Node classification

lecturer: Radoslav Neychev

Graph Machine Learning

Slides by I. Makarov & L.E. Zhukov

Preliminary information

- Course Lecturer: Radoslav Neychev
- Prerequisites: Machine Learning, Algorithms and Data Structure, Discrete Mathematics, Statistics

The course materials developed by Ilya Makarov and Leonid E. Zhukov.
The course is based on materials prepared within courses taught by authors at HSE University, BigData Academy MADE from Mail.ru Group, and MIPT.

Lecture outline

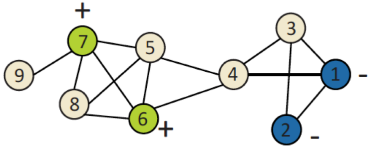
1. Node Classification
   - Label propagation and iterative classification
2. Semi-supervised learning
   - Random walk based methods. Regularization
3. Matrix Factorization

Graph machine learning

- Node classification (attribute inference)
- Link prediction (missing/hidden links inference)
- Community detection (clustering nodes in graph)
- Graph visualization (cluster projections)

Node classification

- Node classification - labeling of all nodes in a graph structure
- Subset of nodes is labeled: categorical/numeric/binary values
- Extend labeling to all nodes on the graph (class/class probability/regression)
- Classification in networked data, network classification, structured inference, relational learning



Node classification

- Structure can help only if labels/values of linked nodes are correlated
- Social networks show assortative mixing - bias in favor of connections between network nodes with similar characteristics:
  – homophily: similar characteristics $\rightarrow$ connections
  – influence: connections $\rightarrow$ similar characteristics
- Can apply to constructed (induced) similarity networks
- Node classification by label propagation

Node classification

Supervised learning approach

- Given graph nodes $V = V_l \cup V_u$:
  – nodes V_l given labels Y_l
  – nodes V_u do not have labels
- Need to find Y_u
- Labels can be binary, multi-class, real values
- Features (attributes) can be computed for every node ϕ_i:
  – local node features (if available)
  – link features available (labels from neighbors, attributes from neighbors, node degrees, connectivity patterns)

Iterative relational classifiers

- Weighted-vote relational neighbor classifier:

$$P(y_i = c|\mathcal{N}_i) = \frac{1}{Z} \sum_{j \in \mathcal{N}_i} A_{ij} P(y_j = c|\mathcal{N}_j)$$

- Network only Naive Bayes classifier:

$$P(y_i = c|\mathcal{N}_i) = \frac{P(\mathcal{N}_i|c)P(c)}{P(\mathcal{N}_i)}$$

where

$$P(\mathcal{N}_i|c) = \frac{1}{Z} \prod_{j \in \mathcal{N}_i} P(y_j = \hat{y}_j | y_i = c)$$

Semi-supervised learning

- Graph-based semi-supervised learning
- Given partially labeled dataset
- Data: $\mathrm{X} = X_l \cup X_u$
  – small set of labeled data (X_l, Y_l)
  – large set of unlabeled data X_u
- Similarity graph over data points $G(V, E)$, where every vertex v_i corresponds to a data point x_i
- Transductive learning: learn a function that predicts labels Y_u for the unlabeled input X_u

Random walk methods

- Consider random walk with absorbing states - labeled nodes V_l
- Probability $\hat{y}_i[c]$ for node $v_i \in V_u$ to have label c,

$$\hat{y}_i[c] = \sum_{j \in V_l} p_{ij}^{\infty} y_j[c]$$

  where $y_i[c]$ - probability distribution over labels,
  $p_{ij} = P(i \to j)$ - one step probability transition matrix
- If output requires single label per node, assign the most probable
- In matrix form

$$\hat{Y} = P^{\infty} Y$$

  where $Y = (Y_l, 0)$, $\hat{Y} = (Y_l, \hat{Y}_u)$

Random walk methods

- Random walk matrix: $P = D^{-1}A$
- Random walk with absorbing states

$$P = \begin{pmatrix} P_{ll} & P_{lu} \\ P_{ul} & P_{uu} \end{pmatrix} = \begin{pmatrix} I & 0 \\ P_{ul} & P_{uu} \end{pmatrix}$$

