epsilon)d(x_0, X - \{x_0\})$ .

## 2. Optimality of the Johnson-Lindenstrauss lemma by Larseni and Nelson.

This paper proves a lower bound for JL Lemma on the dimension  $m$  of the image space. Through literature review, a lower bound is obtained for only *linear* mappings and for a selected range of error  $\epsilon$  or sufficiently large size  $n$ . The main contribution of this paper is giving a lower bound of  $m$  and thus proving the optimality of the JL Lemma. For thm.2, we get that: for any integers  $n, d \geq 2$  and  $\epsilon \in (\log^{0.5001} n / \sqrt{\min(n, d)}, 1)$ , there exists a set of points  $X \subset \mathbb{R}^d$  of size  $n$ , s.t. any map  $f : X \rightarrow \mathbb{R}^m$  providing the guarantee of JL must have  $m = \Omega(\epsilon^{-2} \log n)$

We proved JL Lemma through random projection theories and indeed, all known proofs of the JL lemma proceed by instantiating distributions  $D_{\epsilon, \delta}$  satisfying the guarantee of the below DJL lemma. (Actually JL lemma is a colloary of DJL Lemma when  $\delta < 1/\binom{n}{2}$ )

For any integer  $d \geq 1$  and any  $0 < \epsilon, \delta < \frac{1}{2}$ , there exists a distribution  $D_{\epsilon, \delta}$  over  $m \times d$  real matrices for some  $m \lesssim \epsilon^{-2} \log(\frac{1}{\delta})$  s.t.

$$\forall u \in \mathbb{R}^d, \mathbb{P}_{\Pi \sim D_{\epsilon, \delta}} (||\Pi u||_2 - ||u||_2| > \epsilon ||u||_2) < \delta \quad (1)$$

We want to prove the result by constructing a large family  $\mathcal{P} = \{P_1, P_2, \dots\}$  of very different sets of  $n$  points in  $\mathbb{R}^d$ . Through the whole proof, we assume all point sets in  $\mathcal{P}$  can be embedded into  $\mathbb{R}^m$  while preserving all pairwise distances to within  $(1 + \epsilon)$ . If the data sets  $P_i$  are very different between each other, we know we cannot embed them into a very low-dimensional space. And the main idea is to construct special sets to argue that  $m$  should at least at some level to let this assumption hold.

First assume  $d = \frac{n}{\log(1/\epsilon)}$  and  $\epsilon \in (\log^{0.5001} n / \sqrt{d}, 1)$ . For any set  $S \subset [d]$  of  $k = -\epsilon^{-2}/256$  indices, define  $y_S := \sum_{j \in S} \frac{e_j}{\sqrt{k}}$ , where  $e_i$ 's denote the standard unit vectors

in  $\mathbb{R}^d$ . So that  $\langle e_j, y_S \rangle$  equals to 0 if  $j \notin S$  and  $16\epsilon$  if  $j \in S$ . We then have  $T = \{0, e_1, \dots, e_d, y_S\}$ , where  $\forall u, v \in T, \langle f(u), f(v) \rangle \in (\langle u, v \rangle - 4\epsilon, \langle u, v \rangle + 4\epsilon)$ .

Secondly, to extend  $d$  to any range, we give an encoding argument. Based on the assumption that the embedding preserves pairwise distances to within  $(1 + \epsilon)$ , we can take any point set  $T \in \mathcal{P}$  and encode it into a bit string of length  $O(nm)$ . (The encoding guarantees that  $T$  can be uniquely recovered from the encoding.) The encoding algorithm thus effectively defines an injective mapping  $g$  from  $\mathcal{P}$  to  $\{0, 1\}^{O(nm)}$ . Since  $g$  is injective, we must have  $|\mathcal{P}| \leq 2^{O(nm)}$ . But  $|\mathcal{P}| = \binom{d}{k}^Q = (\epsilon^2 n / \log(\frac{1}{\epsilon}))^{\Omega(\epsilon^{-2}n)}$  and we can conclude  $m = \Omega(\epsilon^{-2} \log(\epsilon^2 n / \log(\frac{1}{\epsilon})))$ . For  $\epsilon > \frac{1}{n^{0.4999}}$ , this is  $m = \Omega(\epsilon^{-2} \log n)$ .

Then it proposes the idea to reduce the length of the encoding to  $O(mn)$ . We can encode approximations  $\hat{f}(e_j)$  by specifying indices into a covering  $C_2$  of  $(1 + \epsilon)B_2^m$  by  $\epsilon B_2^m$ . Define a  $d \times m$  matrix  $A$  having  $\hat{f}(e_j) = c_2 f(e_j)$  as rows. Then by utilizing the matrix and the structure of  $\mathcal{P}$ , we can get down to just  $O(m)$  bits. Denote  $W$  as the subspace of  $\mathbb{R}^d$  spanned by the columns of  $A$  and define  $U := B_\infty^d \cap W$  as the convex body. Now let  $C_\infty$  be a minimum cardinality covering of  $(22\epsilon)U$  by translated copies of  $\epsilon U$ . By the following lemma and corollary, we have  $|C_\infty| \leq 2^{m \log 45}$ . For lemma 2 in the paper: Let  $E$  be an  $m$ -dimensional normed space and let  $B_E$  denote its unit ball. For any  $0 < \epsilon < 1$ , one can cover  $B_E$  using at most  $2^{m \log(1+2/\epsilon)}$  translated copies of  $\epsilon B_E$ . And we have the corollary: Let  $T$  be an origin symmetric convex body in  $\mathbb{R}^m$ . For any  $0 < \epsilon < 1$ , one can cover  $T$  using at most  $2^{m \log(1+2/\epsilon)}$  translated copies of  $\epsilon T$ .

