Label propagation on graphs

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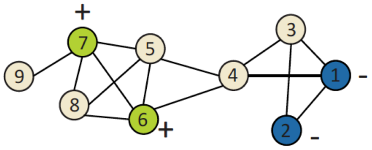
Lecture outline

1. Label propagation problem
2. Collective classification
   - Iterative classification
3. Semi-supervised learning
   - Random walk based methods
   - Graph regularization

Label propagation

- Label propagation - 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



Label propagation problem

- 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

Network 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)
- Feature (design) matrix $\Phi = (\Phi_l, \Phi_u)$

Network learning components

- **Local classifier**. This is a local learned model, predicts node label based on node attributes. No network information
- **Relational classier**. Takes into account labels and attributes of node neighbors. Uses neighborhood network information
- **Collective classifier**. Estimates unknown values together applying relational classifier iteratively. Strongly depends on network structure

Relational classifiers

- Weighted-vote relational neighbor classifier:

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

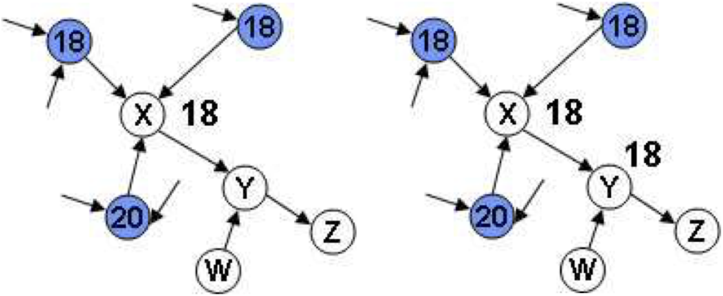
- Network only Naive Bayes classifier:

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

where

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

Iterative classification



(a) Step 1

(b) Step 2

Collective classification

Algorithm: Iterative classification method

Input: Graph $G(V, E)$, labels Y_l

Output: labels $\hat{Y}$

Compute $\Phi^{(0)}$

Train classifier on $(\Phi_l^{(0)}, Y_l)$

Predict $Y_u^{(0)}$

repeat

  Compute $\Phi_u^{(t)}$

  Train classifier on $(\Phi^{(t)}, Y^{(t)})$

  Predict $Y_u^{(t+1)}$ from $\Phi_u^{(t)}$

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

$\hat{Y} \leftarrow Y^{(t)}$

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 stept 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

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

$t \leftarrow t + 1$

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]:

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

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

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

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 $L = D - A$:

$$L e_j = \lambda_j e_j$$

- 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

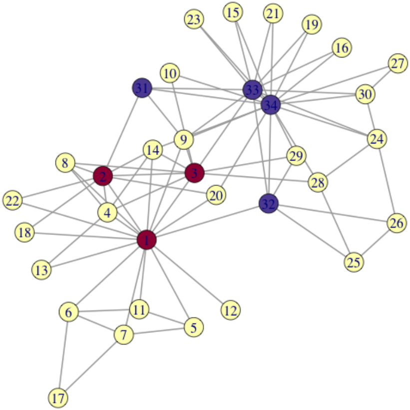
Algorithm: Laplacian regularization, Belkin and Niyogy, 2003

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 $a_1...a_p$
$\arg\ \min_{a_1,...a_p} \sum_{i=1}^{l}(y_i - \sum_{j=1}^{p} a_j e_{ji})^2, \quad a = (E^T E)^{-1} E^T Y_l$
Label v_i by the $sign(\sum_{j=1}^{p} a_j e_{ji})$

Label propagation example



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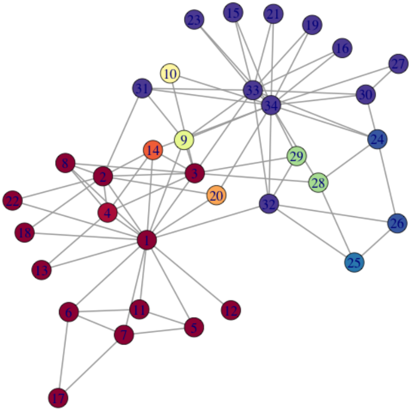

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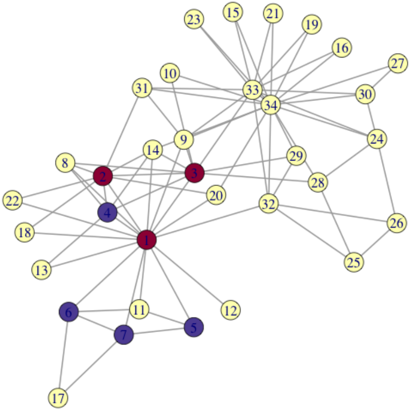

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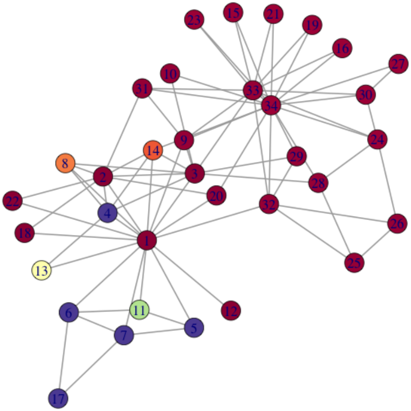

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