CS724: Topics in Algorithms
Spectral Clustering

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We present a treatment of clusterings starting from a finite similarity space $\mathcal{S} = (V, s)$ defined on the set of objects V.

Definition

The *similarity graph* associated to $\mathcal{S}$ is the weighted graph $\mathcal{G}_{\mathcal{S}} = (V, E, s)$, where $E = \{(v, v') \in V \times V \mid s(v, v') > 0\}$ and the weight of an edge (v, v') is $s(v, v')$ for $v, v' \in V$.

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A clustering of the objects in V is a partition $\kappa = \{C_1, \ldots, C_n\}$ of V. The blocks C_i of κ are the *clusters*.
In terms of similarity spaces, the goal of any clustering algorithm is to gather in a cluster all objects that are similar to each other and to place in distinct clusters pairs of objects that have low similarities.

There are several ways to contruct a similarity space (or a similarity graph) for a set of points $V = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$.
For example, an undirected graph $G_t = (V, E_t)$ can be defined by

$$E_t = \{\{\mathbf{x}_i, \mathbf{x}_j\} \mid d(\mathbf{x}_i, \mathbf{x}_j) \leqslant t\},$$

where t is a given threshold.

Another option is to use the k-nearest neighbor graph $G_{nn,k}$, where an edge $(\mathbf{v}, \mathbf{w})$ exists if $\mathbf{w}$ is among the k nearest neighbors of $\mathbf{v}$. This leads, of course to a directed graph; however, an undirected graph can be readily obtained by ignoring the orientation of the edges. An alternative undirected graph $G'_{nn,k}$ can be obtained by considering an edge $\{\mathbf{v}, \mathbf{w}\}$ if $\mathbf{w}$ is among the k closest neighbors of $\mathbf{v}$ and $\mathbf{v}$ is among the k closest of $\mathbf{w}$.

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Finally, it is possible to use a weighted complete graph on the set V and define for each pair of objects a similarity measure $k(\mathbf{v}, \mathbf{w})$. The function k is referred in the specialized **R** package `kernlab` as a *kernel*.

A *radial basis function* (rbf) is a real-valued function $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ whose value $f(\mathbf{x})$ depends only on the distance from the origin $\| \mathbf{x} \|$, that is, $f(\mathbf{x}) = f(\| \mathbf{x} \|)$.

Examples of such kernels are $k(\mathbf{v}, \mathbf{w}) = e^{-\|\mathbf{v}-\mathbf{w}\|^2}$ named the `rbfdot` or $e^{-\|\mathbf{v}-\mathbf{w}\|}$ named the `laplacedot`, etc.

As usual, a clustering of the objects in $V = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$, where $V \subseteq \mathbb{R}^m$ is a partition $\kappa = \{C_1, \ldots, C_k\}$ of V. The blocks C_i of κ are the *clusters*. Let $\kappa = \{C_1, \ldots, C_k\}$ be a clustering of the objects of the set $V = \{v_1, \ldots, v_n\}$. For a block C_i we denote by $\bar{C}_i$ the complement of C_i relative the set V. Clearly, $\bar{C}_i = \bigcup\{C_j \mid j \in \{1, \ldots, k\} - \{i\}\}$ for every i, $1 \leqslant i \leqslant k$.

Definition

The *cut* of κ is the number

$$\begin{aligned} cut(\kappa) &= \sum_{i=1}^{k} cut(C_i, \bar{C}_i) \\ &= \sum_{p=1}^{n}\sum_{q=1}^{n}\{s(v_p, v_q) \mid v_p \text{ and } v_q \text{belong to different clusters}\} \end{aligned}$$

Definition

Let $G = (V, E)$ be a graph and let S be a set of vertices. The *edge boundary* of S is the set of edges of G that join S to its complement. This set is denoted by $\partial(S)$. Clearly, $\partial(V - S) = \partial(S)$.

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Theorem

Let $G = (V, E)$ be a graph with $V = \{v_1, \ldots, v_n\}$ and let S be a subset of V. Then

$$\alpha(\mathcal{G}) \leq \frac{n|\partial(S)|}{|S|(n - |S|)},$$

where $\partial(S)$ is the edge boundary of the set S.