And finally we analyse the size of the encoding produced by the above procedure and derive a lower bound on  $m$ . Recall that the encoding procedure produces  $O(mn)$  bits but  $|\mathcal{P}| \geq (d/2k)^{kQ} \geq (d/2k)^{kn/2}$ . Therefore  $m = \Omega(\epsilon^{-2} \log(\epsilon^2 n / \log(1/\epsilon)))$ . With the assumption  $\epsilon > \log^{0.5001} n / \sqrt{d}$  and this can be simplified to  $m = \omega(\epsilon^{-2} \log(\epsilon^2 n))$ .

To note that in the previous steps we utilize some lemma to get our conclusion.

For every  $e_j$  and  $y_{sl}$  in  $T$ , we have

$$|\langle \hat{f}(e_j), \hat{f}(y_{sl}) \rangle - \langle e_j, y_{sl} \rangle| \leq 6\epsilon$$

Finally we make some handling toward other values of  $d$  by differently constructing the point sets in  $\mathcal{P}$  and discuss the cases in which  $d > n / \log(1/\epsilon)$  and in which  $d > n / \log(1/\epsilon)$  and  $\epsilon \in (\log^{0.5001} n / \sqrt{d}, 1)$  through proof by contradiction.

## Problem 2

For any  $u, v \in S$ , denote  $x = u - v$ . We want show that for any  $0 < \epsilon < 1/2$  there exists a linear map  $f : \mathbb{R}^D \rightarrow \mathbb{R}^d$  s.t.

$$(1 - \epsilon)\|u - v\| \leq \|f(u) - f(v)\| \leq (1 + \epsilon)\|u - v\|$$

For a linear map  $f$ , we have  $f(u) - f(v) = f(u - v) = f(x)$ , and  $f(x) = \|x\|f(\frac{x}{\|x\|})$ . So it is suffice to show that for any  $x$  in the unit ball of  $S$ ,

$$(1 - \epsilon)\|x\| \leq \|f(x)\| \leq (1 + \epsilon)\|x\| \quad (2)$$

Let  $\epsilon_0 = \epsilon/3$ , so we have  $0 < \epsilon_0 < 1/6 < 1/2$ . Let  $r = \frac{\epsilon}{3+\epsilon}$ , so we have  $\frac{r}{1-r} = \epsilon/3$ . Denote  $S_0$  as the unit ball of  $S$ .  $S_0 \subset S \subset \mathbb{R}^D$ , and  $S_0$  is close and bounded, so it is compact. Hence we can find a finite  $r$ -cover on  $S_0$ , denote this cover as  $C$ . Because  $C$  is finite, we can apply JL-Lemma to  $C$ . That is, for  $\epsilon_0$ , there exists a linear map  $f : C \rightarrow \mathbb{R}^d$  (with  $d = O(k/\epsilon^2)$ ), such that for all  $u, v \in C$ ,

$$(1 - \epsilon_0)\|u - v\| \leq \|f(u) - f(v)\| \leq (1 + \epsilon_0)\|u - v\| \quad (3)$$

Because  $\mathbb{R}^D$  and  $\mathbb{R}^d$  are finite dimensional vector spaces with defined basis, we know  $f$  can be represented by a  $d \times D$  matrix  $A$ . So consider  $\phi : S_0 \rightarrow \mathbb{R}^d$  such that  $\phi(x) = Ax$  for  $x \in S_0$ .  $\phi$  is a linear map. So  $\phi(0) = \phi(u - u) = \phi(u) - \phi(u) = 0$ . Let  $v = 0$  in equation (2) and we get for all  $u \in C$ ,

$$1 - \epsilon_0 = (1 - \epsilon_0)\|u\| \leq \|f(u)\| = \|\phi(u)\| \leq (1 + \epsilon_0)\|u\| = 1 + \epsilon_0 \quad (4)$$

So we know that

$$\max_{x \in C} \|\phi(x)\| \leq 1 + \epsilon_0 \quad (5)$$

$$\min_{x \in C} \|\phi(x)\| \geq 1 - \epsilon_0 \quad (6)$$

Then for any  $x$  in  $S_0$ , since  $C$  is an  $r$ -cover of  $S_0$ , there exists a  $x_c \in C$  such that  $x = x_c + x_r$  and  $\|x_r\| \leq r$ .

$$\|\phi(x)\| = \|\phi(x_c) + \phi(x_r)\| \leq \|\phi(x_c)\| + \|\phi(x_r)\| \quad (7)$$

Recall Question 4(iv) of HW1, we know that

$$\max_{x \in S_0} \|\phi(x)\| \leq \frac{\max_{x \in C} \|\phi(x)\|}{1 - r} \leq \frac{1 + \epsilon_0}{1 - r}$$

