# Manifold Learning for Signal and Visual Processing Lecture 3: Introduction to Graphs, Graph Matrices, and Graph Embeddings

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#### Outline of Lecture 3

- What is spectral graph theory?
- Some graph notation and definitions
- The adjacency matrix
- Laplacian matrices
- Spectral graph embedding

#### Material for this lecture

- F. R. K. Chung. Spectral Graph Theory. 1997. (Chapter 1)
- M. Belkin and P. Niyogi. Laplacian Eigenmaps for Dimensionality Reduction and Data Representation. Neural Computation, 15, 1373–1396 (2003).
- U. von Luxburg. A Tutorial on Spectral Clustering. Statistics and Computing, 17(4), 395–416 (2007). (An excellent paper)
- Software: http://open-specmatch.gforge.inria.fr/index.php.
   Computes, among others, Laplacian embeddings of very large graphs.

# Spectral graph theory at a glance

- The spectral graph theory studies the properties of graphs via the eigenvalues and eigenvectors of their associated graph matrices: the adjacency matrix, the graph Laplacian and their variants.
- These matrices have been extremely well studied from an algebraic point of view.
- The Laplacian allows a natural link between discrete representations (graphs), and continuous representations, such as metric spaces and manifolds.
- Laplacian embedding consists in representing the vertices of a graph in the space spanned by the smallest eigenvectors of the Laplacian – A geodesic distance on the graph becomes a spectral distance in the embedded (metric) space.

# Spectral graph theory and manifold learning

- ullet First we construct a graph from  $oldsymbol{x}_1, \dots oldsymbol{x}_n \in \mathbb{R}^D$
- ullet Then we compute the d smallest eigenvalue-eigenvector pairs of the graph Laplacian
- Finally we represent the data in the  $\mathbb{R}^d$  space spanned by the corresponding orthonormal eigenvector basis. The choice of the dimension d of the embedded space is not trivial.
- ullet Paradoxically, d may be larger than D in many cases!

# Basic graph notations and definitions

We consider *simple graphs* (no multiple edges or loops),  $\mathcal{G} = \{\mathcal{V}, \mathcal{E}\}$ :

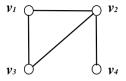
- $V(G) = \{v_1, \dots, v_n\}$  is called the *vertex set* with n = |V|;
- $\mathcal{E}(\mathcal{G}) = \{e_{ij}\}$  is called the *edge set* with  $m = |\mathcal{E}|$ ;
- An edge  $e_{ij}$  connects vertices  $v_i$  and  $v_j$  if they are adjacent or neighbors. One possible notation for adjacency is  $v_i \sim v_j$ ;
- The number of neighbors of a node v is called the *degree* of v and is denoted by d(v),  $d(v_i) = \sum_{v_i \sim v_j} e_{ij}$ . If all the nodes of a graph have the same degree, the graph is *regular*; The nodes of an *Eulerian* graph have even degree.
- A graph is complete if there is an edge between every pair of vertices.

# The adjacency matrix of a graph

• For a graph with n vertices, the entries of the  $n \times n$  adjacency matrix are defined by:

$$\mathbf{A} := \left\{ \begin{array}{ll} A_{ij} = 1 & \text{ if there is an edge } e_{ij} \\ A_{ij} = 0 & \text{ if there is no edge} \\ A_{ii} = 0 \end{array} \right.$$

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



# Eigenvalues and eigenvectors

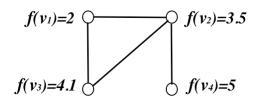
- A is a real-symmetric matrix: it has n real eigenvalues and its n real eigenvectors form an orthonormal basis.
- Let  $\{\lambda_1, \ldots, \lambda_i, \ldots, \lambda_r\}$  be the set of *distinct* eigenvalues.
- The eigenspace  $S_i$  contains the eigenvectors associated with  $\lambda_i$ :

$$S_i = \{ \boldsymbol{x} \in \mathbb{R}^n | \mathbf{A}\boldsymbol{x} = \lambda_i \boldsymbol{x} \}$$

- For real-symmetric matrices, the algebraic multiplicity is equal to the geometric multiplicity, for all the eigenvalues.
- The dimension of  $S_i$  (geometric multiplicity) is equal to the multiplicity of  $\lambda_i$ .
- If  $\lambda_i \neq \lambda_j$  then  $S_i$  and  $S_j$  are mutually orthogonal.