Proof

Recall that we have shown that

$$\begin{aligned}\alpha(G) &= \min_{\mathbf{x}}\{\mathbf{x}' L_G \mathbf{x} \mid \mathbf{x} \in S_n\} \\ &= \min_{\mathbf{x}} \sum\{(x_i - x_j)^2 \mid \mathbf{x} \in S_n, i < j \text{ and } \{v_i, v_j\} \in E\},\end{aligned}$$

where $S_n = \{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{x}'\mathbf{1}_n = 0 \text{ and } \| \mathbf{x} \| = 1\}$.

Proof cont'd

Let $\mathbf{r} \in \mathbb{R}^n$ be a vector defined by

$$r_i = \begin{cases} n - |S| & \text{if } v_i \in S, \\ -|S| & \text{if } v_i \notin S, \end{cases}$$

for $1 \leq i \leq n$.
It is clear that $\mathbf{r}'\mathbf{1}_n = 0$, that is, $\mathbf{r}$ is orthogonal on $\mathbf{1}_n$. Therefore, we have:

$$\alpha(\mathcal{G}) \leq \frac{\sum_{(v_i,v_j)\in E}(r_i - r_j)^2}{\| \mathbf{r} \|^2} = \frac{n^2|\partial(S)|}{|S|(n-|S|)^2 + (n-|S|)|S|^2} = \frac{n\partial(S)}{|S|(n-|S|)}.$$

Definition

Let $G = (V, E)$ be a graph. The *conductance* of G is the number

$$\mathrm{cd}(G) = \min \left\{ \frac{|\partial(S)|}{|S|} \mid S \subseteq V, |S| \leq \frac{|V|}{2} \right\}.$$

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Example

To compute the conductance of a complete graph $\mathcal{K}_n$ note that each vertex v is linked to $n-1$ other vertices of the graph. Thus, for a set of vertices S we have $\partial(S) = S \times (V - S)$, so $|\partial(S)| = |S|(n - |S|)$. Thus,

$$\text{cd}(\mathcal{K}_n) = \min\left\{n - |S| \mid S \subseteq V, |S| \leq \frac{n}{2}\right\} = \lceil \frac{n}{2} \rceil.$$

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Example

Let $G = (V, E)$ be a graph such that $|V| = n$.
If $|S| \leq \frac{n}{2}$, then $\text{cd}(G) \leq \frac{\partial(S)}{|S|}$, so $|\partial(S)| \geq \text{cd}(G)|S|$. If $\text{cd}(G)$ is large, then the vertices of S have many neighbors outside S.
Suppose that $\{G_n = (V_n, E_n) \mid n \in \mathbb{N}\}$ be a sequence of graphs with $|V_n| = n$ such that each graph G_n is k-regular and the there exists a lower bound b of the sequence $\{\text{cd}(G_n) \mid n \in \mathbb{N}\}$. We refer to such a sequence of graphs as an *expander*. Note that $|E_n| = \frac{kn}{2}$, which means that the graphs grow increasingly sparse.
The existence of a lower bound for conductances guarantees that there exist many neighbors for a set S of vertices.

Theorem

Let $G = (V, E)$ be a graph. We have

$$cd(G) \geq \frac{\alpha(G)}{2}.$$

Proof

In the definition of the conductance we require $|S| \leq \frac{|V|}{2}$ so

$$\frac{|V|}{|V| - |S|} = \frac{1}{1 - \frac{|S|}{|V|}} \leq 2.$$

Therefore, since $\alpha(G) \leq \frac{n|\partial(S)|}{|S|(n-|S|)}$, it follows that

$$\alpha(G) \leq \frac{n|\partial(S)|}{|S|(n - |S|)} = \frac{|\partial(S)|}{|S|} \cdot \frac{n}{n - |S|} \leq 2\mathrm{cd}G).$$

This theorem shows that $\frac{\alpha(G)}{2}$ provides a lower bound for the conductance of a graph, whose computation is intractable.

