Graphs in Machine Learning

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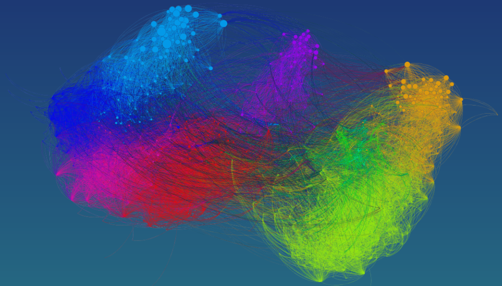
TA: Pierre Perrault

Partially based on material by: Ulrike von Luxburg, Gary Miller, Doyle & Schnell, Daniel Spielman



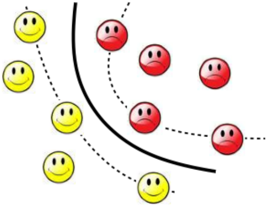
Previous lecture

- where do the graphs come from?
  - social, information, utility, and biological networks
  - we create them from the flat data
  - random graph models
- specific applications and concepts
  - maximizing influence on a graph **gossip propagation, submodularity**, proof of the approximation guarantee
  - Google pagerank **random surfer process, steady state vector, sparsity**
  - online semi-supervised learning **label propagation, backbone graph, online learning, combinatorial sparsification, stability analysis**
  - Erdős number project, real-world graphs, **heavy tails, small world** – when did this happen?
- PS: some students have started working on their projects already

This lecture

- similarity graphs
  - different types
  - construction
  - practical considerations
- **Laplacians** and their properties
- spectral graph theory
- random walks
- recommendation on a bipartite graph
- resistive networks
  - recommendation score as a resistance?
  - Laplacian and resistive networks
  - resistance distance and random walks

Statistical Machine Learning in Paris!



https://sites.google.com/site/smileinparis/sessions-2016--17

Speaker: Anna Ben-Hamou (UMPC LSTA)

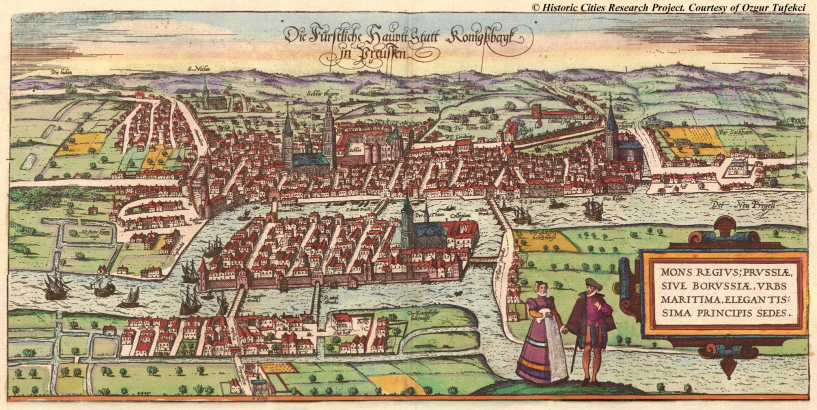
Topic: Estimating graph parameters via random walks with restarts

Date: Monday, October 9, 2017

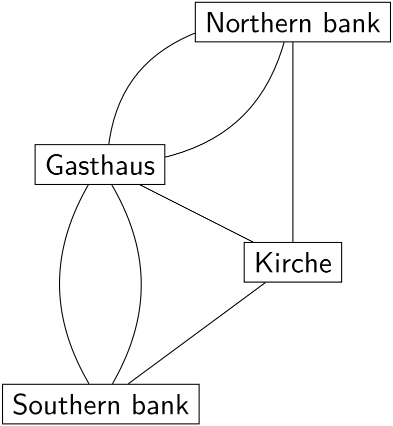
Time: 13:30 - 14:30 (this is pretty soon)