### Real-valued functions on graphs

- We consider real-valued functions on the set of the graph's vertices,  $f: \mathcal{V} \longrightarrow \mathbb{R}$ . Such a function assigns a real number to each graph node.
- ullet f is a vector indexed by the graph's vertices, hence  $f\in\mathbb{R}^n$ .
- Notation:  $\boldsymbol{f} = (f(v_1), \dots, f(v_n)) = (f_1, \dots, f_n)$ .
- The eigenvectors of the adjacency matrix,  $\mathbf{A}x = \lambda x$ , can be viewed as *eigenfunctions*.



# Matrix A as an operator and quadratic form

The adjacency matrix can be viewed as an operator

$$\boldsymbol{g} = \mathbf{A}\boldsymbol{f}; g(i) = \sum_{i \sim j} f(j)$$

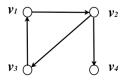
It can also be viewed as a quadratic form:

$$\boldsymbol{f}^{\top} \mathbf{A} \boldsymbol{f} = \sum_{e_{ij}} f(i) f(j)$$

# The incidence matrix of a graph

- Let each edge in the graph have an arbitrary but fixed orientation;
- The incidence matrix of a graph is a  $|\mathcal{E}| \times |\mathcal{V}|$   $(m \times n)$  matrix defined as follows:

$$\bigtriangledown := \left\{ \begin{array}{ll} \bigtriangledown_{ev} = -1 & \text{if } v \text{ is the initial vertex of edge } e \\ \bigtriangledown_{ev} = 1 & \text{if } v \text{ is the terminal vertex of edge } e \\ \bigtriangledown_{ev} = 0 & \text{if } v \text{ is not in } e \end{array} \right.$$



# The incidence matrix: A discrete differential operator

- The mapping  $f \longrightarrow \nabla f$  is known as the *co-boundary mapping* of the graph.

$$\begin{bmatrix} -1 & 1 & 0 & 0 \\ 1 & 0 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & -1 & 0 & +1 \end{bmatrix} \begin{pmatrix} f(1) \\ f(2) \\ f(3) \\ f(4) \end{pmatrix} = \begin{pmatrix} f(2) - f(1) \\ f(1) - f(3) \\ f(3) - f(2) \\ f(4) - f(2) \end{pmatrix}$$

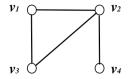
# The Laplacian matrix of a graph

- $\mathbf{L} = \nabla^{\top} \nabla$
- $(\mathbf{L}\mathbf{f})(v_i) = \sum_{v_i \sim v_i} (f(v_i) f(v_j))$
- Connection between the Laplacian and the adjacency matrices:

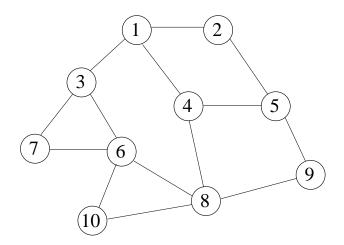
$$L = D - A$$

• The degree matrix:  $\mathbf{D} := D_{ii} = d(v_i)$ .

$$\mathbf{L} = \begin{bmatrix} 2 & -1 & -1 & 0 \\ -1 & 3 & -1 & -1 \\ -1 & -1 & 2 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix}$$



# Example: A graph with 10 nodes



# The adjacency matrix

# The Laplacian matrix

$$\mathbf{L} = \begin{bmatrix} 3 & -1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 2 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 3 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 3 & -1 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & -1 & 3 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 4 & -1 & -1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 & -1 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & -1 & 0 & 4 & -1 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 2 & 0 & 0 \end{bmatrix}$$

# The Eigenvalues of this Laplacian

$$\Lambda = \begin{bmatrix}
0.0000 & 0.7006 & 1.1306 & 1.8151 & 2.4011 \\
3.0000 & 3.8327 & 4.1722 & 5.2014 & 5.7462
\end{bmatrix}$$