There are several criteria for choosing clusterings defined on similarity spaces.
The simplest such criterion is the minimal value of $cut(\kappa)$. This will ensure that the objects of each cluster C_i are as dissimilar as possible to the objects from the other clusters.
For bipartitions the algorithm is based on the observation that if x, y are two vertices of a weighted graph $G = (V, E, w)$ and $\pi = \{X, Y\}$ is a bipartition of V such that $x \in X$ and $y \in Y$, then the value of a minimum cut $cut(\pi)$ is the smaller of a minimum (x, y)-cut and a minimum cut of $G/\{x, y\}$, where $G/\{x, y\}$ is the graph obtained from G by merging x and y and removing the edge (x, y) if such an edge exists.
Indeed, either there exists a minimum cut of G that separates x and y (and in this case a minimum (x, y)-cut is a minimum cut of G), or there is no such cut and, in this case, a minimum cut of $G/\{x, y\}$ is a minimum cut of π.

Let $\kappa = \{C_1, \ldots, C_k\}$ be a partition of a set $V = \{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$ of n objects into k clusters.
Starting from a similarity matrix $S \in \mathbb{R}^{n \times n}$ for the objects of V we can define a *similarity graph* of V as $G = (V, E, s)$, where $s(\mathbf{v}_i, \mathbf{v}_\ell) = s_{i\ell}$ for $1 \leqslant i, \ell \leqslant n$.
The *indicator vector* $\mathbf{c}_j \in \mathbb{R}^n$ of the cluster C_j is

$$(\mathbf{c}_j)_i = \begin{cases} \frac{1}{\sqrt{|C_j|}} & \text{if } \mathbf{v}_i \in C_j \\ 0 & \text{otherwise,} \end{cases}$$

where $1 \leqslant i \leqslant n$ and $1 \leqslant j \leqslant i$.

Since κ is a partition of V, the matrix $C = (\mathbf{c}_1 \ \cdots \ \mathbf{c}_k)$ has an orthonormal set of columns, so $C'C = I_k$. Note that, in terms of the entries of C we have

$$\mathbf{c}_j = \begin{pmatrix} c_{1j} \\ c_{2j} \\ \vdots \\ c_{ij} \\ \vdots \\ c_{nj} \end{pmatrix}$$

for $1 \leqslant j \leqslant k$.
We claim that

$$\mathbf{c}_j' L_G \mathbf{c}_j = \frac{1}{2} \frac{cut(C_j, \bar{C}_j)}{|C_j|}$$

By a previous result we have:

$$\mathbf{c}_j' L_G \mathbf{c}_j = \frac{1}{2} \sum_{i=1}^{k} \sum_{\ell=1}^{k} s_{i\ell} (c_{ij} - c_{\ell j})^2.$$

If $\mathbf{v}_i \in C_j$ and $\mathbf{v}_\ell \notin C_j$ we have $c_{ij} = \frac{1}{\sqrt{|C_j|}}$ and $c_{\ell j} = 0$; in this case

$$s_{i\ell} (c_{ij} - c_{\ell j})^2 = \frac{s_{ij}}{|C_j|}.$$

Otherwise, that is, if both $\mathbf{v}_i$ and $\mathbf{v}_\ell$ belong to C_j, or neither vertex belongs to C_j we have

$$s_{i\ell} (c_{ij} - c_{\ell j})^2 = 0.$$

This implies

$$\mathbf{c}_j' L_G \mathbf{c}_j = \sum_{v_i \in C_j} \sum_{v_\ell \notin C_j} \frac{s_{ij}}{|C_j|} = \frac{1}{2} \frac{cut(C_j, \bar{C}_j)}{|C_j|}$$

and $\mathbf{c}_j' L_G \mathbf{c}_j = (C' L_G C)_{jj}$.