- At the $t \to \infty$ limit:

$$\lim_{t\to\infty} P^t = \begin{pmatrix} I & 0 \\ \left(\sum_{n=0}^{\infty} P_{uu}^n\right) P_{ul} & P_{uu}^{\infty} \end{pmatrix} = \begin{pmatrix} I & 0 \\ (I - P_{uu})^{-1} P_{ul} & 0 \end{pmatrix}$$

Random walk methods

- Matrix equation

$$\begin{pmatrix} \hat{Y}_l \\ \hat{Y}_u \end{pmatrix} = \begin{pmatrix} I & 0 \\ (I - P_{uu})^{-1} P_{ul} & 0 \end{pmatrix} \begin{pmatrix} Y_l \\ Y_u \end{pmatrix}$$

- Solution

$$\begin{aligned} \hat{Y}_l &= Y_l \\ \hat{Y}_u &= (I - P_{uu})^{-1} P_{ul} Y_l \end{aligned}$$

- $(I - P_{uu})$ is non-singular for all label connected graphs (is always possible to reach a labeled node from any unlabeled node)

Label propagation

Algorithm: Label propagation, Zhu et. al 2002

Input: Graph $G(V, E)$, labels Y_l
Output: labels $\hat{Y}$
Compute $D_{ii} = \sum_j A_{ij}$
Compute $P = D^{-1}A$
Initialize $Y^{(0)} = (Y_l, 0)$, t=0
repeat
  $Y^{(t+1)} \leftarrow P \cdot Y^{(t)}$
  $Y_l^{(t+1)} \leftarrow Y_l^{(t)}$
until $Y^{(t)}$ *converges*;
$\hat{Y} \leftarrow Y^{(t)}$

Solution: $\hat{Y} = \lim_{t\to\infty} Y^{(t)} = (I - P_{uu})^{-1} P_{ul} Y_l$

Label spreading

Algorithm: Label spreading, Zhou et. al 2004

Input: Graph $G(V, E)$, labels Y_l
Output: labels $\hat{Y}$
Compute $D_{ii} = \sum_j A_{ij}$,
Compute $\mathcal{S} = D^{-1/2} A D^{-1/2}$
Initialize $Y^{(0)} = (Y_l, 0)$, t=0
repeat

$\quad Y^{(t+1)} \leftarrow \alpha \mathcal{S} Y^{(t)} + (1-\alpha) Y^{(0)}$

$\quad t \leftarrow t + 1$

until $Y^{(t)}$ *converges*;

Solution: $\hat{Y} = (1-\alpha)(I - \alpha\mathcal{S})^{-1} Y^{(0)}$

Regression on graphs

Find labeling $\hat{Y} = (\hat{Y}_l, \hat{Y}_u)$ that

- Consistent with initial labeling:

$$\sum_{i \in V_l} (\hat{y}_i - y_i)^2 = ||\hat{Y}_l - Y_l||^2$$

- Consistent with graph structure (regression function smoothness):

$$\frac{1}{2} \sum_{i,j \in V} A_{ij} (\hat{y}_i - \hat{y}_j)^2 = \hat{Y}^T (D - A) \hat{Y} = \hat{Y}^T L \hat{Y}$$

- Stable (additional regularization):

$$\epsilon \sum_{i \in V} \hat{y}_i^2 = \epsilon ||\hat{Y}||^2$$

Regularization on graphs

Minimization with respect to $\hat{Y}$, $\arg\min_{\hat{Y}} Q(\hat{Y})$

- Label propagation [Zhu, 2002]:

$$Q(\hat{Y}) = \frac{1}{2}\sum_{i,j\in V} A_{ij}(\hat{y}_i - \hat{y}_j)^2 = \hat{Y}^T L \hat{Y}, \quad \text{with fixed} \quad \hat{Y}_l = Y_l$$