So we know that

$$\max_{\|x_\delta\|=\delta} \|\phi(x_\delta)\| = \delta \max_{\|x_\delta\|=\delta} \|\phi(x_\delta/\delta)\| = \delta \max_{\|x\|=1} \|\phi(x)\| \leq \delta \frac{1 + \epsilon_0}{1 - r}$$

So we have

$$\max_{\|x_r\| \leq r} \|\phi(x_r)\| \leq \frac{r(1 + \epsilon_0)}{1 - r} \quad (8)$$

Therefore we can derive from equation(4)(6)(7) that

$$\begin{aligned}
 \max_{x \in S_0} \|\phi(x)\| &\leq \max_{x_c \in C} \|\phi(x_c)\| + \max_{\|x_r\| \leq r} \|\phi(x_r)\| \\
 &\leq (1 + \epsilon_0) + \frac{r(1 + \epsilon_0)}{1 - r} \\
 &= \frac{1 + \epsilon/3}{1 - \frac{\epsilon}{3+\epsilon}} \\
 &= (\epsilon + 3)^2/9 \\
 &\leq 1 + \epsilon
 \end{aligned}$$

From here we have proved the right part of (1). For the other part, we need to estimate the lower bound of  $\|\phi(x)\|$ .

$$\|\phi(x)\| = \|\phi(x_c) + \phi(x_r)\| \geq \phi(x_c) - \phi(x_r) \quad (9)$$

We need to estimate the minimum of  $\|\phi(x)\|$ . From equation (5)(7)(8)

$$\begin{aligned}
 \min_{x \in S_0} \|\phi(x)\| &\geq \min_{x_c \in C} \|\phi(x_c)\| - \max_{\|x_r\| \leq r} \|\phi(x_r)\| \\
 &\geq 1 - \epsilon_0 - \frac{r(1 + \epsilon_0)}{1 - r} \\
 &= 1 - \epsilon/3 - (1 + \epsilon/3)\epsilon/3 \\
 &= 1 - 2\epsilon/3 - \epsilon^2/9 \\
 &\geq 1 - 2\epsilon/3 - \epsilon/3 \\
 &= 1 - \epsilon
 \end{aligned}$$

So now we have proved that for any  $x$  in the unit ball, equation (1) is correct.

Finally we estimate  $d$ . Recall Question 4(iii) of HW1, we know that  $r$ -cover number  $\geq (\frac{1}{r})^k$ , so from JL-Lemma we know that

$$d = \Omega\left(\frac{\log n}{\epsilon_0^2}\right) = \Omega\left(\frac{k \log \frac{1}{r}}{\epsilon_0^2}\right) = \Omega\left(\frac{k \log(1 + \frac{3}{\epsilon})}{\epsilon^2/9}\right) = \Omega(k/\epsilon^2)$$

Therefore we have proved the JL-type result in a fixed but unknown  $k$ -dimensional affine space. #

- Reference: Discuss with Yuze Zhou.

### Problem 3

1. Since  $P$  is the projection onto the orthogonal complement of  $\text{span}(\mathbf{1}_v)$ , we have  $P = I - \frac{1}{n} \mathbf{1}_v \mathbf{1}_v^T$ , and  $P \mathbf{1}_S = \mathbf{1}_S - \frac{|S|}{n} \mathbf{1}_v$ . Then we have  $\|P \mathbf{1}_S\|_2^2 = |S| + \frac{|S|^2}{n} - 2 \frac{|S|^2}{n} = |S| - \frac{|S|^2}{n}$ . Since  $|S| \leq \frac{|V|}{2}$  we have

$$\frac{\|P \mathbf{1}_S\|_2^2}{\|\mathbf{1}_S\|_2^2} = 1 - \frac{|S|}{n} \geq 1 - \frac{1}{2} = \frac{1}{2}$$

Recall the properties we've derived in the class and in homework 1 and 2, we know  $L$  has an eigenpair  $(0, \mathbf{1})$ , so  $I(L) \subset \text{span}(\mathbf{1}_v)^\perp$ , here  $I(L)$  denotes the image of  $L$ . Thus  $PL = L = LP$ . So we have

$$\phi = \min_{x \in \{\mathbf{1}_S : |S| \leq \frac{|V|}{2}\}} \frac{1}{d} \frac{x^T L x}{\|x\|_2^2} = \min_{x \in \{\mathbf{1}_S : |S| \leq \frac{|V|}{2}\}} \frac{1}{d} \frac{(Px)^T L P x}{\|Px\|_2^2} \frac{\|Px\|_2^2}{\|x\|_2^2}$$

$$\forall x \in \text{span}(\mathbf{1}_v)^\perp, R(x) \geq \lambda_2,$$

$$\frac{1}{d} \frac{(Px)^T L P x}{\|Px\|_2^2} \frac{\|Px\|_2^2}{\|x\|_2^2} \geq \frac{1}{d} \lambda_2 \frac{\|Px\|_2^2}{\|x\|_2^2} \geq \frac{\lambda_2}{2d}$$

Minimize both side on  $x$ , and so we get  $\phi \geq \frac{\lambda_2}{2d}$ .