Since

$$C' L_G C = \begin{pmatrix} \mathbf{c}_1' \\ \vdots \\ \mathbf{c}_k' \end{pmatrix} L_G (\mathbf{c}_1 \ \cdots \ \mathbf{c}_k),$$

we have

$$\begin{aligned} \sum_{j=1}^{k} \mathbf{c}_j' L_G \mathbf{c}_j &= \sum_{j=1}^{k} (C' L_G C)_{jj} \\ &= trace(C' L_G C) = \frac{1}{2} \sum_{j=1}^{k} \frac{cut(C_j, \bar{C}_j)}{|C_j|} = \frac{1}{2} cutratio(\kappa). \end{aligned}$$

To minimize $cutratio(\kappa)$ is tantamount to seeking the matrix C such that $trace(C' L_G C)$ is minimal subjected to the constraint $C'C = I_k$.
To obtain a practical solution this optimization problem is relaxed by allowing C to range over $\mathbb{R}^{n \times k}$. By Ky Fan's Theorem the minimum is obtained by choosing C such that its columns consist of the eigenvectors $\mathbf{c}_1, \ldots, \mathbf{c}_k$ of L_G that correspond to the k smallest eigenvalues of the Laplacian L_G.

The original set of points $V = \{\mathbf{v}_1, \ldots, \mathbf{v}_n\} \subseteq \mathbb{R}^m$ is transformed now into a set $\{\mathbf{y}_1, \ldots, \mathbf{y}_n\}$ in a lower-dimensional space $\mathbb{R}^k$, where $\mathbf{y}'_1, \ldots, \mathbf{y}'_n$ are the rows of the matrix $C \in \mathbb{R}^{\times}$ whose columns are the k eigenvectors $\mathbf{c}_1, \ldots, \mathbf{c}_k$ of L_G, as shown next.

Unnormalized Spectral Clustering

Data: Similarity matrix $S \in \mathbb{R}^{n \times n}$, number k of clusters
Result: A clustering $\kappa = \{C_1, \ldots, C_k\}$
let A be its weighted adjacency matrix;
compute the ordinary Laplacian L;
compute the first k eigenvectors $\mathbf{c}_1, \ldots, \mathbf{c}_k$ of L;
let $C = (\mathbf{c}_1, \ldots, \mathbf{c}_k) \in \mathbb{R}^{n \times k}$;
define $\mathbf{y}_1, \ldots, \mathbf{y}_n \in \mathbb{R}^k$ such that $C' = (\mathbf{y}_1 \ \cdots \ \mathbf{y}_n)$;
cluster $\{\mathbf{y}_1, \ldots, \mathbf{y}_n\} \subseteq \mathbb{R}^k$ using the k-means algorithm into κ;

Another approach to spectral clustering uses the normalized cut of a partition. As before, let $\kappa = \{C_1, \ldots, C_k\}$ be a partition of a set $V = \{v_1, \ldots, v_n\}$ of n objects into k clusters for which we have a similarity matrix $S \in \mathbb{R}^{n \times n}$. Define the characteristic vector $\mathbf{h}_j$ of C_j as

$$(\mathbf{h}_j)_i = \begin{cases} \frac{1}{\sqrt{vol(C_j)}} & \text{if } v_i \in C_j, \\ 0 & \text{otherwise,} \end{cases}$$

for $1 \leqslant j \leqslant k$ and let $H = (\mathbf{h}_1 \ \cdots \ \mathbf{h}_k)$ be the matrix of these vectors. We have

$$\mathbf{h}_j' D_G \mathbf{h}_j = \sum_{i=1}^{n} \sum_{\ell=1}^{n} (\mathbf{h}_j)_i d_{i\ell} (\mathbf{h}_j)_\ell.$$

The non-zero terms in this sum are such that $i = \ell$ and $v_i \in C_j$. Thus, $\mathbf{h}_j' D_G \mathbf{h}_j = \frac{1}{vol(C_j)} \sum_{v \in C_j} d(v) = 1$. On the other had, $\mathbf{h}_j' D_G \mathbf{h}_m = 0$ if $j \neq m$, so $H' D_G H = I_k$. A similar computation yields

$$\mathbf{h}_j' A_G \mathbf{h}_j = \sum_{i=1}^{n} \sum_{\ell=1}^{n} (\mathbf{h}_j)_i s_{i\ell} (\mathbf{h}_j)_\ell = \frac{1}{vol(C_j)} \sum_{v_i, v_\ell \in C_j} s(v_i, v_\ell).$$

