

Graphs in Machine Learning

Michal Valko

Inria Lille - Nord Europe, France

TA: Pierre Perrault

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

October 10th, 2018

MVA 2018/2019

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?
- similarity graphs
 - different types
 - construction

practical considerations

This lecture

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

PS: some students have started working on their projects already



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:

$$s_{ij} = \cos(heta) = \left(rac{\mathbf{x}_i^{\intercal} \mathbf{x}_j}{\|\mathbf{x}_i\| \|\mathbf{x}_j\|}
ight)$$

Typical Kernels



Similarity Graphs



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



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

L = D - W graph Laplacian ...the only matrix that matters

Innia

Graph Laplacian

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





Properties of Graph Laplacian

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

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

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



Recap: Eigenwerte und Eigenvektoren

A vector **v** is an **eigenvector** of matrix **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 **M** with $\lambda_1 \neq \lambda_2$ then $\mathbf{v}_1 \perp \mathbf{v}_2$, i.e., $\mathbf{v}_1^\mathsf{T} \mathbf{v}_2 = 0$.

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

For symmetric **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 **v** is an **eigenvector** of matrix **M** of **eigenvalue** λ

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

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

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

Q has eigenvectors in columns and Λ has eigenvalues on its diagonal.

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

$$\mathbf{M} = \mathbf{M} \mathbf{Q} \mathbf{Q}^{\mathsf{T}} = \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^{\mathsf{T}} \Leftarrow \sum_{i} \lambda_{i} \mathbf{v}_{i} \mathbf{v}_{i}^{\mathsf{T}}$$



M = **L**: Properties of Graph Laplacian

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

 $\boldsymbol{\mathsf{L}}$ is symmetric

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 **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 L.



Properties of Graph Laplacian

The multiplicity of eigenvalue 0 of 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 $0 = \frac{1}{2} \sum_{i,j \le N} w_{i,j} (f_i - f_j)^2$. Therefore, **f** is constant on each connected component. If there are *k* components, then **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 L_i (eigenvectors of 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 $\mathbf{L} = \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^{\mathsf{T}}$ be the eigendecomposition of the Laplacian.

- Diagonal matrix Λ whose diagonal entries are eigenvalues of L.
- Columns of Q are eigenvectors of L.
- Columns of **Q** form a basis.

• α : Unique vector such that $\mathbf{Q}\alpha = \mathbf{f}$ Note: $\mathbf{Q}^{\mathsf{T}}\mathbf{f} = \alpha$

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

$$S_{G}(\mathbf{f}) = \mathbf{f}^{\mathsf{T}} \mathbf{L} \mathbf{f} = \mathbf{f}^{\mathsf{T}} \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^{\mathsf{T}} \mathbf{f} = \boldsymbol{\alpha}^{\mathsf{T}} \mathbf{\Lambda} \boldsymbol{\alpha} = \| \boldsymbol{\alpha} \|_{\mathbf{\Lambda}}^{2} = \sum_{i=1}^{N} \lambda_{i} \alpha_{i}^{2}$$

Smoothness and regularization: Small value of

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



Smoothness of the Function and Laplacian

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

Eigenvectors are graph functions too!

What is the smoothness of an eigenvector?

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

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

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



Laplacian of the Complete Graph K_N

What is the eigenspectrum of L_{K_N} ?



$$\kappa_{\mathcal{K}_N} = \left(egin{array}{ccccccc} N-1 & -1 & -1 & -1 & -1 \ -1 & N-1 & -1 & -1 & -1 \ -1 & -1 & N-1 & -1 & -1 \ -1 & -1 & -1 & N-1 & -1 \ -1 & -1 & -1 & -1 & N-1 \end{array}
ight)$$

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

If $\mathbf{v} \neq \mathbf{0}_N$ 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 $\mathbf{v}_1 \neq 0$).

L

$$(\mathbf{L}_{\mathcal{K}_{\mathcal{N}}}\mathbf{v})_{1}=(\mathcal{N}-1)\mathbf{v}_{1}-\sum_{i=2}^{N}\mathbf{v}_{i}=\mathcal{N}\mathbf{v}_{1}.$$

What are the remaining eigenvalues/vectors?



Normalized Laplacians

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

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

 (λ, \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

 L_{sym} and L_{rw} are PSD with non-negative real eigenvalues $0 = \lambda_1 \le \lambda_2 \le \lambda_3 \le \dots \le \lambda_N$

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

 $(0, \mathbf{1}_N)$ 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 L_{rw} or L_{sym} equals to the number of connected components.