2. With the assumption that there exist  $\mathcal{D}$  such that  $\mathbb{P}_{k \sim \mathcal{D}} \left( \phi(S_k) \leq \sqrt{\frac{2\lambda_2}{d}} \right) > 0$ ,

$$0 < \mathbb{P}_{k \sim \mathcal{D}} \left( \phi(S_k) \leq \sqrt{\frac{2\lambda_2}{d}} \right) = \mathbb{E}_{k \sim \mathcal{D}} \left( \mathbb{I}_{\left\{ \phi(S_k) \leq \sqrt{\frac{2\lambda_2}{d}} \right\}} \right)$$

So there exist at least one  $k$  such that satisfies  $\phi(S_k) \leq \sqrt{\frac{2\lambda_2}{d}}$ . So we have our algorithm as follows.

**Algorithm 1** edge expansion algorithm

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1: function EDGEEXPANSION( $G(V,E)$ )  $\triangleright V = \{v_1, \dots, v_n\}$ 
2:   Compute  $x$  as the minimizer of modified relaxation problem
3:   Resort all the nodes such that  $x_1 \leq x_2 \leq \dots \leq x_n$ ,  $T = S_1 = \phi(\{v_1\})$ ,  $Out = \{v_1\}$ 
4:   for  $i = 2:(n - 1)$  do
5:     Construct  $S_i = \{v_1, \dots, v_i\}$ 
6:     if  $\phi(S_i) \leq T$  then
7:        $T = \phi(S_i)$ 
8:       if  $|S_i| \leq \frac{n}{2}$  then
9:          $Out = S_i$ 
10:      else
11:         $Out = V \setminus S_i$ 
12:      end if
13:    end if
14:  end for
15:   $T$  and  $Out$ 
16: end function

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3. Since  $L$  has only one eigenvalue that equals to 0, and all other eigenvalues are greater than 0. We obtain the min  $v$  from

$$R(v) = \min_{x \in \text{span}(\mathbf{1}_v)^\perp} \frac{x^T L x}{\|x\|_2^2}$$

Let  $v'$  be the eigenvector corresponding to  $\lambda_2$ , so we have

$$R(v') = \frac{\lambda_2 \|v'\|_2^2}{\|v'\|_2^2} = \lambda_2 \geq R(v)$$

By Rayleigh quotient and SVD, we know  $v'$  is also a solver to the minimization problem.

If  $u = \alpha(v + \beta \mathbf{1}_v)$ , so

$$R(u) = \frac{\alpha^2 (v + \beta \mathbf{1}_v)^T L (v + \beta \mathbf{1}_v)}{\alpha^2 \|v + \beta \mathbf{1}_v\|_2^2} = \frac{v^T L v}{\|v + \beta \mathbf{1}\|_2^2} = \frac{v^T L v}{\|v\|_2^2 + \beta^2 \|\mathbf{1}_v\|_2^2} \leq \frac{v^T L v}{\|v\|_2^2} = R(v)$$

This holds since  $v$  and  $\mathbf{1}_v$  are orthogonal and  $\mathbf{1}_v$  is the eigenvector of  $L$  corresponding to eigenvalue 0.

4. If  $(i, j) \in E$  and  $i < j$ , we have

$$\mathbb{P}_{k \sim D}(i \leq k < j) = \mathbb{P}_{k \sim D}((i, j) \in E(S_k, \bar{S}_k)) = \sum_{k=i}^{j-1} |u_{k+1}^2 - u_k^2|$$

$$\text{If } u_i \geq 0 \text{ or } u_j \leq 0, \mathbb{P}_{k \sim D}(i \leq k < j) = |u_j^2 - u_i^2| = |u_i - u_j| |u_i + u_j| \leq |u_i - u_j| (|u_i| + |u_j|).$$



If  $u_i < 0 < u_j$ , find index  $t$  such that  $u_t \leq 0$  and  $u_{t+1} \geq 0$ , (actually  $t = \lfloor \frac{|V|}{2} \rfloor - 1$ ) then

$$\mathbb{P}_{k \sim D}(i \leq k < j) = u_i^2 - u_t^2 + u_j^2 - u_{t+1}^2 \leq u_i^2 + u_j^2 \leq (|u_i| + |u_j|)^2 = |u_i - u_j|(|u_i| + |u_j|)$$

Moreover, we can compute the expectation of the cardinality of the cut as

$$\mathbb{E}_{k \sim D}(|E(S_k, \bar{S}_k)|) = \mathbb{E}_{k \sim D} \left( \sum_{(i,j) \in E, i < j} (\mathbb{I}_{(i,j) \in E(S_k, \bar{S}_k)}) \right) = \sum_{(i,j) \in E, i < j} \mathbb{P}_{k \sim D}(i \leq k < j)$$

$$\text{Therefore } \mathbb{E}_{k \sim D}(|E(S_k, \bar{S}_k)|) \leq \sum_{(i,j) \in E, i < j} |u_i - u_j|(|u_i| + |u_j|)$$

5. If  $i < \frac{|V|}{2}$ ,  $i$  would be assigned to  $S_k$  if and only if  $i \leq k < \frac{|V|}{2}$ . Since  $u_{\lfloor \frac{|V|}{2} \rfloor - 1} = 0$

$$P(i \in S_k) = \sum_{j=i}^{\lfloor \frac{|V|}{2} \rfloor - 1} |u_{j+1}^2 - u_j^2| = \sum_{j=i}^{\lfloor \frac{|V|}{2} \rfloor} (u_j^2 - u_{j+1}^2) = u_i^2 - u_{\lfloor \frac{n}{2} \rfloor}^2 = u_i^2$$