These computations allow us to write

$$\begin{aligned} \mathbf{h}_j' L_G \mathbf{h}_j &= \mathbf{h}_j' (D_G - A_G) \mathbf{h}_j = I_k - \mathbf{h}_j' A_G \mathbf{h}_j = 1 - \frac{1}{vol(C_j)} \sum_{v_i, v_\ell \in C_j} s(v_i, v_\ell) \\ &= \frac{vol(C_j) - \sum_{v_i, v_\ell \in C_j} s(v_i, v_j)}{vol(C_j)} = \frac{cut(C_j, \bar{C}_j)}{vol(C_j)}. \end{aligned}$$

Therefore,

$$trace(H' L_G H) = \sum_{j=1}^{k} \mathbf{h}_j' L_G \mathbf{h}_j = \sum_{j=1}^{k} \frac{cut(C_j, \bar{C}_j)}{vol(C_j)} = ncut(\kappa).$$

To minimize the normalized cut we need to minimize $trace(H'L_G H)$ subjected to the constraint $H'DH = I_k$. Let $M = D^{\frac{1}{2}}H$. Then, in terms of the matrix M, the optimization problem amounts to minimizing $trace(M'D^{-\frac{1}{2}}L_G D^{-\frac{1}{2}}M) = trace(M'L_{G,\text{sym}}M)$ subjected to the restriction $M'M = I_k$. By allowing M to range over $\mathbb{R}^{n\times k}$, the optimum can be achieved by $M = (\mathbf{m}_1, \ldots, \mathbf{m}_k)$, where $\mathbf{m}_1, \ldots, \mathbf{m}_k$ are the first k eigenvectors of the symmetric Laplacian $L_{G,\text{sym}}$.

$D^{-\frac{1}{2}}\mathbf{m}_1, \ldots, D^{-\frac{1}{2}}\mathbf{m}_k$ are the first k eigenvectors of the of the random walk Laplacian and these are exactly the columns of the matrix H. So, the optimal value of H is obtained by choosing its columns to be equal to the eigenvectors that correspond to the first k eigenvalues of $L_{G,\text{rw}}$.

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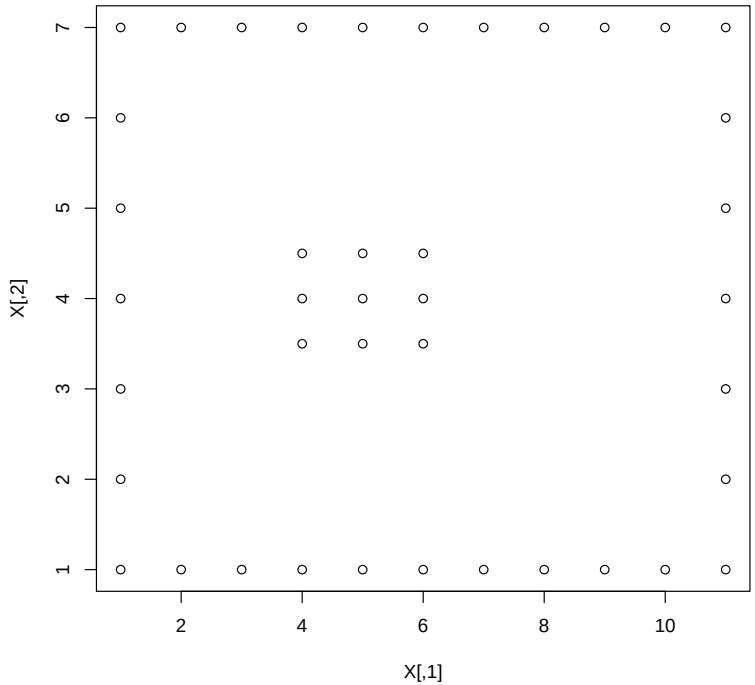
Next we discuss the implementation of spectral clustering in **R** .
We consider a set of 41 points in $\mathbb{R}^2$ placed into two squares and encoded as pairs of numbers in the matrix X.

```
X <- matrix(c(1,1,1,2,1,3,1,4,1,5,1,6,1,7,
              11,1,11,2,11,3,11,4,11,5,11,6,11,7,
              2,1,3,1,4,1,5,1,6,1,7,1,8,1,9,1,10,1,
              2,7,3,7,4,7,5,7,6,7,7,7,8,7,9,7,10,7,
              4,3.5,4,4,4,4.5,
              5,3.5,5,4,5,4.5,
              6,3.5,6,4,6,4.5),
              nrow = 41, byrow=TRUE)
```

