DAI-Labor
TU Berlin

Learning Spectral Graph Transformations for Link Prediction

Jérôme Kunegis & Andreas Lommatzsch

DAI-Labor, Technische Universität Berlin

kunegis@dai-lab.de, andreas@dai-lab.de

Abstract

We present a unified framework for learning link prediction and edge weight prediction functions in large networks, based on the transformation of a graph's algebraic spectrum. Our approach generalizes several graph kernels and dimensionality reduction methods and provides a method to estimate their parameters efficiently. We show how the parameters of these prediction functions can be learned by reducing the problem to a one-dimensional regression problem whose runtime only depends on the method's reduced rank and that can be inspected visually. We derive variants that apply to undirected, weighted, unweighted, unipartite and bipartite graphs. We evaluate our method experimentally using examples from social networks, collaborative filtering, trust networks, citation networks, authorship graphs and hyperlink networks.

Graph Kernels as Spectral Transformations

Name	***F(A) =***	***f(x) =***	***$f_{odd}(x)$ =***
Polynomial [nonneg.]	$\sum_i \alpha_i \mathbf{A}^i$ $[\alpha_i \geq 0]$	$\sum_i \alpha_i x^i$ $[\alpha_i \geq 0]$	$\sum_{i=2k+1} \alpha_i x^i$ $[\alpha_i \geq 0]$
Exponential	$e^{\alpha \mathbf{A}}$	$e^{\alpha x}$	$\sinh(\alpha x)$
Von Neumann	$(\mathbf{I} - \alpha \mathbf{A})^{-1}$	$1 / (1 - \alpha x)$	$\alpha x / (1 - \alpha^2 x^2)$
Comb. Laplacian	$\mathbf{L}^+$	$1/x$ when $x > 0$, 0 when $x = 0$	
Regul. Laplacian	$(\mathbf{I} + \alpha \mathbf{L})^{-1}$	$1 / (1 + \alpha x)$	
Heat diffusion	$e^{-\alpha \mathbf{L}}$	$e^{-\alpha x}$	
Rank reduction	$\mathbf{U}_{(k)} \mathbf{\Lambda}_{(k)} \mathbf{U}_{(k)}^T$	x when $\lvert x \rvert \geq \lvert \mathbf{\Lambda}_{kk} \rvert$, 0 otherwise	

Derivation of Least Squares

$$\min \left\| F(\mathbf{A}) - \mathbf{B} \right\|_F$$

$$= \min \left\| \mathbf{U} F(\mathbf{\Lambda}) \mathbf{U}^T - \mathbf{B} \right\|_F$$

$$= \min \left\| F(\mathbf{\Lambda}) - \mathbf{U}^T \mathbf{B} \mathbf{U} \right\|_F$$

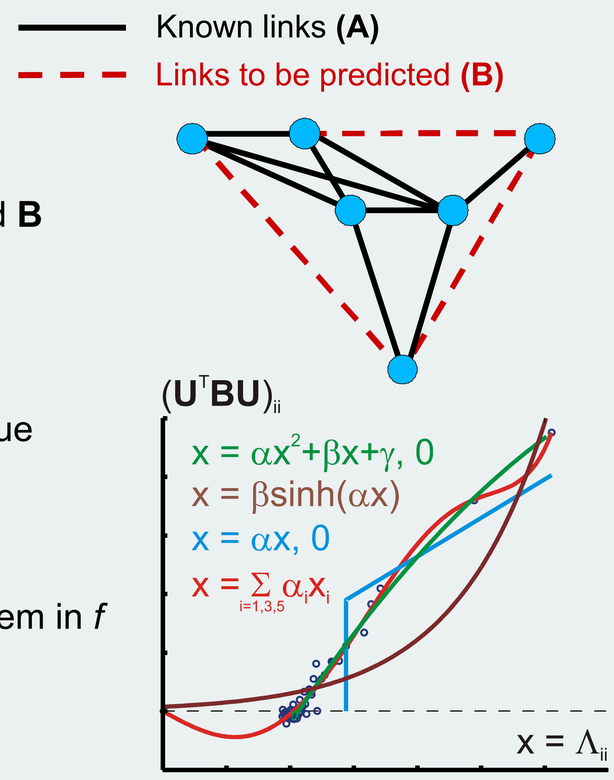
(The Frobenius norm is invariant under multiplication with orthogonal matrices)