Place: Institut Henri Poincaré, room 421

Graph theory refresher



Graph theory refresher



Graph theory refresher

- 250 years of graph theory
- Seven Bridges of Königsberg (Leonhard Euler, 1735)
- necessary for Eulerian circuit: 0 or 2 nodes of odd degree
- after bombing and rebuilding there are now 5 bridges in Kaliningrad for the nodes with degrees $[2, 2, 3, 3]$
- the original problem is solved but not practical
  `http://people.engr.ncsu.edu/mfms/SevenBridges/`

Similarity Graphs

Input: $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \ldots, \mathbf{x}_N$

- raw data
- flat data
- vectorial data

Similarity Graphs

Similarity graph: $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ — **(un)weighted**

Task 1: For each pair i, j: define a **similarity function** s_{ij}

Task 2: Decide which edges to include

ε-neighborhood graphs – connect the points with the distances smaller than ε

k-NN neighborhood graphs – take k nearest neighbors

fully connected graphs - consider everything

This is art (not much theory exists).

http://www.informatik.uni-hamburg.de/ML/contents/people/luxburg/publications/Luxburg07_tutorial.pdf

Similarity Graphs: ε-neighborhood graphs

Edges connect the points with the distances smaller than ε.

- distances are roughly on the same scale (ε)
- weights may not bring additional info $\rightarrow$ unweighted
- equivalent to: similarity function is at least ε
- theory [Penrose, 1999]: $\varepsilon = ((\log N)/N)^d$ to guarantee connectivity N nodes, d dimension
- practice: choose ε as the length of the longest edge in the MST - minimum spanning tree

What could be the problem with this MST approach?

Similarity Graphs: k-nearest neighbors graphs

Edges connect each node to its k-nearest neighbors.

- asymmetric (or directed graph)
  - option OR: ignore the direction
  - option AND: include if we have both direction (mutual k-NN)
- how to choose k?
- $k \approx \log N$ - suggested by asymptotics (practice: up to $\sqrt{N}$)
- for mutual k-NN we need to take larger k
- mutual k-NN does not connect regions with different density
- why don't we take $k = N - 1$?

Similarity Graphs: Fully connected graphs

Edges connect everything.

- choose a "meaningful" similarity function s
- default choice:

$$s_{ij} = \exp\left(\frac{-\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2}\right)$$

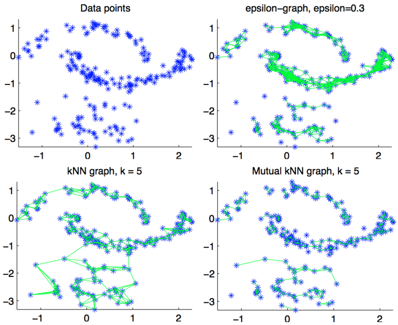
- why the exponential decay with the distance?
- σ controls the width of the neighborhoods
  - similar role as ε
  - **a** practical rule of thumb: 10% of the average empirical std
  - possibility: learn σ_i for each feature independently
- metric learning (a whole field of ML)

Similarity Graphs: Important considerations

- *calculate all s_{ij} and threshold* has its limits ($N \approx 10000$)
- graph construction step can be a huge bottleneck
- want to go higher? (we often have to)
  - down-sample
  - approximate NN
    - **LSH** - Locally Sensitive Hashing
    - **CoverTrees**
    - **Spectral sparsifiers**
  - sometime we may not need the graph (just the final results)
  - yet another story: when we start with a large graph and want to make it sparse (later in the course)
- these rules have little theoretical underpinning
- similarity is very data-dependent

Similarity Graphs: ε or k-NN?

