COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

Cameron Musco
University of Massachusetts Amherst. Fall 2019.
Lecture 14
• Midterm grades are on Moodle.
• Average was 32.67, median 33, standard deviation 6.8
• Come to office hours if you would like to see your exam/discuss solutions.
Last Few Weeks: Low-Rank Approximation and PCA
Summary

Last Few Weeks: Low-Rank Approximation and PCA

- Compress data that lies close to a $k$-dimensional subspace.
- Equivalent to finding a low-rank approximation of the data matrix $X$: $X \approx XVV^T$.
- Optimal solution via PCA (eigendecomposition of $X^TX$ or equivalently, SVD of $X$).
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This Class: Non-linear dimensionality reduction.
**SUMMARY**

**Last Few Weeks: Low-Rank Approximation and PCA**

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- Equivalent to finding a low-rank approximation of the data matrix $X$: $X \approx XVV^T$.
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**This Class: Non-linear dimensionality reduction.**

- How do we compress data that does not lie close to a $k$-dimensional subspace?
- Spectral methods (SVD and eigendecomposition) are still key techniques in this setting.
- Spectral graph theory, spectral clustering.
\[ \mathbb{R}^d \rightarrow \mathbb{R}^{d'} \quad d' < d \]

**End of Last Class:** Embedding objects other than vectors into Euclidean space.
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- Documents (for topic-based search and classification)
- Words (to identify synonyms, translations, etc.)
- Nodes in a social network
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- Documents (for topic-based search and classification)
- Words (to identify synonyms, translations, etc.)
- Nodes in a social network

Usual Approach: Convert each item into a high-dimensional feature vector and then apply low-rank approximation
EXAMPLE: LATENT SEMANTIC ANALYSIS

Term Document Matrix $X$

Low-Rank Approximation via SVD

$X \approx U_k \Sigma_k V_k^T$
EXAMPLE: LATENT SEMANTIC ANALYSIS

Term Document Matrix X

doc_1
0 0 1 0 0 1 1 0 0
doc_2
0 0 0 1 0 1 0 0 0

...  

doc_n
1 0 0 0 0 0 0 1 1

Low-Rank Approximation via SVD

\[ X \approx Y Z^T \]
EXAMPLE: LATENT SEMANTIC ANALYSIS

Term Document Matrix X

<table>
<thead>
<tr>
<th></th>
<th>car</th>
<th>loan</th>
<th>house</th>
<th>...</th>
<th>car</th>
<th>loan</th>
<th>house</th>
<th>...</th>
</tr>
</thead>
<tbody>
<tr>
<td>doc_1</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>doc_2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
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<tr>
<td>...</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
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<td>1</td>
</tr>
<tr>
<td>doc_n</td>
<td>0</td>
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<td>0</td>
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<td>0</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>doc_n</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

Low-Rank Approximation via SVD

\[
X \approx Y Z^T
\]
EXAMPLE: LATENT SEMANTIC ANALYSIS

Term Document Matrix $X$

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<thead>
<tr>
<th></th>
<th>car</th>
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<th>house</th>
<th>...</th>
<th>car</th>
<th>car</th>
</tr>
</thead>
<tbody>
<tr>
<td>doc_1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>doc_2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
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</tr>
<tr>
<td>...</td>
<td>1</td>
<td>0</td>
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<td>doc_n</td>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

Low-Rank Approximation via SVD

$X \approx Y Z^T$

- If the error $\|X - YZ^T\|_F$ is small, then on average,

$$X_{i,a} \approx (YZ^T)_{i,a} = \langle \vec{y}_i, \vec{z}_a \rangle$$
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· I.e., $\langle \vec{y}_i, \vec{z}_a \rangle \approx 1$ when $doc_i$ contains $word_a$. 

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• I.e., $\langle \vec{y}_i, \vec{z}_a \rangle \approx 1$ when $doc_i$ contains $word_a$.

• If $doc_i$ and $doc_j$ both contain $word_a$, $\langle \vec{y}_i, \vec{z}_a \rangle \approx \langle \vec{y}_j, \vec{z}_a \rangle \ll 1$. 

