Clustering Phenomena in Large Networks and Reducible Matrices.

An oral exam presented in partial fulfillment of the requirements of the PhD in mathematics at the University of Georgia

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6th June 2016

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The Research Questions

Question 1

Given $A \in \mathbb{R}^{n \times n}$, symmetric and non-negative, does there exist a **permutation matrix** *P such that PAP^T is block diagonal? That is:*

$$PAP^T = B = \begin{bmatrix} B_{11} & 0 & \cdots & 0 \\ 0 & B_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & B_{kk} \end{bmatrix} \tag{1}$$

If such a P exists, can we find it?

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If such a P exists, can we find it?

Answer 1

Yes and yes. Exist $\mathcal{O}(n)$, graph-based methods.

The Research Questions

Question 2

Given $A \in \mathbb{R}^{n\times n}$, symmetric and non-negative, can we find a permutation matrix P such that

$$PAP^T = B + E$$

with B block diagonal and symmetric as in (1) and E is a small (symmetric) perturbation? ($||E|| << ||B||$)

The Research Questions

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Answer 2

Yes, but existing methods are slow, typically $\mathcal{O}(n^3)$.

The Research Questions

Question 3

Suppose $A \in \mathbb{R}^{n\times n}$ is no longer symmetric. Can we find a permutation matrix P such that

$$PAP^T = B = \begin{bmatrix} B_{11} & B_{12} & \cdots & B_{1,r} \\ 0 & B_{22} & \cdots & B_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & B_{kk} \end{bmatrix},$$

Or $PAP^T = B + E$ *with* $||E|| << ||B||$

The Research Questions

Question 4

What if A is no longer square? Say $A \in \mathbb{R}^{m \times n}$ with $m < n$, can we find permutation matrices $P \in \mathbb{R}^{m \times m}$ and $Q \in \mathbb{R}^{n \times n}$ such that $PAQ = B + E$ with

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and $||E|| << ||B||$.

The Research Questions

Question 5

Why should we care?

Motivating Example 1: Large Networks

- Prevalent in many areas of science, social science and engineering ([1]).

[1] Lovasz, "Very large graphs".

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- Some networks are **directed** (eg. Twitter, Citation Networks) making community detection more subtle.

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Motivating Example 1: Large Networks

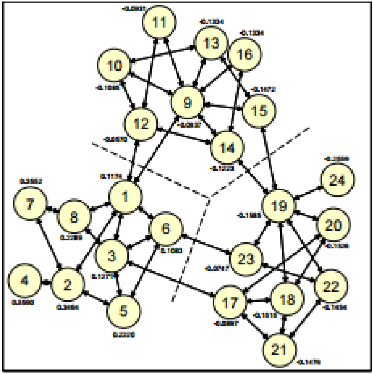

Figure: Graph with vertices ordered into clusters. (from Bertrand and Moonen, "Distributed computation of the Fiedler vector with application to topology inference in ad hoc networks")

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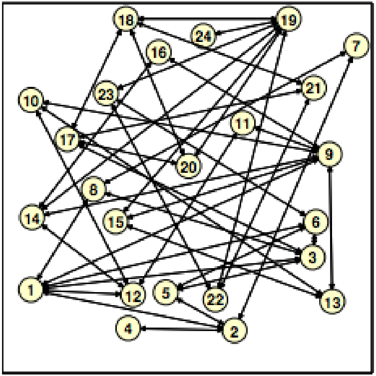

Figure: Same graph with vertices randomly positioned. (from Bertrand and Moonen, "Distributed computation of the Fiedler vector with application to topology inference in ad hoc networks")

Motivating Example 2: Unsupervised Learning[2,3]

- Suppose given a large, high-dimensional dataset $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\} \subset \mathbb{R}^m$.

[2] Ng, Jordan, and Weiss, "On Spectral Clustering: Analysis and Algorithm".

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Motivating Example 2: Unsupervised Learning[2][3]

- Suppose given a large, high-dimensional dataset $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\} \subset \mathbb{R}^m$.
- Want to sort into k clusters $C_1, \ldots, C_k$ of similar data points.

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- Another approach: Form a graph G with vertices $\{1, \ldots, n\}$ and an edge between i and j iff $d(\mathbf{x}_i, \mathbf{x}_j) < \epsilon$
- Find clusters in G, reducing this problem to previous one.