DEMO IN CLASS



http://www.ml.uni-saarland.de/code/GraphDemo/DemoSpectralClustering.htm

http://www.tml.cs.uni-tuebingen.de/team/luxburg/publications/Luxburg07_tutorial.pdf

Generic Similarity Functions

Gaussian similarity function/Heat function/RBF:

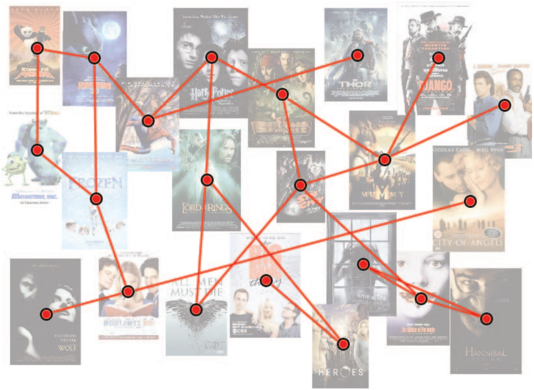
$$s_{ij} = \exp\left(\frac{-\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2}\right)$$

Cosine similarity function:

$$s_{ij} = \cos(\theta) = \left(\frac{\mathbf{x}_i^\mathsf{T}\mathbf{x}_j}{\|\mathbf{x}_i\|\|\mathbf{x}_j\|}\right)$$

Typical Kernels

Similarity Graphs



$\mathcal{G} = (\mathcal{V}, \mathcal{E})$ - with a set of **nodes** $\mathcal{V}$ and a set of **edges** $\mathcal{E}$

Sources of Real Networks

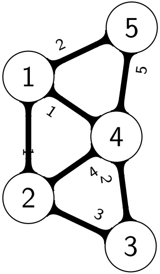
- **http://snap.stanford.edu/data/**
- http://www-personal.umich.edu/~mejn/netdata/
- http://proj.ise.bgu.ac.il/sns/datasets.html
- http://www.cise.ufl.edu/research/sparse/matrices/
- http://vlado.fmf.uni-lj.si/pub/networks/data/default.htm

Graph Laplacian

$\mathcal{G} = (\mathcal{V}, \mathcal{E})$ - with a set of **nodes** $\mathcal{V}$ and a set of **edges** $\mathcal{E}$

$\mathbf{A}$	adjacency matrix
$\mathbf{W}$	weight matrix
$\mathbf{D}$	(diagonal) degree matrix
$\mathbf{L} = \mathbf{D} - \mathbf{W}$	graph **Laplacian** matrix

$$\mathbf{L} = \begin{pmatrix} 4 & -1 & 0 & -1 & -2 \\ -1 & 8 & -3 & -4 & 0 \\ 0 & -3 & 5 & -2 & 0 \\ -1 & -4 & -2 & 12 & -5 \\ -2 & 0 & 0 & -5 & 7 \end{pmatrix}$$



L is SDD!

Properties of Graph Laplacian

Graph function: a vector $\mathbf{f} \in \mathbb{R}^N$ assigning values to nodes:

$$\mathbf{f} : \mathcal{V}(\mathcal{G}) \to \mathbb{R}.$$

$$\mathbf{f}^\mathsf{T}\mathbf{L}\mathbf{f} = \frac{1}{2}\sum_{i,j \leq N} w_{i,j}(f_i - f_j)^2 = S_G(\mathbf{f})$$

Recap: Eigenwerte und Eigenvektoren

A vector $\mathbf{v}$ is an **eigenvector** of matrix $\mathbf{M}$ of **eigenvalue** λ

$$\mathbf{M}\mathbf{v} = \lambda\mathbf{v}.$$

If $(\lambda_1, \mathbf{v}_1)$ are $(\lambda_2, \mathbf{v}_2)$ **eigenpairs** for symmetric $\mathbf{M}$ with $\lambda_1 \neq \lambda_2$ then $\mathbf{v}_1 \perp \mathbf{v}_2$, i.e., $\mathbf{v}_1^\intercal \mathbf{v}_2 = 0$.

If $(\lambda, \mathbf{v}_1)$, $(\lambda, \mathbf{v}_2)$ are eigenpairs for $\mathbf{M}$ then $(\lambda, \mathbf{v}_1 + \mathbf{v}_2)$ is as well.