- Label spread [Zhou, 2003]:

$$Q(\hat{Y}) = \frac{1}{2}\sum_{ij\in V} A_{ij}\left(\frac{\hat{y}_i}{\sqrt{d}_i} - \frac{\hat{y}_j}{\sqrt{d}_j}\right)^2 + \mu\sum_{i\in V}(\hat{y}_i - y_i)^2$$

$$Q(\hat{Y}) = \hat{Y}^T \mathcal{L}\hat{Y} + \mu||\hat{Y} - Y||^2$$

$\mathcal{L} = I - \mathcal{S} = I - D^{-1/2}AD^{-1/2}$

Regularization on graphs

- Laplacian regularization [Belkin, 2003]

$$Q(\hat{Y}) = \frac{1}{2}\sum_{ij\in V} A_{ij}\,(\hat{y}_i - \hat{y}_j)^2 + \mu \sum_{i\in V_l}(\hat{y}_i - y_i)^2$$

$$Q(\hat{Y}) = \hat{Y}^T L \hat{Y} + \mu||\hat{Y}_l - Y_l||^2$$

- Use eigenvectors $(e_1..e_p)$ from smallest eigenvalues of $L = D - A$:

$$Le_j = \lambda_j e_j$$

- Construct classifier (regression function) on eigenvectors

$$Err(a) = \sum_{i\in V_l}(y_i - \sum_{j=1}^{p} a_j e_{ji})^2$$

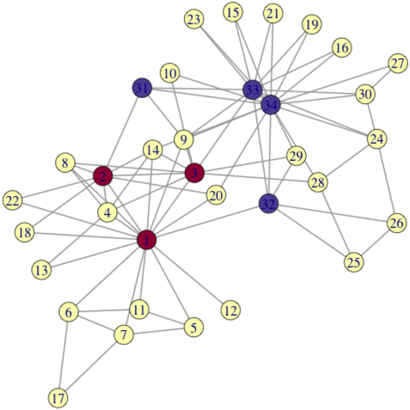
- Predict value (classify) $\hat{y}_i = \sum_{j=1}^{p} a_j e_{ji}$, class $c_i = sign(\hat{y}_i)$

Laplacian regularization

Algorithm: Laplacian regularization, Belkin and Niyogy, 2003

Input: Graph $G(V, E)$, labels Y_l
Output: labels $\hat{Y}$
Compute $D_{ii} = \sum_j A_{ij}$
Compute $L = D - A$
Compute p eigenvectors $e_1..e_p$ with smallest eigenvalues of L, $Le = \lambda e$
Minimize over $a_1...a_p$
$\arg\ \min_{a_1,\dots a_p} \sum_{i=1}^{l}(y_i - \sum_{j=1}^{p} a_j e_{ji})^2, \quad a = (E^T E)^{-1} E^T Y_l$
Label v_i by the $sign(\sum_{j=1}^{p} a_j e_{ji})$

Label propagation example



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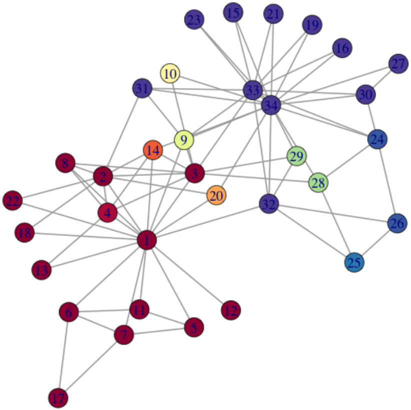