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Motivating Example 2: Unsupervised Learning [4]

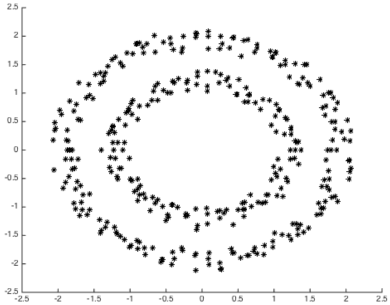

Figure: An artificial data set which appears to have two distinct clusters

[4]see (Jain, "Data clustering: 50 years beyond K-means")

Motivating Example 2: Unsupervised Learning

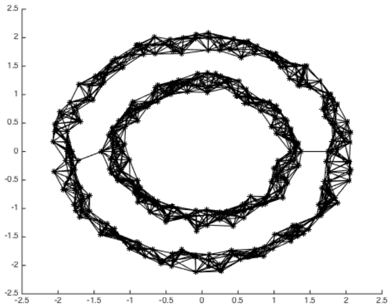

Figure: unweighted graph constructed by connecting data points which are close

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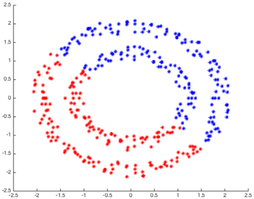
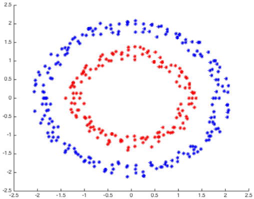


(a) k-means clustering



(b) Graph-based clustering

Figure: Comparison of clustering methods.

Motivating Example 2: Unsupervised Learning

We will relate detecting clusters in graphs to ‘almost block-diagonalizing’ symmetric matrices by permutation matrices (question 2) in section 2

Motivating Example 3: Natural Language Processing

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- Would like to find which words occur frequently together in documents, and which documents are similar.
- We can:
- Choose n keywords.
- Assign i-th document a vector $\mathbf{x}_i \in \mathbb{R}^n$ where $x_{ij} = \#$ times j-th word occurs in i-th document.
- Form matrix $A \in \mathbb{R}^{n \times m}$ with columns $\mathbf{x}_i$.

Motivating Example 3: Natural Language Processing[5]

- Find permutation matrices P and Q such that $PAQ = B + E$ with $||E|| << ||B||$ and:

$$B = \begin{bmatrix} B_{11} & 0 & \cdots & 0 & 0 \\ 0 & B_{22} & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & B_{rr} & 0 \end{bmatrix}$$

[5] see: Dhillon, "Co-clustering documents and words using Bipartite spectral graph partitioning".

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- Rows represent words. Hence rows of B_{ii} represent words which frequently occur together.
- Columns represent documents. Hence columns of B_{ii} represent documents with similar patterns of occurrences of words.
- Have solved two problems simultaneously (co-clustering).

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Reducible matrices

Definition

A matrix A is said to be **reducible** *if there exists a permutation matrix P such that:*

$$PAP^T = \begin{pmatrix} B_{11} & B_{12} \\ 0 & B_{22} \end{pmatrix} \quad (2)$$

and **irreducible** *if no such P exists. We say PAP^T is* **reduced**.

Reducible Matrices

Definition

If there exists a $k > 1$ and permutation matrix P such that:

$$PAP^{\top} = B = \begin{bmatrix} B_{11} & B_{12} & \cdots & B_{1,r} \\ 0 & B_{22} & \cdots & B_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & B_{kk} \end{bmatrix}, \qquad (3)$$

where each B_{ii} is a square matrix and is either irreducible or 0*, we say A is* **k-reducible** *and B is* **k-reduced**.

Reducible Matrices

Remark

If A is symmetric and reducible it can be **block diagonalized** *by a permutation matrix:*

$$PAP^T = \begin{bmatrix} B_{11} & 0 & \cdots & 0 \\ 0 & B_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & B_{kk} \end{bmatrix},$$

with each B_{ii} square and symmetric.

Almost Reducible Matrices

Definition

A is **almost reducible**[6] *if there exists a permutation P such that*

$$PAP^T = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} \tag{4}$$

with $||B_{21}|| << ||B_{11}||$ *and* $||B_{21}|| << ||B_{22}||$.

[6] Bolt and Santitissadeekorn, *Applied and Computational Measurable Dynamics*.

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with $||B_{21}|| << ||B_{11}||$ and $||B_{21}|| << ||B_{22}||$.
Equivalently:

$$PAP^T = \tilde{B} + E$$

with $\tilde{B}$ reduced and $||E|| << ||\tilde{B}||$.