The set of points in $\mathbb{R}^2$ looks like:



The function `neighbor_graph(X,k)` is used for building a k-nearest neighbor graph $G_{nn,k}$, where an edge $(\mathbf{v}, \mathbf{w})$ exists if $\mathbf{w}$ is among the k nearest neighbors of $\mathbf{v}$. The adjacency matrix K of this graph is symmetrized (using the operation `K <- K + t(K)` to yield the symmetric adjacency matrix of an undirected graph.

```
neighbor_graph <- function(X,k)
{
   D <- as.matrix(dist(X))
   K <- matrix(0,nrow=nrow(X),ncol=nrow(X))

   for(i in 1:nrow(X)) {
     neighbor_index <- order(D[i,])[2:k]
     K[i,][neighbor_index] <-1
   }
   # K is a matrix having 1s in position (i,j) if j is among
   # the first k neighbors of i
   K <- K + t(K)
   K[K == 2] = 1
   return(K)
}
```

The function spectral_clustering makes use of the function laplacian and the functineighbor_graph defined above. The **R** script of this function is given next.

```
spectral_clustering <- function(X,k,num_eig)
{
   G = neighbor_graph(X,k)
   L = laplacian(G,FALSE)
   eig = eigen(L,symmetric=TRUE)
   n = nrow(L)
   return(eig$vectors[,(n - num_eig):(n-1)])
   # this returns the eigenvectors of the num_eig smallest eigenvalu
}
```

Finally, the set of eigenvectors returned by `spectral_clustering` is clustered using the k-means function as in:

```
X_sc <- spectral_clustering(X,k,num_eig)
X_final <- kmeans(X_sc,num_clust)
```

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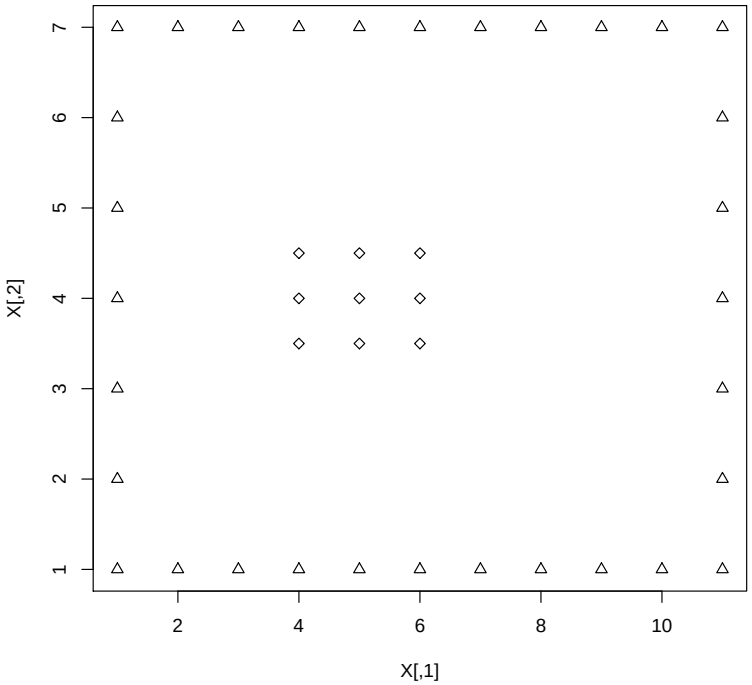
A direct application of the function `specc` of the package `kernlab`

```
sc<- specc(X,centers=2,kernel=''rbfdot'')
```

followed by a call to the `pdf` function

```
> pdf(''squares.pdf'')
> plot(X,pch=sc+22)
> dev.off()
```

will produce the plot shown next.


X[,2]
X[,1]
1
2
3
4
5
6
7
2
4
6
8
10