Variants

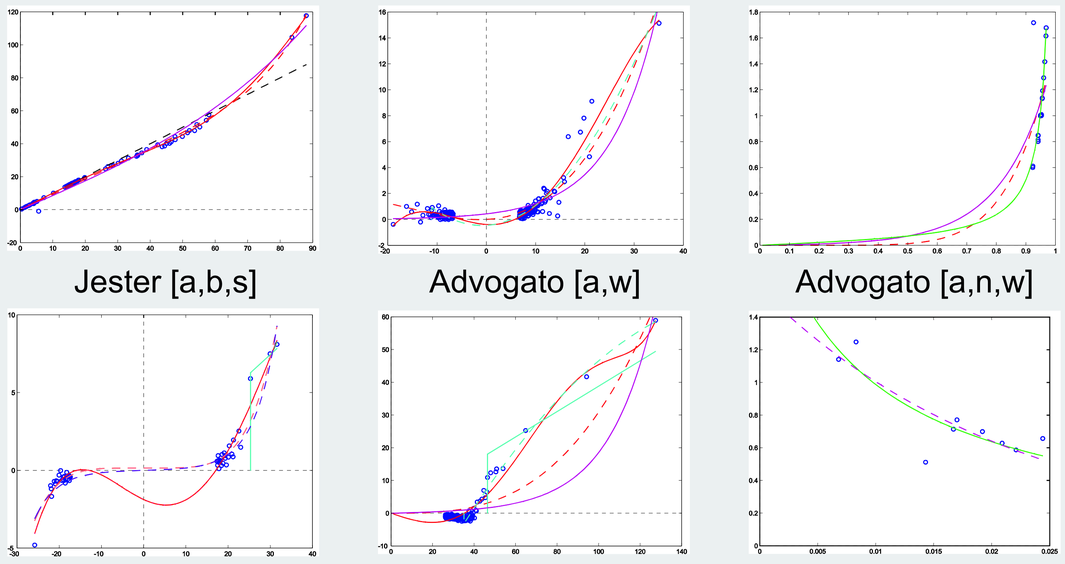
- Weighted, directed and signed graphs [w] [d] [s]
- Bipartite graphs: $f(x)$ must be odd [b]
- Other base matrices: Laplacian $\mathbf{L} = \mathbf{D} - \mathbf{A}$ [l], $\mathbf{D}^{-1/2} \mathbf{A} \mathbf{D}^{-1/2}$ [n]
  - For signed graphs $D_{ii} = \sum_j |A_{ij}|$
- Learn $(\mathbf{A} + \mathbf{B})$ instead of $\mathbf{B}$ [a]

Method

- Use training set **A** to learn edges in test set **B**
- Use adjacency matrices **A** and **B**
- Search a prediction function
  $F(\mathbf{A}) = \mathbf{B}$
- Assume F is a spectral transformation of the eigenvalue decomposition $\mathbf{A} = \mathbf{U} \mathbf{\Lambda} \mathbf{U}^T$
  $F(\mathbf{A}) = \mathbf{U}\, F(\mathbf{\Lambda})\, \mathbf{U}^T = \mathbf{B}$
- Reduce the problem to a one-dimensional curve fitting problem in f
  $F(\mathbf{\Lambda}) = \mathbf{U}^T \mathbf{B} \mathbf{U}$
  $f(\mathbf{\Lambda}_{ii}) = (\mathbf{U}^T \mathbf{B} \mathbf{U})_{ii}$



Curve Fitting



Evaluation

Dataset	***Edges***	***Weights***	***k***	***Description***	***Best F***
DBLP	49,779	{1}	126	Citation graph	Regul. Laplacian [l]
Hep-th	352,807	{1}	54	Citation graph	Exponential [n]
Advogato	57,627	{0.6, 0.8, 1.0}	192	Trust network	Regul. Laplacian [n,l]
Slashdot	488,440	{±1}	24	Friend/foe network	Nonneg. odd polynomial [s]
Epinions	841,372	{±1}	14	Trust/distrust network	Nonneg. odd polynomial [a,s]
WWW	1,497,135	{1}	49	Hyperlink graph	Regul. Laplacian [a,l]
WT10G	8,063,026	{1}	49	Hyperlink graph	Rank reduction [d]
eo-wiki	803,383	{1}	26	Authorship graph	Nonneg. odd polynomial [a]
Jester	616,912	[-10, +10]	100	Joke ratings	Polynomial [n,s]
MovieLens	1,000,209	{1, 2, 3, 4, 5}	202	Movie ratings	Hyperbolic sine [a,s]