Laplacian and Random Walks on Undirected Graphs

- stochastic process: vertex-to-vertex jumping
- transition probability $v_i \rightarrow v_j$ is $p_{ij} = w_{ij}/d_i$

•
$$d_i \stackrel{\text{def}}{=} \sum_j w_j$$

▶ 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 → unique stationary distribution π = (π₁, π₂, π₃,..., π_N) where π_i = d_i/vol(V)
 vol(G) = vol(V) = vol(W) ^{def}= ∑_i d_i = ∑_{i,j} w_{ij}

•
$$\pi = \frac{\mathbf{1}^{\mathsf{T}} \mathbf{W}}{\operatorname{vol}(\mathbf{W})}$$
 verifies $\pi \mathbf{P} = \pi$ as:

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

What's the difference from the PageRankTM?



SCOTe(V, m)recommendation on a bipartite graph ...with the graph Laplacian!

naío

Use of Laplacians: Movie recommendation

How to do movie recommendation on a bipartite graph?



Question: Do we recommend Capitaine Superslip to Adam?

Let's compute some score(v, m)!



Use of Laplacians: Movie recommendation

How to compute the score(v, m)? Using some graph distance!

Idea₁: maximally weighted path

 $\operatorname{score}(v, m) = \max_{v P m} \operatorname{weight}(P) = \max_{v P m} \sum_{e \in P} \operatorname{ranking}(e)$

Idea₂: change the path weight

 $\operatorname{score}_2(v, m) = \max_{v \in m} \operatorname{weight}_2(P) = \max_{v \in m} \min_{e \in P} \operatorname{ranking}(e)$

Idea₃: consider everything

score₃(v, m) = max flow from m to v

Laplacians and Resistive Networks

How to compute the score(v, m)?

Idea₄: view edges as conductors

 $score_4(v, m) = effective resistance between m and v$



- $C \equiv {\rm conductance}$
- $R \equiv \text{resistance}$
 - $i \equiv \text{current}$
- $V \equiv \mathrm{voltage}$

$$C = \frac{1}{R}$$
 $i = CV = \frac{V}{R}$

Resistive Networks: Some high-school physics





Resistive Networks

resistors in series

$$R = R_1 + \dots + R_n$$
 $C = \frac{1}{\frac{1}{c_1} + \dots + \frac{1}{c_N}}$ $i = \frac{V}{R}$

conductors in parallel

$$C = C_1 + \cdots + C_N$$
 $i = VC$

Effective Resistance on a graph

Take two nodes: $a \neq b$. Let V_{ab} be the voltage between them and i_{ab} the current between them. Define $R_{ab} = \frac{V_{ab}}{i_{ab}}$ and $C_{ab} = \frac{1}{R_{ab}}$.

We treat the entire graph as a resistor!

Resistive Networks: Optional Homework (ungraded)

Show that R_{ab} is a metric space.

1.
$$R_{ab} \ge 0$$

2. $R_{ab} = 0$ iff $a = b$
3. $R_{ab} = R_{ba}$

$$4. \ R_{ac} \leq R_{ab} + R_{bc}$$

The effective resistance is a distance!

nría

How to compute effective resistance?

Kirchhoff's Law \equiv flow in = flow out



 $V = \frac{C_1}{C}V_1 + \frac{C_2}{C}V_2 + \frac{C_3}{C}V_3 \text{ (convex combination)}$ residual current = $CV - C_1V_1 - C_2V_2 - C_3V_3$ Kirchhoff says: This is zero! **There is no residual current!**



Resistors: Where is the link with the Laplacian?

General case of the previous! $d_i = \sum_j c_{ij} = \text{sum of conductances}$

$$\mathbf{L}_{ij} = egin{cases} d_i & ext{if } i=j, \ -c_{ij} & ext{if } (i,j) \in E, \ 0 & ext{otherwise.} \end{cases}$$

 $\mathbf{v} = \mathbf{voltage \ setting}$ of the nodes on graph.

 $(\mathbf{Lv})_i$ = residual current at \mathbf{v}_i — as we derived

Use: setting voltages and getting the current

Inverting \equiv injecting current and getting the voltages

The net injected has to be zero \equiv Kirchhoff's Law.

Resistors and the Laplacian: Finding *R*_{ab}

Let's calculate R_{1N} to get the **movie recommendation score**!

$$\mathbf{L}\begin{pmatrix} 0\\ v_2\\ \vdots\\ v_{n-1}\\ 1 \end{pmatrix} = \begin{pmatrix} i\\ 0\\ \vdots\\ 0\\ -i \end{pmatrix}$$
$$i = \frac{V}{R} \qquad V = 1 \qquad R = \frac{1}{i}$$
Return $R_{1N} = \frac{1}{i}$

Doyle and Snell: Random Walks and Electric Networks https://math.dartmouth.edu/~doyle/docs/walks.pdf



Resistors and the Laplacian: Finding R_{1N}

$$\mathbf{Lv} = (i, 0, \dots, -i)^{\mathsf{T}} \equiv \mathbf{boundary valued problem}$$

For R_{1N}

 V_1 and V_N are the **boundary** $(v_1, v_2, ..., v_N)$ is **harmonic**: $V_i \in interior$ (not boundary)

 V_i is a convex combination of its neighbors



Resistors and the Laplacian: Finding R_{1n}

From the properties of electric networks (cf. Doyle and Snell) we inherit the useful properties of the Laplacians!