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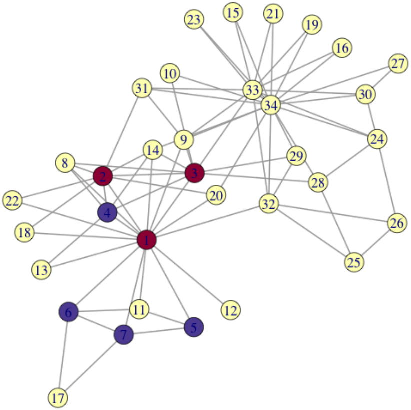
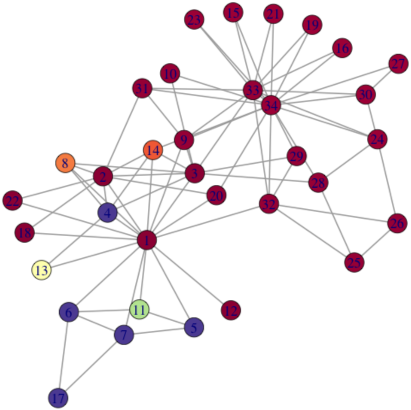


Label propagation example



Matrix Factorization: Dimension Reduction

The idea of solving node classification lies in decomposing structural and context features from graph for efficient node representation.

- Multidimensional scaling (MDS): Approximating MSE over $A_{ij} - |u_i - u_j|_2^2$
- Indexing by latent semantic analysis (LSI): SVD decomposition of A adjacency matrix
- Dimension reduction for A: PCA (principal components analysis), LDA (linear discriminant analysis), etc.

from Makarov et al., 2021[1]

[1] https://peerj.com/articles/cs-357/

Matrix Factorization: Proximity Matrix

Instead of extracting features from A alone, take into account node neighbors in the approximation framework.

A Global Geometric Framework for Nonlinear Dimensionality Reduction (**Isomap**)

- Take graph as an input from some metric learning task, for e.g.
- Compute its k-distance matrix by Floyd-Warshall algorithm.
- Use dimension reduction to extract meaningful components.

Nonlinear Dimensionality Reduction by Locally Linear Embedding (**LLE**)

$$LLE_{error}(W) = MSE(A - W^t U)$$

where U contains neighbors of points from A. In this way, locally, each point is presented as linear combinations of neighbor vector representations.

from Makarov et al., 2021[2]

[2] `https://peerj.com/articles/cs-357/`

Matrix Factorization: Spectral Decomposition

Find eigen-vector decomposition, producing low-dimensional space representation.

Laplacian Eigenmaps and Spectral Techniques for Embedding and Clustering (**LE**)

- Take graph as an input from some metric learning task, and allow heat kernels for weights from features F.
- Solve the equation $Lx = \lambda Dx$, $L = D - A$ is Laplacian
- $X = (x_1 \cdots x_n)$, $X^t F$ get a low dimension representation.

The goal for Laplacian Eigenmaps class of models lies in preserving first-order similarities giving a larger penalty using graph Laplacian if two nodes with larger similarity are embedded far apart.

Locality Preserving Projections (**LPP**)

- Take graph as an input from some metric learning task, and allow heat kernels for weights from features F.
- Solve the equation $FLF^t x = \lambda FDF^t x$, $L = D - A$ is Laplacian
- $X = (x_1 \cdots x_n)$, $X^t F$ get a low dimension representation.

Matrix Factorization: Second-order proximities

Find eigen-vector decomposition, producing low-dimensional space representation.
Continuous nonlinear dimensionality reduction by kernel eigenmaps (**Kernel Eigenmaps**) present a kernel-based mixture of affine maps from the ambient space to the target space, in which local PCA can be run.
Cauchy Graph Embedding enhance the local topology preserving with the similarity relationships of the original data.
Structure Preserving Embedding (**SPE**) aims to use LE combined with preserving spectral decomposition representing the cluster structure of the graph. SPE is formulated as a semidefinite program that learns a low-rank kernel matrix constrained by a set of linear inequalities which captures the input graph.
Graph Factorization minimize $MSE(A_{ij}, < Z_i, Z_j >)$ with L_2 regularization on 'Z' representations.

from Makarov et al., 2021[4]

[4] https://peerj.com/articles/cs-357/

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