For symmetric $\mathbf{M}$, the **multiplicity** of λ is the dimension of the space of eigenvectors corresponding to λ.

$N \times N$ symmetric matrix has N eigenvalues (w/ multiplicities).

Eigenvalues, Eigenvectors, and Eigendecomposition

A vector $\mathbf{v}$ is an **eigenvector** of matrix $\mathbf{M}$ of **eigenvalue** λ

$$\mathbf{M}\mathbf{v} = \lambda\mathbf{v}.$$

Vectors $\{\mathbf{v}_i\}_i$ form an **orthonormal** basis with $\lambda_1 \leq \lambda_2 \leq \dots \lambda_N$.

$$\forall i \quad \mathbf{M}\mathbf{v}_i = \lambda_i \mathbf{v}_i \qquad \equiv \qquad \mathbf{MQ} = \mathbf{Q\Lambda}$$

$\mathbf{Q}$ has eigenvectors in columns and $\mathbf{\Lambda}$ has eigenvalues on its diagonal.

Right-multiplying $\mathbf{MQ} = \mathbf{Q\Lambda}$ by $\mathbf{Q}^\mathsf{T}$ we get the **eigendecomposition** of $\mathbf{M}$:

$$\mathbf{M} = \mathbf{MQQ}^\mathsf{T} = \mathbf{Q\Lambda Q}^\mathsf{T} = \sum_i \lambda_i \mathbf{v}_i \mathbf{v}_i^\mathsf{T}$$

$\mathbf{M} = \mathbf{L}$: Properties of Graph Laplacian

We can assume **non-negative weights**: $w_{ij} \geq 0$.

$\mathbf{L}$ is symmetric

$\mathbf{L}$ positive semi-definite $\leftarrow \mathbf{f}^\mathsf{T}\mathbf{L}\mathbf{f} = \frac{1}{2}\sum_{i,j \leq N} w_{i,j}(f_i - f_j)^2$

Recall: If $\mathbf{L}\mathbf{f} = \lambda\mathbf{f}$ then λ is an **eigenvalue** (of the Laplacian).

The smallest eigenvalue of $\mathbf{L}$ is 0. Corresponding eigenvector: $\mathbf{1}_N$.

All eigenvalues are non-negative reals $0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_N$.

Self-edges do not change the value of $\mathbf{L}$.

Properties of Graph Laplacian

The multiplicity of eigenvalue 0 of $\mathbf{L}$ equals to the number of connected components. The eigenspace of 0 is spanned by the components' indicators.

Proof: If $(0, \mathbf{f})$ is an eigenpair then $0 = \frac{1}{2}\sum_{i,j\leq N} w_{i,j}(f_i - f_j)^2$. Therefore, $\mathbf{f}$ is constant on each connected component. If there are k components, then $\mathbf{L}$ is k-block-diagonal:

$$\mathbf{L} = \begin{bmatrix} \mathbf{L}_1 & & & \\ & \mathbf{L}_2 & & \\ & & \ddots & \\ & & & \mathbf{L}_k \end{bmatrix}$$

For block-diagonal matrices: the spectrum is the union of the spectra of $\mathbf{L}_i$ (eigenvectors of $\mathbf{L}_i$ padded with zeros elsewhere).

For $\mathbf{L}_i$ $(0, \mathbf{1}_{|V_i|})$ is an eigenpair, hence the claim.