# Matrices of an Undirected Weighted Graph

• We consider *undirected weighted graphs*; Each edge  $e_{ij}$  is weighted by  $w_{ij} > 0$ . We obtain:

$$oldsymbol{\Omega} := \left\{ egin{array}{ll} \Omega_{ij} = w_{ij} & ext{ if there is an edge } e_{ij} \\ \Omega_{ij} = 0 & ext{ if there is no edge} \\ \Omega_{ii} = 0 & ext{ } \end{array} 
ight.$$

ullet The degree matrix:  $\mathbf{D} = \sum_{i \sim j} w_{ij}$ 

# The Laplacian on an undirected weighted graph

- $L = D \Omega$
- The Laplacian as an operator:

$$(\mathbf{L}f)(v_i) = \sum_{v_j \sim v_i} w_{ij} (f(v_i) - f(v_j))$$

• As a quadratic form:

$$\mathbf{f}^{\top} \mathbf{L} \mathbf{f} = \frac{1}{2} \sum_{e_{ij}} w_{ij} (f(v_i) - f(v_j))^2$$

- L is symmetric and positive semi-definite  $\leftrightarrow w_{ij} \ge 0$ .
- L has n non-negative, real-valued eigenvalues:  $0 = \lambda_1 < \lambda_2 < \ldots < \lambda_n$ .

# Other adjacency matrices

The normalized weighted adjacency matrix

$$\mathbf{\Omega}_N = \mathbf{D}^{-1/2} \mathbf{\Omega} \mathbf{D}^{-1/2}$$

• The *transition* matrix of the Markov process associated with the graph:

$$\mathbf{\Omega}_R = \mathbf{D}^{-1}\mathbf{\Omega} = \mathbf{D}^{-1/2}\mathbf{\Omega}_N \mathbf{D}^{1/2}$$

# Several Laplacian matrices

- The unnormalized Laplacian which is also referred to as the combinatorial Laplacian  $\mathbf{L}_C$ ,
- ullet the normalized Laplacian  ${f L}_N$ , and
- ullet the random-walk Laplacian  ${f L}_R$  also referred to as the discrete Laplace operator.

#### We have:

$$\mathbf{L}_C = \mathbf{D} - \mathbf{\Omega}$$
  
 $\mathbf{L}_N = \mathbf{D}^{-1/2} \mathbf{L}_C \mathbf{D}^{-1/2} = \mathbf{I} - \mathbf{\Omega}_N$   
 $\mathbf{L}_R = \mathbf{D}^{-1} \mathbf{L}_C = \mathbf{I} - \mathbf{\Omega}_R$ 

# Relationships between all these matrices

$$\mathbf{L}_{C} = \mathbf{D}^{1/2} \mathbf{L}_{N} \mathbf{D}^{1/2} = \mathbf{D} \mathbf{L}_{R}$$
 $\mathbf{L}_{N} = \mathbf{D}^{-1/2} \mathbf{L}_{C} \mathbf{D}^{-1/2} = \mathbf{D}^{1/2} \mathbf{L}_{R} \mathbf{D}^{-1/2}$ 
 $\mathbf{L}_{R} = \mathbf{D}^{-1/2} \mathbf{L}_{N} \mathbf{D}^{1/2} = \mathbf{D}^{-1} \mathbf{L}_{C}$ 

# Some spectral properties of the Laplacians

Laplacian	Null space	Eigenvalues	Eigenvectors
$\mathbf{L}_C =$	$u_1 = 1$	$0 = \lambda_1 < \lambda_2 \le$	
$\mathbf{U}\mathbf{\Lambda}\mathbf{U}^{ op}$		$  \ldots   \leq \lambda_n \leq 1$	$\mid oldsymbol{u}_i^ op oldsymbol{u}_j = \delta_{ij}  \mid$
		$2 \max_i(d_i)$	
$\mathbf{L}_N =$	$oldsymbol{w}_1 = \mathbf{D}^{1/2} 1$	$0 = \gamma_1 < \gamma_2 \le$	$egin{aligned} oldsymbol{w}_{i>1}^{ op} \mathbf{D}^{1/2} 1 = \end{aligned}$
$\mathbf{W} \mathbf{\Gamma} \mathbf{W}^ op$		$\ldots \leq \gamma_n \leq 2$	0,
			$egin{aligned} oldsymbol{w}_i^ op oldsymbol{w}_j = \delta_{ij} \end{aligned}$
	$oldsymbol{t}_1 = oldsymbol{1}$	$0 = \gamma_1 < \gamma_2 \le$	
$\mathbf{T}\mathbf{\Gamma}\mathbf{T}^{-1}$		$\ldots \leq \gamma_n \leq 2$	$egin{aligned} oldsymbol{t}_i^{ op} \mathbf{D} oldsymbol{t}_j = \delta_{ij} \end{aligned}$
$\mathbf{T} =$			
$\mathbf{D}^{-1/2}\mathbf{W}$			