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Equivalently:

$$A = \tilde{A} + D$$

with $\tilde{A}$ reducible and $||D|| << ||\tilde{A}||$.

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Suppose A is symmetric and k-almost-reducible:

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- Equivalently $A = \tilde{A} + D$ with $\tilde{A}$ and D symmetric, $\tilde{A}$ k-reducible and $||D|| << ||\tilde{A}||$.
- Thus A is a perturbation of a symmetric k-reducible matrix by a ‘small’ symmetric matrix.

Graph Theory[7]

Definition

A **graph** *G is a set of vertices V together with a subset $E \subset V \times V$ of edges. G is:*

- **Weighted** *if every edge $e \in E$ has a weight $a_e \in \mathbb{R}_{>0}$*
- **Directed** *if we distinguish between an edge from u to v or from v to u.*

[7] Bollobas, *Graph theory: an introductory course.*

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Remark

Some Conventions:

- *Henceforth shall assume all graphs weighted and undirected.*
- *If $|V| = n < \infty$ we shall identify V with $\{1, 2, \ldots, n\}$.*

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Definition

*G is **connected** if given any $i, j \in V$ there exists a path between them. Otherwise, G is **disconnected**.*

Clusters in Graphs

Definition

A **k-clustering** *of G is a partition $\pi = \{C_1, \ldots, C_k\}$ of V into k subsets with 'many' edges between vertices in C_a for any a, and 'few' edges between vertices in C_a and vertices in C_b for $a \neq b$.*

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Definition

$$Rcut(\pi) = \frac{1}{2}\sum_{a=1}^{k}\frac{W(C_a, \bar{C}_a)}{|C_a|} \quad \text{where } W(C_a, \bar{C}_a) = \sum_{i \in C_a, j \notin C_a} a_{ij}$$

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Although there are (many) other measures ([8]).

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Clusters in Graphs

We say π is a good clustering if $\text{Rcut}(\pi)$ is 'small'.

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Definition (The Clustering Problem)

Given a graph G, find π such that:

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Remark

An ideal clustering would be k connected components, as this would have $Rcut = 0$. Thus finding clusters is a 'perturbation' of the problem of finding connected components.

Graphs and Associated Matrices

Definition

Given a graph G, its **Adjacency Matrix** *A is a non-negative $n \times n$ matrix defined by:*

$$A_{ij} = \begin{cases} a_{ij} & \text{if } \{i,j\} \in E \\ 0 & \text{otherwise} \end{cases}$$

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A is **symmetric** if G is **undirected**, **binary** if G is **unweighted**.

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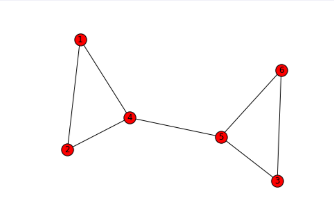
Remark

Given any permutation matrix P, $B = PAP^T$ is adjacency matrix of same graph G, just with labels of vertices permuted.

Graphs and Associated Matrices

Example

Consider the following graph G:



Which has adjacency matrix:

$$A = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 \end{bmatrix}$$

Graphs and Associated Matrices

Example

G clearly has two clusters. Moreover if P is the permutation matrix swapping the third and fourth rows (so P^T swaps the third and fourth columns) then:

$$PAP^T = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{bmatrix}$$

Which is 2-almost-reduced. (But note there are other P such that PAP^T is 2-almost-reduced.)

Graphs and Associated Matrices

Theorem

G has k connected components iff A is k reducible.
G has a good k clustering iff $A = \tilde{A} + E$ is k-almost-reducible and $||E||$ is small .

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Remark

Can associate a graph G to any symmetric, non-negative matrix A, thus question 1 and 2 are equivalent to graph-theoretic problems.

Graphs and Associated Matrices

Definition

Let A be the adjacency matrix of an undirected graph G.
Let $D = diag(d_1, \ldots, d_n)$.
The (unnormalized) **Graph Laplacian** *is defined as:*

$$L = D - A$$

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The (unnormalized) **Graph Laplacian** *is defined as:*

$$L = D - A$$

Note that $d_i = \sum_j a_{ij}$ and L can be defined for any symmetric non-negative matrix A.

Graphs and Associated Matrices

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Proof.

(See Chung, *Spectral graph theory*) □

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- Easier in practice to work with L than A, and A is (almost-) reduced iff L is (almost-) reduced.