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**EXAMPLE: LATENT SEMANTIC ANALYSIS**

![Term Document Matrix X](image1)

![Low-Rank Approximation via SVD](image2)
If \( \text{doc}_i \) and \( \text{doc}_j \) both contain \( \text{word}_a \), \( \langle \vec{y}_i, \vec{z}_a \rangle \approx \langle \vec{y}_j, \vec{z}_a \rangle = 1 \)
If \( doc_i \) and \( doc_j \) both contain \( word_a \), \( \langle \tilde{y}_i, \tilde{z}_a \rangle \approx \langle \tilde{y}_j, \tilde{z}_a \rangle = 1 \)

**Another View:** Each column of \( Y \) represents a ‘topic’. \( \tilde{y}_i(j) \) indicates how much \( doc_i \) belongs to topic \( j \). \( \tilde{z}_a(j) \) indicates how much \( word_a \) associates with that topic.
• Just like with documents, $\tilde{z}_a$ and $\tilde{z}_b$ will tend to have high dot product if word
  $a$ and word $b$ appear in many of the same
documents.

$$\langle \tilde{y}_i, \tilde{y}_j \rangle = \tilde{z}_i(k) \tilde{y}_j(k)$$
• Just like with documents, $\bar{z}_a$ and $\bar{z}_b$ will tend to have high dot product if $word_i$ and $word_j$ appear in many of the same documents.

• In an SVD decomposition we set $Z = \Sigma_k V^T_k$. 
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• The columns of $V_k$ are equivalently: the top $k$ eigenvectors of $XX^T$. 
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- The columns of \( \mathbf{V}_k \) are equivalently: the top \( k \) eigenvectors of \( \mathbf{X} \mathbf{X}^T \). The eigendecomposition of \( \mathbf{X} \mathbf{X}^T \) is \( \mathbf{X} \mathbf{X}^T = \mathbf{V} \mathbf{\Sigma}^2 \mathbf{V}^T \).
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</tr>
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<tbody>
<tr>
<td>cat</td>
<td>loan</td>
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</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0</td>
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- The columns of $V_k$ are equivalently: the top $k$ eigenvectors of $XX^T$. The eigendecomposition of $XX^T$ is $XX^T = V \Sigma^2 V^T$.

- What is the best rank-$k$ approximation of $XX^T$? I.e.

$\arg \min_{\text{rank} - k} B \| XX^T - B \|_F$

$XX^TV_kV_k^T = V \Sigma^2 [V_k^TV_k]V_k^T \Rightarrow V_k \Sigma_k^2 V_k^T$
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\arg\min_{rank - k} B \|XX^T - B\|_F$

$XX^T \approx V_k \Sigma_k^2 V_k^T = ZZ^T$. 
EXAMPLE: WORD EMBEDDING

LSA gives a way of embedding words into $k$-dimensional space.

- Embedding is via low-rank approximation of $\mathbf{X}\mathbf{X}^T$: where $(\mathbf{X}\mathbf{X}^T)_{a,b}$ is the number of documents that both $\text{word}_a$ and $\text{word}_b$ appear in.
LSA gives a way of embedding words into $k$-dimensional space.

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$$words \rightarrow \text{s}im\text{ilarity matrix} \rightarrow \text{LR approx embedding of words}$$

- Think about $XX^T$ as a similarity matrix (gram matrix, kernel matrix) with entry $(a, b)$ being the similarity between $word_a$ and $word_b$. 
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- Many ways to measure similarity: number of sentences both occur in, number of time both appear in the same window of \( w \) words, in similar positions of documents in different languages, etc.
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- Many ways to measure similarity: number of sentences both occur in, number of time both appear in the same window of $w$ words, in similar positions of documents in different languages, etc.

- Replacing $XX^T$ with these different metrics (sometimes appropriately transformed) leads to popular word embedding algorithms: word2vec, GloVe, fastText, etc.
EXAMPLE: WORD EMBEDDING
Note: word2vec is typically described as a neural-network method, but it is really just low-rank approximation of a specific similarity matrix. *Neural word embedding as implicit matrix factorization*, Levy and Goldberg.
A common way of encoding similarity is via a graph. E.g., a $k$-nearest neighbor graph.