Example: Semi-Supervised Learning Using Gaussian Fields and Harmonic Functions (later in the course)

Maximum Principle

If $\mathbf{f} = \mathbf{v}$ is harmonic then min and max are on the boundary.

Uniqueness Principle

If f and ${\bf g}$ are harmonic with the same boundary then $f={\bf g}$

nnía

Resistors and the Laplacian: Finding R_{1N}

Alternative method to calculate R_{1N} :

$$\mathbf{L}\mathbf{v} = \begin{pmatrix} 1\\ 0\\ \vdots\\ 0\\ -1 \end{pmatrix} \stackrel{\text{def}}{=} \mathbf{i}_{\text{ext}} \quad \text{Return} \quad R_{1N} = \mathbf{v}_1 - \mathbf{v}_N \qquad \text{Why?}$$

Question: Does v exist? L does not have an inverse :(. Not unique: 1 in the nullspace of L : L(v + c1) = Lv + cL1 = LvMoore-Penrose pseudo-inverse solves LS Solution: Instead of $v = L^{-1}i_{ext}$ we take $v = L^{+}i_{ext}$ We get: $R_{1N} = v_1 - v_N = i_{ext}^{T}v = i_{ext}^{T}L^{+}i_{ext}$. Notice: We can reuse L^{+} to get resistances for any pair of nodes!



What? A pseudo-inverse?

Eigendecomposition of the Laplacian:

$$\mathbf{L} = \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^{\mathsf{T}} = \sum_{i=1}^{N} \lambda_i \mathbf{q}_i \mathbf{q}_i^{\mathsf{T}} = \sum_{i=2}^{N} \lambda_i \mathbf{q}_i \mathbf{q}_i^{\mathsf{T}}$$

Pseudo-inverse of the Laplacian:

$$\mathbf{L}^+ = \mathbf{Q} \mathbf{\Lambda}^+ \mathbf{Q}^{\mathsf{T}} = \sum_{i=2}^N \frac{1}{\lambda_i} \mathbf{q}_i \mathbf{q}_i^{\mathsf{T}}$$

Moore-Penrose pseudo-inverse solves a least squares problem:

$$\mathbf{v} = \underset{\mathbf{x}}{\arg\min} \left\| \mathbf{L}\mathbf{x} - \mathbf{i}_{\text{ext}} \right\|_2 = \mathbf{L}^+ \mathbf{i}_{\text{ext}}$$



$\operatorname{cut}(A, B) = \frac{1}{2}\mathbf{f}^{\mathsf{T}}\mathbf{L}\mathbf{f}^{\mathsf{T}}$ spectral clustering ...with connectivity beyond compactness

nnin

How to rule the world?

Let's make France great again!



Ínría

Michal Valko - Graphs in Machine Learning

SequeL - 36/43

How to rule the world?



One reason you're seeing this ad is that Donald J. Trump wants to reach people who are part of an audience called "Likely To Engage in Politics (Liberal)". This is based on your activity on Facebook and other apps and websites, as well as where you connect to the internet.

There may be other reasons you're seeing this ad, including that Donald J. Trump wants to reach people ages 25 and older who live near Boston, Massachusetts. This is information based on your Facebook profile and where you've connected to the internet.





How to rule the world: "AI" is here



https://www.washingtonpost.com/opinions/obama-the-big-data-president/2013/06/14/ 1d71fe2e-d391-11e2-b05f-3ea3f0e7bb5a_story.html

https://www.technologyreview.com/s/509026/how-obamas-team-used-big-data-to-rally-voters/

Talk of Rayid Ghaniy: https://www.youtube.com/watch?v=gDM1GuszM_U



Michal Valko - Graphs in Machine Learning

Application of Graphs for ML: Clustering





Michal Valko – Graphs in Machine Learning

Application: Clustering - Recap

What do we know about the clustering in general?

- ▶ ill defined problem (different tasks → different paradigms)
- "I know it when I see it"
- inconsistent (wrt. Kleinberg's axioms)

number of clusters k need often be known

difficult to evaluate

What do we know about k-means?

- "hard" version of EM clustering
- sensitive to initialization
- optimizes for compactness
- yet: algorithm-to-go



Spectral Clustering: Cuts on graphs



Inría

Spectral Clustering: Cuts on graphs



Defining the cut objective we get the clustering!



Spectral Clustering: Cuts on graphs



MinCut:
$$\operatorname{cut}(A,B) = \sum_{i \in A, j \in B} w_{ij}$$



Can be solved efficiently, but maybe not what we want



Next class on Wednesday, October 17th at 14:00!





Michal Valko michal.valko@inria.fr ENS Paris-Saclay, MVA 2018/2019 SequeL team, Inria Lille — Nord Europe https://team.inria.fr/sequel/