# Spectral properties of adjacency matrices

From the relationship between the normalized Laplacian and adjacency matrix:  $\mathbf{L}_N = \mathbf{I} - \mathbf{\Omega}_N$  one can see that their eigenvalues satisfy:

$$\gamma = 1 - \psi$$

Adjacency matrix	Eigenvalues	Eigenvectors
$\mathbf{\Omega}_N = \mathbf{W} \mathbf{W} \mathbf{W}^{T},$	$-1 \le \psi_n \le \ldots \le \psi_2 <$	$oldsymbol{w}_i^ op oldsymbol{w}_j = \delta_{ij}$
$\Psi = \mathrm{I} - \Gamma$	$\psi_1 = 1$	
$\mathbf{\Omega}_R = \mathbf{T} \mathbf{\Psi} \mathbf{T}^{-1}$	$-1 \le \psi_n \le \ldots \le \psi_2 <$	$oldsymbol{t}_i^{ op} \mathbf{D} oldsymbol{t}_j = \delta_{ij}$
	$\psi_1 = 1$	

# Eigenvalue and Eigenvectors of the Normalized and Random Laplacians

Eigenvalues of the normalized adjacent matrix:

$$1 = \psi_1 \ge \psi_2 \ge \ldots \ge \psi_n \ge -1$$

- The largest eigenvalue-eigenvector pair:  $(\psi_1 = 1, \boldsymbol{w}_1 = \mathbf{D}^{1/2} \mathbf{1})$
- The estimation of the smallest non null eigenvalue-eigenvector pairs of  $\mathbf{L}_N$  involves the shifted inverse power method.
- The second, third, etc., largest eigenvalue-eigenvector pair of  $\Omega_N$  can be obtained with the direct power method and deflation:

$$ilde{m{\Omega}}_N = m{\Omega}_N - m{w}_1 m{w}_1^{ op}$$

• Remark: Sparsity is lost by deflation!

# The Laplacian of a graph with one connected component

- $\mathbf{L} \boldsymbol{u} = \lambda \boldsymbol{u}$ .
- L1 = 0,  $\lambda_1 = 0$  is the smallest eigenvalue.
- The *one* vector:  $\mathbf{1} = (1 \dots 1)^{\top}$ .
- $0 = \mathbf{u}^{\top} \mathbf{L} \mathbf{u} = \sum_{i,j=1}^{n} w_{ij} (u(i) u(j))^{2}$ .
- If any two vertices are connected by a path, then  $\boldsymbol{u}=(u(1),\ldots,u(n))$  needs to be constant at all vertices such that the quadratic form vanishes. Therefore, a graph with one connected component has the constant vector  $\boldsymbol{u}_1=\mathbf{1}$  as the only eigenvector with eigenvalue 0.

# A graph with k > 1 connected components

Each connected component has an associated Laplacian.
 Therefore, we can write matrix L as a block diagonal matrix:

$$\mathbf{L} = \left[ egin{array}{cccc} \mathbf{L}_1 & & & \ & \ddots & \ & & \mathbf{L}_k \end{array} 
ight]$$

- ullet The spectrum of  ${f L}$  is given by the union of the spectra of  ${f L}_i$ .
- Each block corresponds to a connected component, hence each matrix  $L_i$  has an eigenvalue 0 with multiplicity 1.
- ullet The spectrum of  ${f L}$  is given by the union of the spectra of  ${f L}_i.$
- The eigenvalue  $\lambda_1 = 0$  has multiplicity k.