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Definition

Suppose $|V| = n$*. For any* $C \subset V$*, define the* **indicator vector** $\mathbf{1}_C \in \mathbb{R}^n$ *as:*

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Follows from Courant-Fischer-Weyl minmax principle / Rayleigh quotient (Bhatia, *Matrix analysis*, Cor. III.1.2) □

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- Hence can think of them as approximations to indicator vectors of optimal clustering.

The Spectral Clustering Algorithm

Algorithm 1 Spectral Algorithm for clustering/ almost reducibility[11]

Given a non-negative, symmetric matrix A:

1. Compute eigenvalues of L, $\lambda_1, \ldots, \lambda_m$ for $1 < m << n$.
2. If $\lambda_1, \ldots, \lambda_k < \epsilon$ and $\lambda_{k+1} >> \epsilon$ then A is k-almost-reducible.
3. Compute eigenvectors $\mathbf{x}_1, \ldots, \mathbf{x}_k$. Let $X = [\mathbf{x}_1, \ldots, \mathbf{x}_k]$.
4. Let $\mathbf{w}^1, \ldots, \mathbf{w}^n$ denote **rows** of X. Sort these into k groups $R_1, \ldots, R_k$ using any linear time clustering algorithm (e.g. k-means).
5. Let $C_a = \{i : \mathbf{w}^i \in R_a\}$ for $a = 1, \ldots, k$.

[11] See: Ng, Jordan, and Weiss, "On Spectral Clustering: Analysis and Algorithm", and references therein.

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- *There exist (pathological) graphs on which Spectral approach will miss the best clustering (See the 'cockroach graphs' of Guattery and Miller, "On the performance of spectral graph partitioning methods")*
- *Observed to work well in practice and be robust to small perturbations.*

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Experimental Results: Artificial Data Set

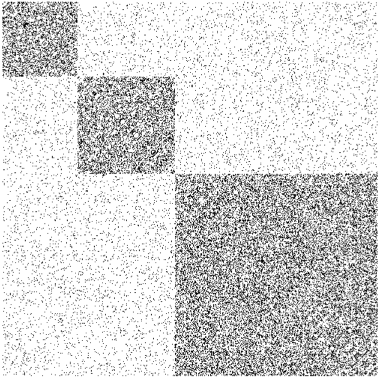

Figure: Original Matrix A

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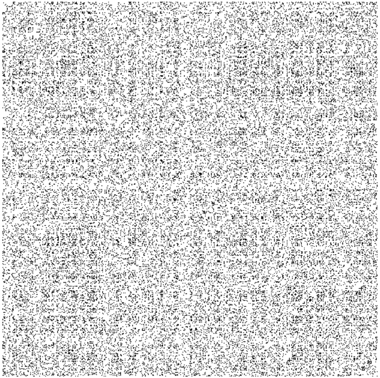

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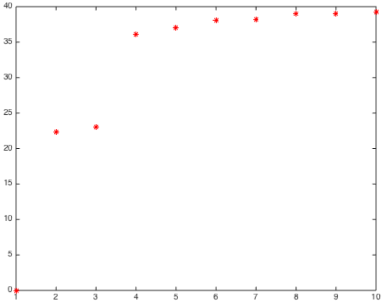

Figure: First 10 eigenvalues of L

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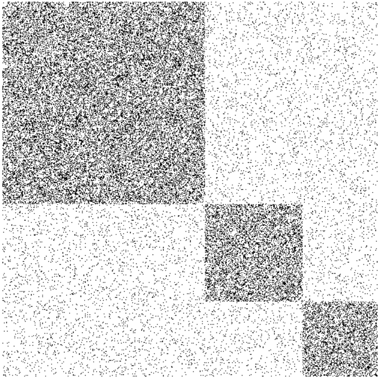


Figure: PAP^T for P found using spectral method

Experimental Results: Facebook Data Set[12]

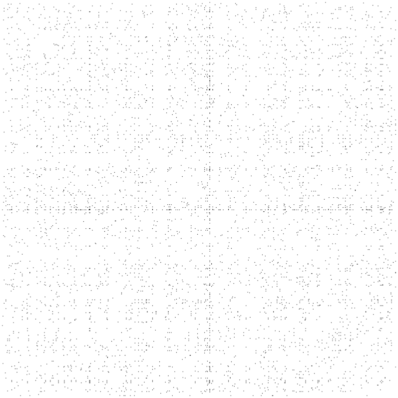
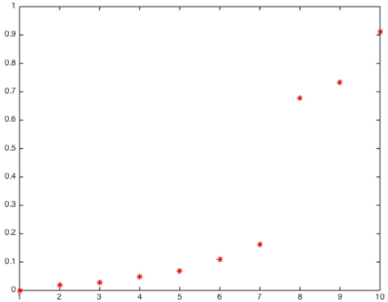