For  $i \geq \frac{|V|}{2}$ ,  $i$  would be assigned to  $S_k$  if and only if  $i > k \geq \frac{|V|}{2}$ ,

$$P(i \in S_k) = \sum_{j=\lfloor \frac{|V|}{2} \rfloor}^{i-1} |u_{j+1}^2 - u_j^2| = \sum_{j=\lfloor \frac{|V|}{2} \rfloor}^{i-1} (u_{j+1}^2 - u_j^2) = u_i^2$$

Thus

$$\mathbb{E}_{k \sim D}(\text{vol}(S_k)) = \mathbb{E}_{k \sim D} \left( d \sum_{i=1}^n \mathbb{I}_{i \in S_k} \right) = d \sum_{i=1}^n P(i \in S_k) = d \sum_{i=1}^n u_i^2$$

6. From (4),  $\mathbb{E}_{k \sim D}(|E(S_k, \bar{S}_k)|) \leq \sum_{(i,j) \in E, i < j} |u_i - u_j|(|u_i| + |u_j|)$ , and Cauchy inequality tells us,

$$\mathbb{E}_{k \sim D}(|E(S_k, \bar{S}_k)|) \leq \sqrt{\sum_{(i,j) \in E, i < j} |u_i - u_j|^2} \sqrt{\sum_{(i,j) \in E, i < j} (|u_i| + |u_j|)^2} = \sqrt{u^T L u} \sqrt{\sum_{(i,j) \in E, i < j} (|u_i| + |u_j|)^2}$$

Therefore

$$\frac{\mathbb{E}_{k \sim D}(|E(S_k, \bar{S}_k)|)}{\mathbb{E}_{k \sim D}(\text{vol}(S_k))} \leq \frac{\sqrt{u^T L u} \sqrt{2d \sum_{i=1}^n u_i^2}}{d \sum_{i=1}^n u_i^2} = \sqrt{\frac{2u^T L u}{d \sum_{i=1}^n u_i^2}} = \sqrt{\frac{2R(u)}{d}}$$

7. Since probability is nonnegative, suppose  $P\left(\frac{X}{Y} \leq \frac{\mathbb{E}X}{\mathbb{E}Y}\right) = 0$ . Then  $\frac{X}{Y} > \frac{\mathbb{E}X}{\mathbb{E}Y}$  holds almost surely. Since  $X$  and  $Y$  are both positive random variables,  $X\mathbb{E}Y > Y\mathbb{E}X$  also holds almost surely. Taking expectation for both sides, and we have  $\mathbb{E}X\mathbb{E}Y > \mathbb{E}Y\mathbb{E}X$ . This causes a contradiction. So we have

$$P\left(\frac{X}{Y} \leq \frac{\mathbb{E}X}{\mathbb{E}Y}\right) > 0$$

8. Since  $\phi(S_k) = \frac{|E(S_k, \bar{S}_k)|}{\text{vol}(S_k)}$ , we have  $\mathbb{P}_{k \sim D} \left( \phi(S_k) \leq \sqrt{\frac{2R(u)}{d}} \right) > 0$ .

From (3) we've prove  $R(u) \leq R(v) = \lambda_2$ , so we have

$$0 < \mathbb{P}_{k \sim D} \left( \phi(S_k) \leq \sqrt{\frac{2R(u)}{d}} \right) \leq \mathbb{P}_{k \sim D} \left( \phi(S_k) \leq \sqrt{\frac{2R(v)}{d}} \right) = \mathbb{P}_{k \sim D} \left( \phi(S_k) \leq \sqrt{\frac{2\lambda_2}{d}} \right)$$

- Reference: Discuss with Linyun He, Yuze Zhou.

## Problem 4

1. From the definition of eigenvalue and eigenvector we have

$$\lambda_i v_i = X X^T v_i \quad (10)$$

$$\mu_i u_i = X^T X u_i \quad (11)$$

**Lemma 1.** *If  $A$  is a  $m \times n$  matrix,  $B$  is a  $n \times m$  matrix,  $m \geq n$ , then we have the non-zero eigenvalues of  $AB$  are the same as the non-zero eigenvalues of  $BA$ , and  $AB$  has  $m - n$  more zero eigenvalues than  $BA$ .*

*Proof.*

$$\begin{bmatrix} I & B \\ 0 & I \end{bmatrix} \begin{bmatrix} 0 & 0 \\ A & AB \end{bmatrix} = \begin{bmatrix} BA & BAB \\ A & AB \end{bmatrix} = \begin{bmatrix} BA & 0 \\ A & 0 \end{bmatrix} \begin{bmatrix} I & B \\ 0 & I \end{bmatrix}$$

So we have  $C_1 = \begin{bmatrix} 0 & 0 \\ A & AB \end{bmatrix}$  and  $C_2 = \begin{bmatrix} BA & 0 \\ A & 0 \end{bmatrix}$  are similar. And thus have same eigenvalues. The eigenvalues of  $C_1$  are the eigenvalues of  $AB$  and  $n$  zeros. The eigenvalues of  $C_2$  are the eigenvalues of  $BA$  and  $m$  zeros. So we know that  $AB$  and  $BA$  have same non-zero eigenvalues, and  $AB$  has  $m - n$  more zero eigenvalues than  $BA$ .  $\square$

From the lemma we know that  $XX^T$  and  $X^T X$  has same non-zero eigenvalues. And the number of zero eigenvalues of  $XX^T$  is  $D - n$  more than the number of zero eigenvalues of  $X^T X$ .

