Spectral Graph Drawing

based on papers by Yehuda Koren

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- Draw edges using only straight segments.
- Goal: place the vertices in *p*-dimensional space to get a "beautiful" layout.

The Graph Drawing Problem



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- vertices connected by an edge to be close to each other
- higher weighted edge: even closer
- but not too close in general

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- Vertex *i* is at coordinates $(x^1(i), \ldots, x^p(i))$.
- Euclidean distance between vertices *i* and *j*

$$d_{ij} = \sqrt{\sum_{k=1}^{p} (x^k(i) - x^k(j))^2}$$

Theorem (1)

Given a symmetric matrix $A_{n \times n}$, denote by v^1, \ldots, v^n its eigenvectors, with corresponding eigenvalues $\lambda_1 \leq \cdots \leq \lambda_n$. Then, v^1, \ldots, v^p are an optimal solution of the constrained minimization problem:

$$\min_{x_1,\ldots,x_p}\sum_{k=1}^p (x^k)^T A x^k$$

subject to

$$(x^k)^T x^l = \delta_{kl}, \quad k, l = 1, \dots, p$$

where δ_{kl} is 1 if k = l, 0 otherwise.

Generalized eigenvector of (L, D) is u s.t.

 $Lu = \mu Du$

Theorem (2)

Given a symmetric matrix $A_{n \times n}$ and a positive definite matrix $B_{n \times n}$, denote by v^1, \ldots, v^n the generalized eigenvectors of (A, B), with corresponding eigenvalues $\lambda_1 \leq \cdots \leq \lambda_n$. Then, v^1, \ldots, v^p are an optimal solution of the constrained minimization problem:

$$\min_{x_1,\dots,x_p} \sum_{k=1}^p (x^k)^T A x^k$$

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Corollary (1)

Given a symmetric matrix $A_{n \times n}$ and a positive definite matrix $B_{n \times n}$, denote by v^1, \ldots, v^n the generalized eigenvectors of (A, B), with corresponding eigenvalues $\lambda_1 \leq \cdots \leq \lambda_n$. Then, v^1, \ldots, v^p are an optimal solution of the constrained minimization problem:

$$\min_{c_1,\dots,x_p} \frac{\sum_{i=1}^p (x^i)^T A x^i}{\sum_{i=1}^p (x^i)^T B x^i}$$

subject to

$$(x^1)^T B x^1 = (x^2)^T B x^2 = \dots = (x^p)^T B x^p$$

 $(x^k)^T B x^l = 0$

Corollary (2)

Given a symmetric matrix $A_{n \times n}$ and a positive definite matrix $B_{n \times n}$, denote by v^1, \ldots, v^n the generalized eigenvectors of (A, B), with corresponding eigenvalues $\lambda_1 \leq \cdots \leq \lambda_n$. Then, v^{k+1}, \ldots, v^{k+p} are an optimal solution of the constrained minimization problem:

$$\min_{c_1,\dots,x_p} \frac{\sum_{i=1}^p (x^i)^T A x^i}{\sum_{i=1}^p (x^i)^T B x^i}$$

subject to

$$(x^{1})^{T}Bx^{1} = (x^{2})^{T}Bx^{2} = \dots = (x^{p})^{T}Bx^{p}$$

 $(x^{i})^{T}Bx^{j} = 0$
 $(x^{i})^{T}Bv^{j} = 0$

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• Minimization problem:

$$\min_{x_1,\ldots,x_p} \frac{\sum_{(i,j)\in E} w_{ij} d_{ij}^2}{\sum_{i < j} d_{ij}^2}$$

subject to
$$\operatorname{Var}(x^1) = \ldots = \operatorname{Var}(x^p)$$

and $\operatorname{Cov}(x^k, x^l) = 0, \quad 1 \le k \ne l \le p$

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• $\operatorname{Cov}(x^k, x^l) = \frac{1}{n} \sum_{i=1}^{n} (x^k(i) - \bar{x}^k) (x^l(i) - \bar{x}^l)$

• We can make $\bar{x}^k = 0$ for each k i.e. $\sum_{i=1}^n x^k(i) = (x^k)^T \cdot 1_n = 0$

Image: A matrix and a matrix

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- Var $(x^k) = \frac{1}{n} \sum_{i=1}^n (x^k(i) \bar{x}^k)^2$ becomes Var $(x^k) = \frac{1}{n} (x^k)^T x^k$

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- Cov $(x^k, x^l) = \frac{1}{n} \sum_{i=1}^n (x^k(i) \bar{x}^k)(x^l(i) \bar{x}^l)$ becomes Cov $(x^k, x^l) = \frac{1}{n} (x^k)^T (x^l)$

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- Thus we can reformulate the problem as

$$\min_{x_1,...,x_p} \frac{\sum_{k=1}^p (x^k)^T L x^k}{\sum_{k=1}^p (x^k)^T x^k}$$

subject to
$$(x^k)^T (x^l) = \delta_{kl}$$
, $k, l = 1, ..., p$
and $(x^k)^T \cdot 1_n = 0$, $k = 1, ..., p$

- We can make $\bar{x}^k = 0$ for each k i.e. $\sum_{i=1}^n x^k(i) = (x^k)^T \cdot 1_n = 0$
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 $k, l = 1, ..., p$
and $(x^k)^T \cdot 1_n = 0,$ $k = 1, ..., p$

• The answer is v^2, \ldots, v^{p+1} .

Degree-Normalized "Force-Directed" Method

• Minimization problem:

$$\min_{x_1,...,x_p} \frac{\sum_{k=1}^p (x^k)^T L x^k}{\sum_{k=1}^p (x^k)^T D x^k}$$

subject to
$$(x^k)^T D(x^l) = \delta_{kl}$$
, $k, l = 1, \dots, p$
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, $k, l = 1, \dots, p$
and $(x^k)^T D1_n = 0$, $k = 1, \dots, p$

• The answer is u^2, \ldots, u^{p+1} , the generalized eigenvectors of (L, D).

Weighted Centroid Characterization

• Aesthetically, a vertex should be at the weighted centroid of its neighbors.

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- Differentiating *x^TLx* with respect to *x*(*i*) gives

$$\frac{\partial x^T L x}{\partial x(i)} = 2 \sum_{j \in N(i)} w_{ij}(x(i) - x(j))$$

which is zero when

$$x(i) = \frac{\sum_{j \in N(i)} w_{ij} x(j)}{\deg(i)}$$

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• This can be written, for all *i* together, as

$$D^{-1}Lx = \mu x$$
$$Lx = \mu Dx$$

which endorses the use of generalized eigenvectors of (L,D)

• Using generalized eigenvectors of (L,D) gives

$$x(i) - \frac{\sum_{j \in N(i)} w_{ij} x(j)}{\deg(i)} = \mu \cdot x(i)$$

• Using Laplacian eigenvectors gives

$$x(i) - \frac{\sum_{j \in N(i)} w_{ij} x(j)}{\deg(i)} = \lambda \cdot \deg(i)^{-1} \cdot x(i)$$

Weighted Centroid Characterization



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- Random walk!

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