Figure: A for a graph G consisting of anonymised Facebook users and their friendship connections

[12]Leskovec and Krevl, *SNAP Datasets: Stanford Large Network Dataset Collection*

Experimental Results: Facebook Data Set[13]



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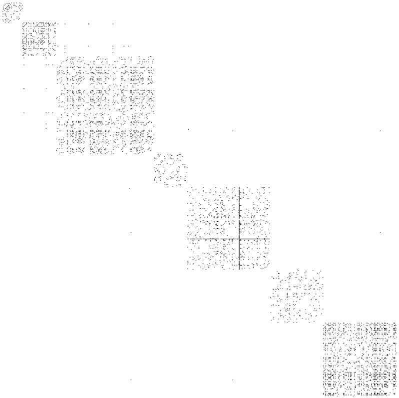

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Generalizations

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- Can we use this additional information to develop an eigenvector finding routine adapted specifically to the case of finding first k eigenvectors of a (graph) Laplacian?

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A Compressed sensing approach

- Consider again case where G has k connected components $C_1, \ldots, C_k$ (equivalently A is k-reducible).

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Idea: $\mathbf{1}_{C_1}$ has the fewest non-zero entries among all elements of $W_0 \setminus \{\mathbf{0}\}$, so we could find it as:

$$\min ||\mathbf{w}||_0 \text{ subject to } L\mathbf{w} = \mathbf{0} \tag{7}$$

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So: $L\mathbf{w} = \mathbf{0}$ and $w_1 = 1 \Leftrightarrow L_{-1}\hat{\mathbf{w}} = -\ell_1$ where $L = [\ell_1, \ell_2, \ldots, \ell_n]$ and $L_{-1} = [\ell_2, \ldots, \ell_n]$

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Lemma

If L is k-reducible the solution then $\mathbf{w}^* = \mathbf{1}_{i^*}$ where $1 \in C_{i^*}$ is the unique solution to (8)

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- Hence $\mathbf{w} = \mathbf{1}_{C_{i^*}}$ is indeed the minimizer.

$\square$

A Compressed sensing approach

Moreover, we can replace the 0 "norm" in (8) by any p norm (for $1 \leq p < \infty$):

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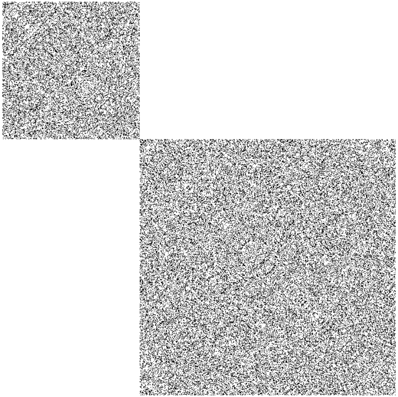

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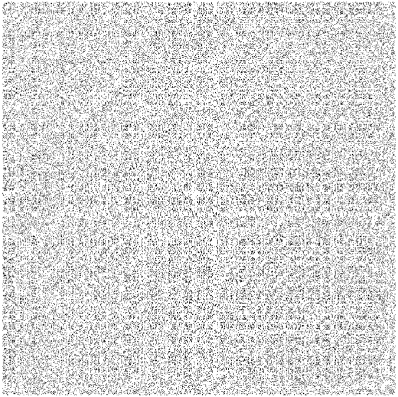

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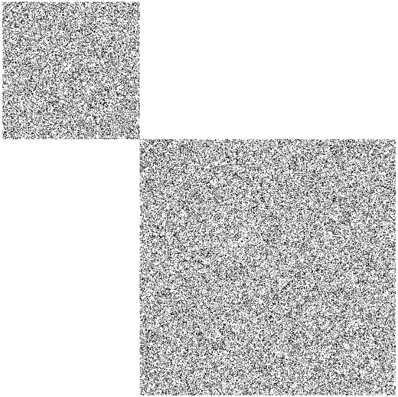

Figure: PAP^T for P found using Compressed Sensing method.