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Is this set of points compressible? Does it lie close to a low-dimensional subspace?
Once we have connected $n$ data points $x_1, \ldots, x_n$ into a graph, we can represent that graph by its (weighted) adjacency matrix.

$$A \in \mathbb{R}^{n \times n} \text{ with } A_{i,j} = \text{ edge weight between nodes } i \text{ and } j$$
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In LSA example, when \( X \) is the term-document matrix, \( X^TX \) is like an adjacency matrix, where \( \text{word}_a \) and \( \text{word}_b \) are connected if they appear in at least 1 document together (edge weight is \# documents they appear in together).
NORMALIZED ADJACENCY MATRIX

What is the sum of entries in the $i^{th}$ column of $A$?
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NORMALIZED ADJACENCY MATRIX

\[ \overrightarrow{\mathbf{A}} = \mathbf{D}^{-1/2} \mathbf{A} \]

\[
\begin{bmatrix}
0 & \frac{1}{\sqrt{3}} & 0 & 0 \\
\frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{6}} & 0 \\
0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{2} \\
0 & \frac{1}{\sqrt{3}} & \frac{1}{2} & 0 \\
\end{bmatrix}
= \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & \frac{1}{\sqrt{3}} & 0 & 0 \\
0 & 0 & \frac{1}{\sqrt{2}} & 0 \\
0 & 0 & 0 & \frac{1}{\sqrt{2}} \\
\end{bmatrix}
\begin{bmatrix}
0 & 1 & 0 & 0 \\
1 & 0 & 1 & 1 \\
0 & 1 & 0 & 1 \\
0 & 1 & 1 & 0 \\
\end{bmatrix}
= \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & \frac{1}{\sqrt{3}} & 0 & 0 \\
0 & 0 & \frac{1}{\sqrt{2}} & 0 \\
0 & 0 & 0 & \frac{1}{\sqrt{2}} \\
\end{bmatrix}
\]

What is the sum of entries in the \(i^{th}\) column of \(\mathbf{A}\)? The (weighted) degree of vertex \(i\).

Often, \(\mathbf{A}\) is normalized as \(\overrightarrow{\mathbf{A}} = \mathbf{D}^{-1/2} \mathbf{A} \mathbf{D}^{-1/2}\) where \(\mathbf{D}\) is the degree matrix.

**Spectral graph theory** is the field of representing graphs as matrices and applying linear algebraic techniques.
How do we compute an optimal low-rank approximation of $A$?
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- Project onto the top \( k \) eigenvectors of \( A^T A = A^2 \).
How do we compute an optimal low-rank approximation of $A$?

- Project onto the top $k$ eigenvectors of $A^TA = A^2$. These are just the eigenvectors of $A$.

\[
A = \mathbf{V}\Lambda\mathbf{V}^T \quad A^2 = \mathbf{V}\Lambda^2\mathbf{V}^T = \mathbf{V}\Lambda^{2}\mathbf{V}^T
\]

\[
A \approx A_{V_k}V_{k}^T = \mathbf{V}\Lambda^{[1]}_{k}V_{k}^T
\]

\[
A \approx V_k\Lambda_kV_k^T \quad \text{best LR approx of } A.
\]
ADJACENCY MATRIX EIGENVECTORS
• Similar vertices (close with regards to graph proximity) should have similar embeddings. I.e., $V_k(i)$ should be similar to $V_k(j)$.
SPECTRAL EMBEDDING

1. Swiss roll

A \in \mathbb{R}^{n \times n}

\phi

V_k

V_i \uparrow \quad \uparrow \quad \uparrow

V_i \quad V_i \quad V_i

n \begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix}

k
A very common task aside from just embedding points via graph based similarity and SVD, is to partition or cluster vertices based on this similarity.
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Non-linearly separable data.
A very common task aside from just embedding points via graph based similarity and SVD, is to partition or cluster vertices based on this similarity.

Community detection in naturally occurring networks.

(a) Zachary Karate Club Graph
**Simple Idea:** Partition clusters along minimum cut in graph.

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Small cuts are often not informative.
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**Solution:** Encourage cuts that separate large sections of the graph.
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Small cuts are often not informative.