Smoothness of the Function and Laplacian

- $\mathbf{f} = (f_1, \ldots, f_N)^\mathsf{T}$: graph function
- Let $\mathbf{L} = \mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^\mathsf{T}$ be the eigendecomposition of the Laplacian.
  - Diagonal matrix $\boldsymbol{\Lambda}$ whose diagonal entries are eigenvalues of $\mathbf{L}$.
  - Columns of $\mathbf{Q}$ are eigenvectors of $\mathbf{L}$.
  - Columns of $\mathbf{Q}$ form a basis.
- $\boldsymbol{\alpha}$: Unique vector such that $\mathbf{Q}\boldsymbol{\alpha} = \mathbf{f}$ Note: $\mathbf{Q}^\mathsf{T}\mathbf{f} = \boldsymbol{\alpha}$

Smoothness of a graph function $S_G(\mathbf{f})$

$$S_G(\mathbf{f}) = \mathbf{f}^\mathsf{T}\mathbf{L}\mathbf{f} = \mathbf{f}^\mathsf{T}\mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^\mathsf{T}\mathbf{f} = \boldsymbol{\alpha}^\mathsf{T}\boldsymbol{\Lambda}\boldsymbol{\alpha} = \|\boldsymbol{\alpha}\|_{\boldsymbol{\Lambda}}^2 = \sum_{i=1}^{N} \lambda_i \alpha_i^2$$

Smoothness and regularization: Small value of

(a) $S_G(\mathbf{f})$ **(b)** $\boldsymbol{\Lambda}$ norm of $\boldsymbol{\alpha}^\star$ **(c)** $\alpha_i^\star$ for large λ_i

Smoothness of the Function and Laplacian

$$S_G(\mathbf{f}) = \mathbf{f}^\mathsf{T}\mathbf{L}\mathbf{f} = \mathbf{f}^\mathsf{T}\mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^\mathsf{T}\mathbf{f} = \boldsymbol{\alpha}^\mathsf{T}\boldsymbol{\Lambda}\boldsymbol{\alpha} = \|\boldsymbol{\alpha}\|_{\boldsymbol{\Lambda}}^2 = \sum_{i=1}^{N}\lambda_i\alpha_i^2$$

Eigenvectors are graph functions too!

What is the smoothness of an eigenvector?

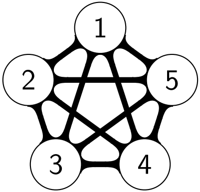
Spectral coordinates of eigenvector $\mathbf{v}_k$: $\mathbf{Q}^\mathsf{T}\mathbf{v}_k = \mathbf{e}_k$

$$S_G(\mathbf{v}_k) = \mathbf{v}_k^\mathsf{T}\mathbf{L}\mathbf{v}_k = \mathbf{v}_k^\mathsf{T}\mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^\mathsf{T}\mathbf{v}_k = \mathbf{e}_k^\mathsf{T}\boldsymbol{\Lambda}\mathbf{e}_k = \|\mathbf{e}_k\|_{\boldsymbol{\Lambda}}^2 = \sum_{i=1}^{N}\lambda_i(\mathbf{e}_k)_i^2 = \lambda_k$$

The smoothness of k-th eigenvector is the k-th eigenvalue.

Laplacian of the Complete Graph K_N

What is the eigenspectrum of $\mathbf{L}_{K_N}$?



$$\mathbf{L}_{K_N} = \begin{pmatrix} N-1 & -1 & -1 & -1 & -1 \\ -1 & N-1 & -1 & -1 & -1 \\ -1 & -1 & N-1 & -1 & -1 \\ -1 & -1 & -1 & N-1 & -1 \\ -1 & -1 & -1 & -1 & N-1 \end{pmatrix}$$

From before: we know that $(0, \mathbf{1}_N)$ is an eigenpair.

If $\mathbf{v} \neq 0_N$ and $\mathbf{v} \perp \mathbf{1}_N \implies \sum_i \mathbf{v}_i = 0$. To get the other eigenvalues, we compute $(\mathbf{L}_{K_N}\mathbf{v})_1$ and divide by $\mathbf{v}_1$ (wlog $\mathbf{v}_1 \neq 0$).

$$(\mathbf{L}_{K_N}\mathbf{v})_1 = (N-1)\mathbf{v}_1 - \sum_{i=2}^{N} \mathbf{v}_i = N\mathbf{v}_1.$$

What are the remaining eigenvalues/vectors?