Preliminary Results

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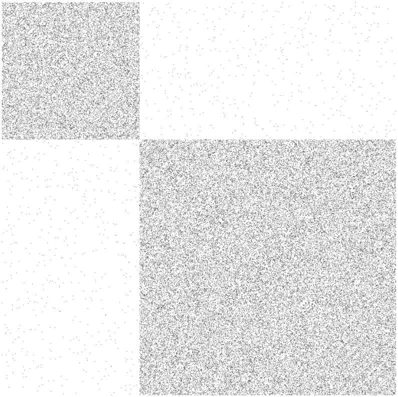

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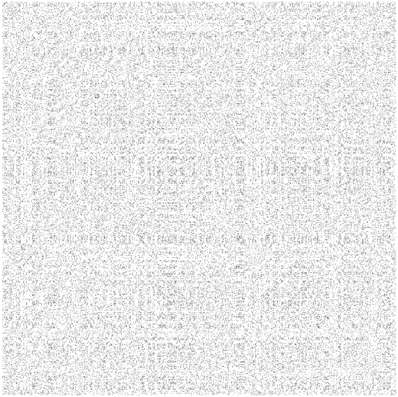

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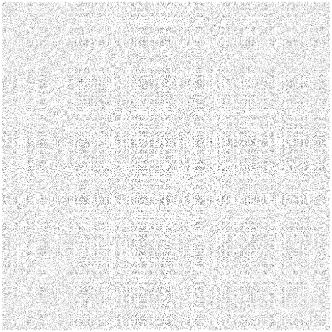

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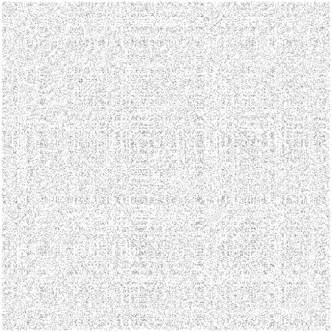

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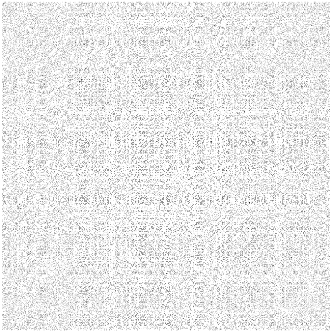

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The eigenspaces, however, are better behaved.

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Problem

For $X \in \mathbb{R}^{n\times k}$ let $\mathbf{r}_X \in \mathbb{R}^n$ denote vector of row sums of X. Find X^* such that:

$$X^* = \mathit{argmin}\{||LX|| \text{ subject to } \mathbf{r}_X = \mathbf{1}\}$$

(Another) Compressed Sensing Approach

Hopefully X^* will provide a good approximation to $\tilde{X}$.

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- Suppose

$$PAP^T = B = \begin{bmatrix} B_{11} & B_{12} & \cdots & B_{1,k} \\ 0 & B_{22} & \cdots & B_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & B_{kk} \end{bmatrix},$$

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- Now need only solve smaller systems

$$\begin{aligned}
\dot{\mathbf{y}}_k &= B_{kk}\mathbf{y}_k \\
\dot{\mathbf{y}}_{k-1} &= B_{k-1,k-1}\mathbf{y}_{k-1} + B_{k-1,k}\mathbf{y}_k \\
&\vdots \\
\dot{\mathbf{y}}_1 &= B_{11}\mathbf{y}_1 + B_{12}\mathbf{y}_2 + \ldots + B_{1r}\mathbf{y}_k
\end{aligned}$$

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- If A is sparse it likely is reducible. Will such a pre-processing step as above speed up numerical solution of this system?
- Even if $PAP^T = B + E$ with $||E|| << B)$ and B k-reduced, might we still find useful approximate solutions like this by ignoring E?

Application 2: Feature recognition in images

- Suppose we have a collection $\{\mathbf{y}_1, \ldots, \mathbf{y}_n]$ of images, each $\mathbf{y}_i \in \mathbb{R}^m$ $(n >> m)$.

[16] Ming-jun Lai. *Nonconvex and Non-Lipschitz Differentiable Minimization for Sparse Solution of Underdetermined Linear Systems*. 2016.

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- Suppose the $\mathbf{y}_i$ are images of k different people's faces, in a variety of angles and conditions.

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- Wish to sort the $\{\mathbf{y}_i\}$ into k groups, each corresponding to a single person.
- **Idea:**[16] each $\mathbf{y}_i$ should be well approximated by a linear combination of a (few) other images of same face.

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- Hence blocks of B should correspond to images of same face.

The End

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Any questions, comments or suggestions?

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