# The eigenspace of $\lambda_1 = 0$ with multiplicity k

• The eigenspace corresponding to  $\lambda_1 = \ldots = \lambda_k = 0$  is spanned by the k mutually orthogonal vectors:

$$egin{aligned} oldsymbol{u}_1 &= oldsymbol{1}_{L_1} \ & \dots \ oldsymbol{u}_k &= oldsymbol{1}_{L_k} \end{aligned}$$

- with  $\mathbf{1}_{L_i} = (00001111110000)^{\top} \in \mathbb{R}^n$
- These vectors are the indicator vectors of the graph's connected components.
- Notice that  $\mathbf{1}_{L_1}+\ldots+\mathbf{1}_{L_k}=\mathbf{1}$

# The Fiedler vector of the graph Laplacian

- The first non-null eigenvalue  $\lambda_{k+1}$  is called the Fiedler value.
- ullet The corresponding eigenvector  $oldsymbol{u}_{k+1}$  is called the Fiedler vector.
- The multiplicity of the Fiedler eigenvalue depends on the graph's structure and it is difficult to analyse.
- The Fiedler value is the *algebraic connectivity of a graph*, the further from 0, the more connected.
- The Fiedler vector has been extensively used for spectral bi-partioning
- Theoretical results are summarized in Spielman & Teng 2007: http://cs-www.cs.yale.edu/homes/spielman/

# Eigenvectors of the Laplacian of connected graphs

- $u_1 = 1, L1 = 0.$
- $u_2$  is the *the Fiedler vector* with multiplicity 1.
- ullet The eigenvectors form an orthonormal basis:  $oldsymbol{u}_i^ op oldsymbol{u}_j = \delta_{ij}.$
- For any eigenvector  $\boldsymbol{u}_i = (\boldsymbol{u}_i(v_1) \dots \boldsymbol{u}_i(v_n))^\top, \ 2 \leq i \leq n$ :

$$\boldsymbol{u}_i^{\top} \mathbf{1} = 0$$

• Hence the components of  $u_i$ ,  $2 \le i \le n$  satisfy:

$$\sum_{j=1}^{n} \boldsymbol{u}_i(v_j) = 0$$

• Each component is bounded by:

$$-1 < \boldsymbol{u}_i(v_i) < 1$$

# Laplacian embedding: Mapping a graph on a line

• Map a weighted graph onto a line such that connected nodes stay as close as possible, i.e., minimize  $\sum_{i,j=1}^{n} w_{ij} (f(v_i) - f(v_j))^2, \text{ or:}$ 

$$\arg\min_{\boldsymbol{f}} \boldsymbol{f}^{\top} \mathbf{L} \boldsymbol{f} \text{ with: } \boldsymbol{f}^{\top} \boldsymbol{f} = 1 \text{ and } \boldsymbol{f}^{\top} \mathbf{1} = 0$$

- The solution is the eigenvector associated with the smallest nonzero eigenvalue of the eigenvalue problem:  $\mathbf{L} f = \lambda f$ , namely the Fiedler vector  $u_2$ .
- Practical computation of the eigenpair  $\lambda_2, u_2$ ): the shifted inverse power method (see lecture 2).

# The shifted inverse power method (from Lecture 2)

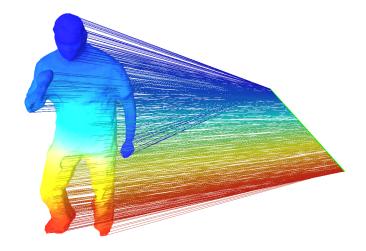
- Let's consider the matrix  $\mathbf{B} = \mathbf{A} \alpha \mathbf{I}$  as well as an eigenpair  $\mathbf{A} \boldsymbol{u} = \lambda \boldsymbol{u}$ .
- $(\lambda \alpha, \mathbf{u})$  becomes an eigenpair of  $\mathbf{B}$ , indeed:

$$\mathbf{B}\boldsymbol{u} = (\mathbf{A} - \alpha \mathbf{I})\boldsymbol{u} = (\lambda - \alpha)\boldsymbol{u}$$

and hence **B** is a **real symmetric** matrix with eigenpairs  $(\lambda_1 - \alpha, \boldsymbol{u}_1), \dots (\lambda_i - \alpha, \boldsymbol{u}_i), \dots (\lambda_D - \alpha, \boldsymbol{u}_D)$ 

- If  $\alpha > 0$  is choosen such that  $|\lambda_j \alpha| \ll |\lambda_i \alpha| \ \forall i \neq j$  then  $\lambda_j \alpha$  becomes the smallest (in magnitude) eivenvalue.
- The inverse power method (in conjuction with the LU decomposition of  $\mathbf{B}$ ) can be used to estimate the eigenpair  $(\lambda_j \alpha, \mathbf{u}_j)$ .