Normalized Laplacians

$$\mathbf{L}_{un} = \mathbf{D} - \mathbf{W}$$
$$\mathbf{L}_{sym} = \mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{W}\mathbf{D}^{-1/2}$$
$$\mathbf{L}_{rw} = \mathbf{D}^{-1}\mathbf{L} = \mathbf{I} - \mathbf{D}^{-1}\mathbf{W}$$

$$\mathbf{f}^{\mathsf{T}}\mathbf{L}_{sym}\mathbf{f} = \frac{1}{2}\sum_{i,j\leq N} w_{i,j}\left(\frac{f_i}{\sqrt{d_i}} - \frac{f_j}{\sqrt{d_j}}\right)^2$$

$(\lambda, \mathbf{u})$ is an eigenpair for $\mathbf{L}_{rw}$ iff $(\lambda, \mathbf{D}^{1/2}\mathbf{u})$ is an eigenpair for $\mathbf{L}_{sym}$

Normalized Laplacians

$\mathbf{L}_{sym}$ and $\mathbf{L}_{rw}$ are PSD with non-negative real eigenvalues

$$0 = \lambda_1 \le \lambda_2 \le \lambda_3 \le \cdots \le \lambda_N$$

$(\lambda, \mathbf{u})$ is an eigenpair for $\mathbf{L}_{rw}$ iff $(\lambda, \mathbf{u})$ solve the generalized eigenproblem $\mathbf{Lu} = \lambda \mathbf{Du}$.

$(0, \mathbf{1}_N)$ is an eigenpair for $\mathbf{L}_{rw}$.

$(0, \mathbf{D}^{1/2}\mathbf{1}_N)$ is an eigenpair for $\mathbf{L}_{sym}$.

Multiplicity of eigenvalue 0 of $\mathbf{L}_{rw}$ or $\mathbf{L}_{sym}$ equals to the number of connected components.

Proof: As for $\mathbf{L}$.

Laplacian and Random Walks on Undirected Graphs

- stochastic process: vertex-to-vertex jumping
- transition probability $v_i \rightarrow v_j$ is $p_{ij} = w_{ij}/d_i$
  - $d_i \stackrel{\text{def}}{=} \sum_j w_{ij}$
- transition matrix $\mathbf{P} = (p_{ij})_{ij} = \mathbf{D}^{-1}\mathbf{W}$ (notice $\mathbf{L}_{rw} = \mathbf{I} - \mathbf{P}$)
- if G is connected and non-bipartite $\rightarrow$ unique **stationary distribution** $\pi = (\pi_1, \pi_2, \pi_3, \ldots, \pi_N)$ where $\pi_i = d_i/\mathrm{vol}(V)$
  - $\mathrm{vol}(G) = \mathrm{vol}(V) = \mathrm{vol}(\mathbf{W}) \stackrel{\text{def}}{=} \sum_i d_i = \sum_{i,j} w_{ij}$
- $\pi = \frac{\mathbf{1}^\mathsf{T}\mathbf{W}}{\mathrm{vol}(\mathbf{W})}$ verifies $\pi\mathbf{P} = \pi$ as:

$$\pi\mathbf{P} = \frac{\mathbf{1}^\mathsf{T}\mathbf{W}\mathbf{P}}{\mathrm{vol}(\mathbf{W})} = \frac{\mathbf{1}^\mathsf{T}\mathbf{D}\mathbf{P}}{\mathrm{vol}(\mathbf{W})} = \frac{\mathbf{1}^\mathsf{T}\mathbf{D}\mathbf{D}^{-1}\mathbf{W}}{\mathrm{vol}(\mathbf{W})} = \frac{\mathbf{1}^\mathsf{T}\mathbf{W}}{\mathrm{vol}(\mathbf{W})} = \pi$$

What's the difference from the PageRank™?

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