Because  $(\mu_i, u_i)$  is the eigenvalue/vector pairs of  $X^T X$ , we have

$$\mu_i u_i = X^T X u_i$$

Left multiply the equation by  $X$ , and we have

$$\mu_i X u_i = X X^T X u_i$$

That is,  $\mu_i (X u_i) = X X^T (X u_i)$ . So we know that if  $X u_i \neq 0$ , the pair  $(\mu_i, X u_i)$  is the eigenvalue/vector of  $XX^T$ .

For  $X u_i = 0$ , from equation (10) we know that LHS = RHS = 0. Since  $u_i \neq 0$ , we know that  $\mu_i = 0$ . So  $\lambda_i = 0$ . Here the corresponding eigenvectors of eigenvalue 0 is the vectors in the null space of  $XX^T$ , which are orthogonal and span the null space of  $XX^T$ .

Therefore we can write  $(\lambda_i, v_i)$  as:

$$\begin{cases} (\mu_i, X u_i) & \text{if } \mu_i \neq 0, \\ (0, v_t), \text{ where } \{v_t\} \text{ are orthogonal and span the null space of } XX^T & \text{if } \mu_i = 0. \end{cases}$$

2. Let's do SVD decomposition of  $X$ , denote  $X = VSU^T$ ,  $V \in \mathbb{R}^{D \times D}$ ,  $S \in \mathbb{R}^{D \times n}$ ,  $U \in \mathbb{R}^{n \times n}$ . So we have  $XX^T = VS^2V^T$ . So we know the diagonal of  $S$  is the square root of  $\lambda_i$ .

We want to project the given data matrix  $X$  into the  $k$  dimensional PCA subspace  $\text{span}(v_1, v_2, \dots, v_k)$ , where  $v_1, \dots, v_k$  is the corresponding eigenvectors of the  $k$  largest eigenvalues of  $XX^T$ . Denote  $V_k = (v_1^T, \dots, v_k^T)^T$ ,  $S_k = \text{diag}(\lambda_1, \dots, \lambda_k)$ ,  $U_k = (u_1^T, \dots, u_k^T)$ . They are the largest  $k$  eigenvalues and corresponding eigenvectors.

$$\tilde{X} = V_k S_k U_k^T = \sum_{i=1}^k v_i \sqrt{\lambda_i} u_i^T = \sum_{i=1}^k \frac{X u_i}{\|X u_i\|} \sqrt{\lambda_i} u_i^T$$

Since

$$\frac{X u_i}{\|X u_i\|} = \frac{X u_i}{\sqrt{u_i^T X^T X u_i}} = \frac{X u_i}{\sqrt{u_i^T \lambda_i u_i}} = \frac{X u_i}{\sqrt{\lambda_i}}$$

So we get

$$\tilde{X} = \sum_{i=1}^k X u_i u_i^T$$

3. For a new datapoint  $x \in \mathbb{R}^D$ , the  $k$ -dimensional PCA projection of  $x$  is

$$\tilde{x} = \sum_{i=1}^k v_i v_i^T x = \sum_{i=1}^k \frac{X u_i}{\sqrt{\lambda_i}} \left( \frac{X u_i}{\sqrt{\lambda_i}} \right)^T x = \sum_{i=1}^k \frac{1}{\lambda_i} X u_i u_i^T X^T x$$

4. First consider a new data point  $x'$ . Let  $\phi(X) = [\phi(x_1), \dots, \phi(x_n)]$  be the coordinates of all data points in the feature space. Then the projection of  $x'$  onto the PCA subspace of the feature space is therefore  $\sum_{i=1}^k \frac{\phi(X) \tilde{u}_i \tilde{u}_i^T \phi(X)^T}{\tilde{\lambda}_i} \phi(x')$ , where  $\tilde{u}_i$  are the top eigenvectors corresponding to the top eigenvalues  $\tilde{\lambda}$  of  $\phi(X)^T \phi(X)$ . Without loss of generalities, let the SVD decomposition of  $K = \phi(X)^T \phi(X)$  is  $\tilde{V} \tilde{\Lambda} \tilde{U}$ , where  $\tilde{\Lambda}$  is a  $D * n$  diagonal matrix containing the singular values  $\sqrt{\tilde{\lambda}_i}$ , and  $\tilde{U} = [\tilde{u}_1, \dots, \tilde{u}_n]$ ,  $\tilde{V} = [\tilde{v}_1, \dots, \tilde{v}_D]$ . Let  $K(X, x') = [K(x_1, x'), \dots, K(x_n, x')]$  be the column vector of the inner product of the projection of  $x'$  onto the PCA subspace of the feature space could be further written as:

$$\begin{aligned} \sum_{i=1}^k \frac{\phi(X) \tilde{u}_i \tilde{u}_i^T \phi(X)^T}{\tilde{\lambda}_i} \phi(x') &= \sum_{i=1}^k \frac{\tilde{v}_i \sqrt{\tilde{\lambda}_i} \tilde{u}_i^T K(X, x')}{\sqrt{\tilde{\lambda}_i}} \\ &= \sum_{i=1}^k \frac{\tilde{u}_i^T K(X, x')}{\sqrt{\tilde{\lambda}_i}} \tilde{v}_i \end{aligned}$$