# Example of mapping a graph on the Fiedler vector



# Laplacian embedding

- Embed the graph in a k-dimensional Euclidean space. The embedding is given by the  $n \times k$  matrix  $\mathbf{F} = [\boldsymbol{f}_1 \boldsymbol{f}_2 \dots \boldsymbol{f}_k]$  where the i-th row of this matrix  $-\boldsymbol{f}^{(i)}$  corresponds to the Euclidean coordinates of the i-th graph node  $v_i$ .
- We need to minimize (Belkin & Niyogi '03):

$$rg \min_{oldsymbol{f}_1 \cdots oldsymbol{f}_k} \sum_{i,j=1}^n w_{ij} \| oldsymbol{f}^{(i)} - oldsymbol{f}^{(j)} \|^2 ext{ with: } \mathbf{F}^ op \mathbf{F} = \mathbf{I}.$$

• The solution is provided by the matrix of eigenvectors corresponding to the k lowest nonzero eigenvalues of the eigenvalue problem  $\mathbf{L} \boldsymbol{f} = \lambda \boldsymbol{f}$ .

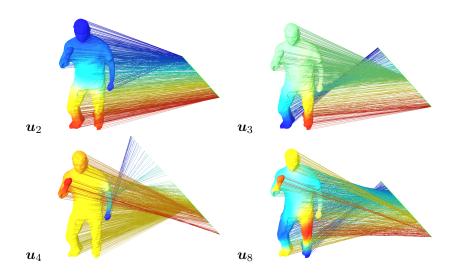
# Spectral embedding using the unnormalized Laplacian

- ullet Compute the eigendecomposition  ${f L}={f D}-{f \Omega}.$
- Select the k smallest non-null eigenvalues  $\lambda_2 \leq \ldots \leq \lambda_{k+1}$
- $\lambda_{k+2} \lambda_{k+1} =$ eigengap.
- We obtain the  $n \times k$  matrix  $\mathbf{U} = [\boldsymbol{u}_2 \dots \boldsymbol{u}_{k+1}]$ :

$$\mathbf{U} = \left[ egin{array}{ccc} oldsymbol{u}_2(v_1) & \dots & oldsymbol{u}_{k+1}(v_1) \ dots & & dots \ oldsymbol{u}_2(v_n) & \dots & oldsymbol{u}_{k+1}(v_n) \end{array} 
ight]$$

- $ullet \ oldsymbol{u}_i^ op oldsymbol{u}_j = \delta_{ij}$  (orthonormal vectors), hence  $\mathbf{U}^ op \mathbf{U} = \mathbf{I}_k$ .
- Column i  $(2 \le i \le k+1)$  of this matrix is a mapping on the eigenvector  $u_i$ .

# Examples of one-dimensional mappings



# Euclidean L-embedding of the graph's vertices

• (Euclidean) L-embedding of a graph:

$$\mathbf{X} = \mathbf{\Lambda}_k^{-rac{1}{2}} \mathbf{U}^ op = [oldsymbol{x}_1 \; \ldots \; oldsymbol{x}_j \; \ldots \; oldsymbol{x}_n]$$

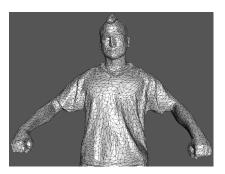
The coordinates of a vertex  $v_i$  are:

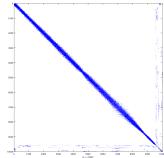
$$oldsymbol{x}_j = \left(egin{array}{c} rac{oldsymbol{u}_2(v_j)}{\sqrt{\lambda_2}} \ dots \ rac{oldsymbol{u}_{k+1}(v_j)}{\sqrt{\lambda_{k+1}}} \end{array}
ight)$$

A formal justification of using this will be provided later.

# The Laplacian of a mesh

A mesh may be viewed as a graph: n=10,000 vertices, m=35,000 edges. ARPACK finds the smallest 100 eigenpairs in 46 seconds.





# Example: Shape embedding