**Solution:** Encourage cuts that separate large sections of the graph.

- Let $\mathbf{v} \in \mathbb{R}^n$ represent a cut: $\mathbf{v}(i) = 1$ if $i \in S$ and $\mathbf{v}(i) = -1$ if $i \in T$. Want $\mathbf{v}$ to have roughly equal numbers of 1s and -1s. I.e., $\mathbf{v}^T \mathbf{1} \approx 0$. 

(a) Zachary Karate Club Graph
For a graph with adjacency matrix $A$ and degree matrix $D$, $L = D - A$ is the graph Laplacian.
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For any vector $\vec{v}$,

$$\vec{v}^T L \vec{v} = \vec{v}^T D \vec{v} - \vec{v}^T A \vec{v} = \sum_{i=1}^{n} d(i) \vec{v}(i)^2 - \sum_{i=1}^{n} \sum_{j=1}^{n} A(i, j) \cdot \vec{v}(i) \cdot \vec{v}(j)$$

$$= \sum_{i,j \in E} (\vec{v}(i) - \vec{v}(j))^2 = \sum_{i,j \in E} [\vec{v}(i)^2 + \vec{v}(j)^2 - 2\vec{v}(i)\vec{v}(j)]$$
For a cut indicator vector $\vec{v} \in \{-1, 1\}^n$ with $\vec{v}(i) = -1$ for $i \in S$ and $\vec{v}(i) = 1$ for $i \in T$:

$$\vec{v}^T L \vec{v} = \sum_{(i,j) \in E} (\vec{v}(i) - \vec{v}(j))^2 = 4 \cdot \text{cut}(S, T).$$

So minimizing $\vec{v}^T L \vec{v}$ corresponds to minimizing the cut size.
For a cut indicator vector $\vec{v} \in \{-1, 1\}^n$ with $\vec{v}(i) = -1$ for $i \in S$ and $\vec{v}(i) = 1$ for $i \in T$:

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So minimizing $\vec{v}^T L \vec{v}$ corresponds to minimizing the cut size.

$$\arg \min_{\vec{v} \in \{-1, 1\}^n} \vec{v}^T L \vec{v}$$
For a cut indicator vector $\vec{v} \in \{-1, 1\}^n$ with $\vec{v}(i) = -1$ for $i \in S$ and $\vec{v}(i) = 1$ for $i \in T$:

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So minimizing $\vec{v}^T L \vec{v}$ corresponds to minimizing the cut size.

$$\max \quad \arg \min \quad \vec{v}^T L \vec{v}$$

$$\vec{v} \in \mathbb{R}^d \text{ with } ||\vec{v}||=1$$
For a cut indicator vector \( \mathbf{v} \in \{-1, 1\}^n \) with \( \mathbf{v}(i) = -1 \) for \( i \in S \) and \( \mathbf{v}(i) = 1 \) for \( i \in T \):

\[
\mathbf{v}^T L \mathbf{v} = \sum_{(i,j) \in E} (\mathbf{v}(i) - \mathbf{v}(j))^2 = 4 \cdot \text{cut}(S, T).
\]

So minimizing \( \mathbf{v}^T L \mathbf{v} \) corresponds to minimizing the cut size.

\[
\mathbf{v}^T L \mathbf{v} = 0 \quad \arg \min_{\mathbf{v} \in \mathbb{R}^d \text{ with } \|\mathbf{v}\| = 1} \mathbf{v}^T L \mathbf{v}
\]

By the Courant-Fischer theorem, \( \mathbf{v} \) is the \textit{smallest} eigenvector of \( L = D - A \).
SMALLEST LAPLACIAN EIGENVECTOR

\[ L = \begin{bmatrix} \Lambda & I \\ -I & A \end{bmatrix} \]

We have:

\[ \vec{v}_n = \frac{1}{\sqrt{n}} \cdot \vec{1} = \arg \min_{\vec{v} \in \mathbb{R}^d \text{ with } \|\vec{v}\| = 1} \vec{v}^T L \vec{v} \]

with \( \vec{v}_n^T L \vec{v}_n = 0. \)
We have:

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with $$\vec{v}_n^T L \vec{v}_n = 0.$$
By Courant-Fischer, second small eigenvector is obtained greedily:

\[ \vec{v}_1 = \arg \min_{\vec{v} \in \mathbb{R}^d \text{ with } \|\vec{v}\|=1} \vec{v}^T L \vec{v} \]

\[ \vec{v}_2 = \arg \min_{\vec{v} \in \mathbb{R}^d \text{ with } \|\vec{v}\|=1, \vec{v}_2 \vec{v}_1 = 0} \vec{v}^T L \vec{v} \]
By Courant-Fischer, second small eigenvector is obtained greedily:

\[
\tilde{v}_1 = \arg \min_{v \in \mathbb{R}^d \text{ with } \|v\| = 1} v^T L \tilde{v}
\]

\[
\tilde{v}_2 = \arg \min_{v \in \mathbb{R}^d \text{ with } \|v\| = 1, \, \tilde{v}_2^T \tilde{v}_1 = 0} v^T L \tilde{v}
\]

If \( \tilde{v}_2 \) were binary \( \{-1, 1\}^d \), orthogonality condition ensures that there are an equal number of vertices on each side of the cut.
By Courant-Fischer, second small eigenvector is obtained greedily:

$$\vec{v}_1 = \arg \min_{\vec{v} \in \mathbb{R}^d \text{with } \|\vec{v}\| = 1} \vec{v}^T L \vec{v}$$

$$\vec{v}_2 = \arg \min_{\vec{v} \in \mathbb{R}^d \text{with } \|\vec{v}\| = 1, \vec{v}_1^T \vec{v}_1 = 0} \vec{v}^T L \vec{v}$$

If $\vec{v}_2$ were binary $\{-1, 1\}^d$, orthogonality condition ensures that there are an equal number of vertices on each side of the cut. When $\vec{v}_2 \in \mathbb{R}^d$, enforces a ‘relaxed’ version of this constraint.
Find a good partition of the graph by computing

\[ \vec{v}_2 = \arg \min_{\vec{v} \in \mathbb{R}^d \text{ with } \|\vec{v}\| = 1, \vec{v}_2 \cdot 1 = 0} \vec{v}^T L \vec{v} \]

Set \( S \) to be all nodes with \( \vec{v}_2(i) < 0 \), \( T \) to be all with \( \vec{v}_2(i) \geq 0 \).
Find a good partition of the graph by computing

\[ \vec{v}_2 = \arg \min_{\vec{v} \in \mathbb{R}^d \text{ with } \|\vec{v}\|=1} \vec{v}^T L \vec{v} \]

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Find a good partition of the graph by computing

$$\vec{v}_2 = \arg\min_{\mathbf{v} \in \mathbb{R}^d \text{with } \|\mathbf{v}\| = 1, \ \vec{v}_2 \mathbf{1} = 0} \mathbf{v}^T L \mathbf{v}$$

Set $S$ to be all nodes with $\vec{v}_2(i) < 0$, $T$ to be all with $\vec{v}_2(i) \geq 0$.

The Shi-Malik normalized cuts algorithm is a commonly used variance on this approach, using the normalize Laplacian $D^{-1/2} L D^{-1/2}$. 
The smallest eigenvectors of $L = D - A$ give the orthogonal ‘functions’ that are smoothest over the graph. I.e., minimize

$$\vec{v}^T L \vec{v} = \sum_{(i,j) \in E} [\vec{v}(i) - \vec{v}(j)]^2.$$
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Embedding points with coordinates given by $[\vec{v}_{n-1}(j), \vec{v}_{n-2}(j), \ldots, \vec{v}_{n-k}(j)]$ ensures that coordinates connected by edges have minimum Euclidean distance.
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The smallest eigenvectors of $\mathbf{L} = \mathbf{D} - \mathbf{A}$ give the orthogonal ‘functions’ that are smoothest over the graph. I.e., minimize

$$\nabla^T \mathbf{L} \nabla = \sum_{(i,j) \in E} [\nabla(i) - \nabla(j)]^2.$$ 

Embedding points with coordinates given by $[\nabla_{n-1}(j), \nabla_{n-2}(j), \ldots, \nabla_{n-k}(j)]$ ensures that coordinates connected by edges have minimum Euclidean distance.

- Laplacian Eigenmaps
- Locally linear embedding
- Isomap
- Etc...
Questions?