Since  $\tilde{v}_1, \dots, \tilde{v}_k$  are the orthonormal vectors that span the  $k$ -dimensional PCA subspace in the feature space. We have the coordinates of the data onto the specific subspace with respect to  $\tilde{v}_1, \dots, \tilde{v}_k$  is  $[\frac{\tilde{u}_1^T K(X, x')}{\sqrt{\tilde{\lambda}_1}}, \dots, \frac{\tilde{u}_k^T K(X, x')}{\sqrt{\tilde{\lambda}_k}}]$ .

Denote  $\tilde{\Lambda}_k^{-1/2} = \text{diag}(1/\sqrt{\tilde{\lambda}_1}, \dots, 1/\sqrt{\tilde{\lambda}_k})$  and  $K = (\langle \phi(x_i), \phi(x_j) \rangle)_{ij}$  be the inner product matrix of all old data points in the feature space, we can get the input data points' coordinates in the subspace is  $\tilde{\Lambda}_k^{-1/2} \tilde{U}_k^T K$ .

5. I use two concentric circles to show the kernalized-PCA result.

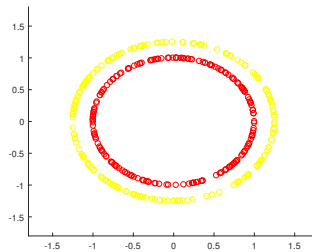


Figure 1: original data

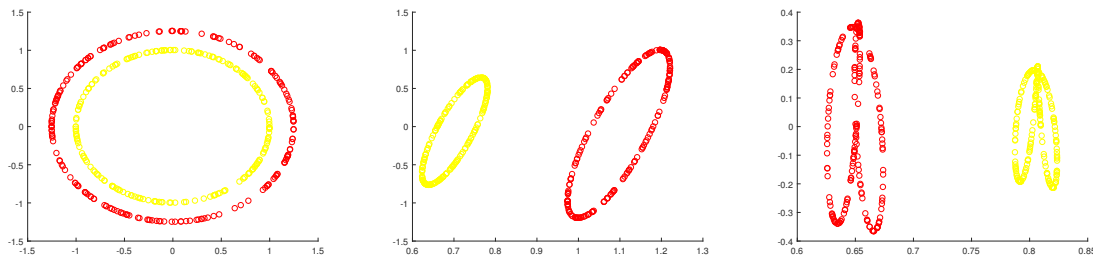


Figure 2: 2D PCA (linear, quadratic, rbf kernels)

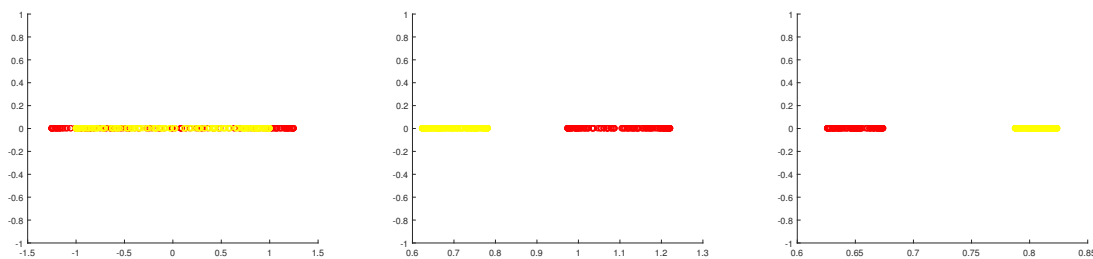


Figure 3: 1D PCA (linear, quadratic, rbf kernels)

We can see that 2D PCA has better result compared to 1D PCA. And rbf kernel has very good results for concentric circles. #

- Reference: <https://stats.stackexchange.com/questions/134282/relationship-between-svd-and-pca-how-to-use-svd-to-perform-pca>
- Discuss with Yuze Zhou

## Problem 5

Here I use two methods to separate audio signals: fourth-order blind identification (FOBI) and fastICA.

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### Algorithm 2 Fourth-order Blind Identification

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**input:** the mixed signals  $X \in \mathbb{R}^{D \times T}$  after centering and whitening, number of signals  $k$ , number of mixtures  $D$ , time sampling number  $T$

**output:** the separated signals  $S \in \mathbb{R}^{k \times T}$

- 1: **function** FOURTH-ORDER BLIND IDENTIFICATION( $X$ )
  - 2:      $\Omega = E(XX^T||x||^2)$
  - 3:      $Y =$  eigenvectors of  $\Omega$  ▷ find the eigenvectors of  $\Omega$
  - 4:     **return**  $Y^T X$
  - 5: **end function**
- 

This method is very efficient and has very good efficient on dataset 1. I plot the original mixture signals and the separated signals as follows:

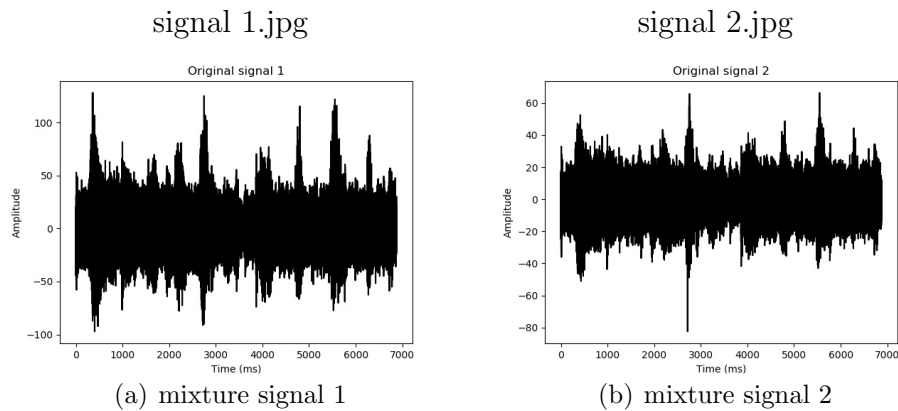


Figure 4: Mixture signals

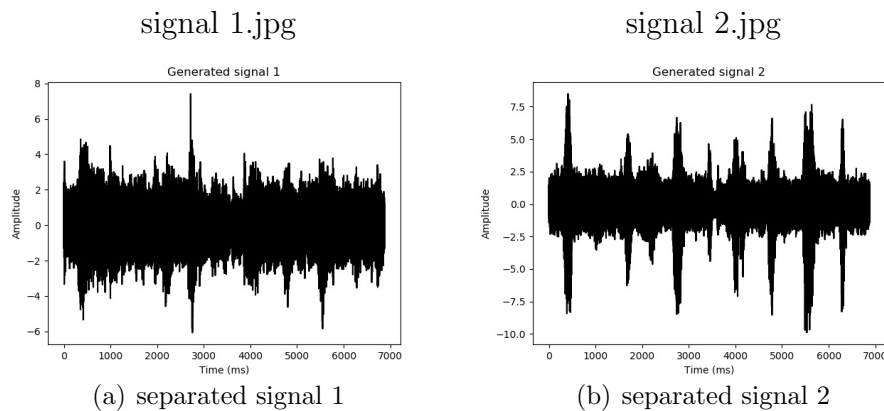


Figure 5: Separated signals using FOBI

So it is obvious that the result of this algorithm can separate the background music apart with the voice. This can also be identified by listening to the output file. Secondly I follow the tutorial and implemented FastICA.

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**Algorithm 3** FastICA
 

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**input:** the mixed signals  $X \in \mathbb{R}^{D \times T}$  after centering and whitening, number of signals  $k$ , number of mixtures  $D$ , time sampling number, maximum iteration number  $T$

**output:** the separated signals  $S \in \mathbb{R}^{k \times T}$

```

1: function FOURTH-ORDER BLIND IDENTIFICATION( $X$ )
2:   for  $i$  in 1 to  $k$  do
3:     Initialize  $W_p$  randomly
4:     while  $W_p$  changes do
5:        $W_p \leftarrow \frac{1}{T} X g(w_p^T X)^T - \frac{1}{T} g'(w_p^T X) \mathbf{1} w_p$        $\triangleright$  Here we choose  $g(u) = \tanh(u)$ 
6:        $W_p \leftarrow W_p - \sum_{j=1}^{i-1} (W_p^T w_j) w_j$ 
7:        $W_p \leftarrow \frac{W_p}{\|W_p\|}$ 
8:     end while
9:   end for
10:  return  $W^T X$ 
11: end function

```

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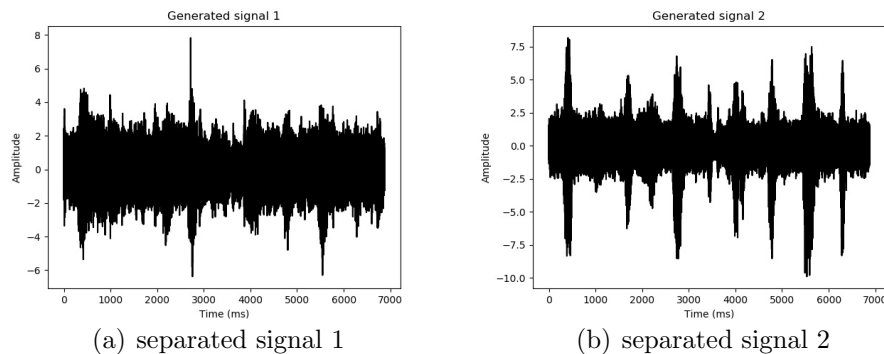


Figure 6: Separated signals using FastICA

It can be seen and also heard that this method has similar performance as FOBI. But for dataset2 and 3, these two algorithms both cannot achieve good results.

- Reference

1. Independent Component Analysis A Tutorial by Hyvriinen and Oja
2. Source Separation Using Higher Order Moments by J.-F. Cardoso
3. [https://www.cs.helsinki.fi/u/ahyvarin/papers/bookfinal\\_ICA.pdf](https://www.cs.helsinki.fi/u/ahyvarin/papers/bookfinal_ICA.pdf)