March 19, 2019

Last week:

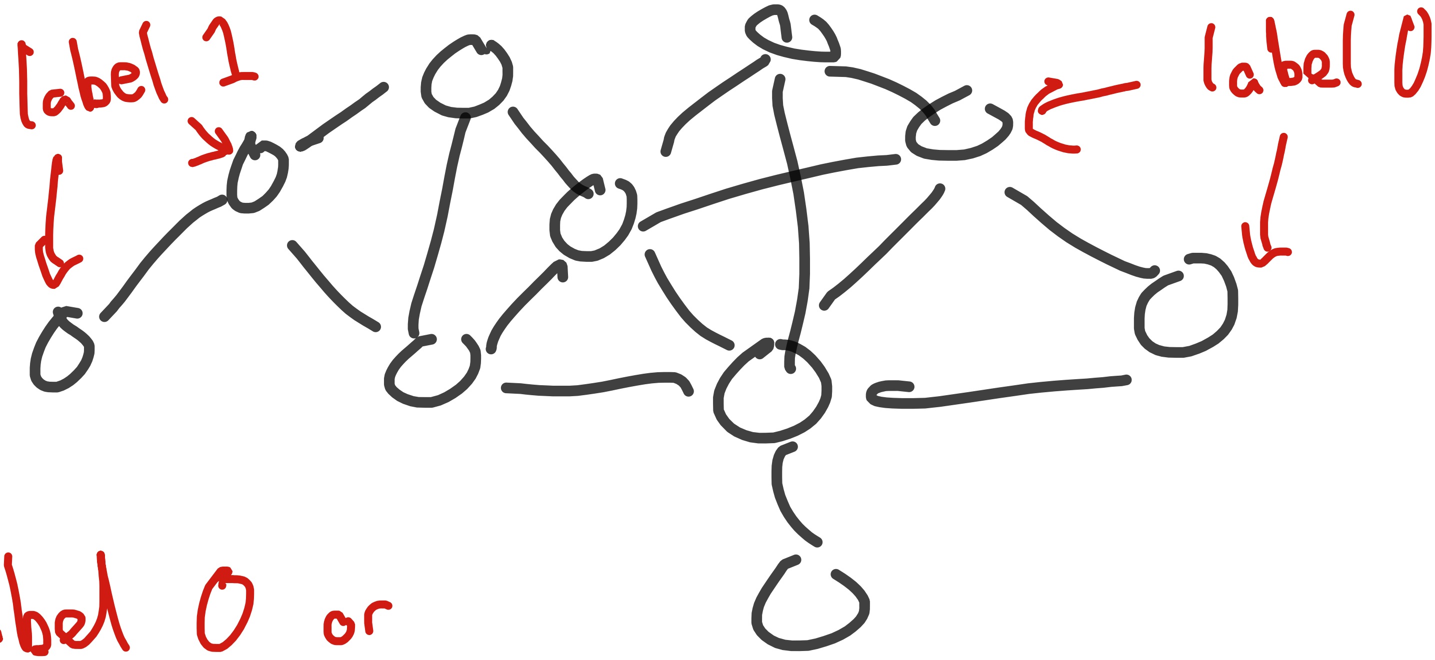
Graph clustering

- NCUT
- RCUT
- Bisection Cut

"unsupervised learning"

Today:

"semi-supervised learning" on graphs



label 0 or
label 1?

Goal: labels on the rest of the graph

$\Rightarrow$ classification

$f : V \to \mathbb{R}$ (labels)

$f(i) = f_i \in \mathbb{R}$

f should be smooth over the graph

(assuming homophily)

Penalty:

$$E(f) = \sum_{(i,j) \in E} (f_i - f_j)^2 = f^T L f$$

Possible opt problem:

$$\min_f \; f^T L f = E(f)$$
$$\text{s.t.} \quad f[H] = l$$

H are labeled nodes

l are labels

$U = V \setminus H$ unlabeled nodes

Lagrangian:

$$\mathcal{L}(f,\lambda) = f^T L f - \sum_{i \in H} \lambda_k (f_i - l_i)$$

$\nabla \mathcal{L} = 0$ at any optimum

$$\begin{aligned}
\nabla_{f_u} &= 2(Lf)_u \\
&= 2\left((Df)_u - (Af)_u\right) \\
&= 2\Big[d_u f_u - \sum_{(u,v)\in E} f_v\Big]
\end{aligned}$$

$$= 0 \iff f_u = \frac{1}{d_u} \sum_{(u,v)\in E} f_v$$

optimal point is mean of neighbors

Alternative:

$$f_U = (Pf)_U \qquad P = A^T D^{-1}$$

$$P = \begin{bmatrix} P_{HH} & P_{UH} \\ P_{UH} & P_{UU} \end{bmatrix}$$

$$(Pf)_U = f_U \qquad u \in U$$

$$f_H = l$$

$$f_U = P_{UH} f_H + P_{UU} f_U$$

$$= P_{UH}\, l + P_{UU} f_U$$

$$\Longleftrightarrow \underbrace{(I - P_{UU})}_{\text{average of neighbors}} f_U = \underbrace{P_{UH}\, l}_{\text{propagate labels}}$$

Claim: If graph connected, then $I - P_{uu}$ is nonsingular

$$D_{uu}(I - P_{uu}) f_u = D_{uu} P_{uL} \ell$$

$$\underbrace{(D_{uu} - A_{uu})}_{M = L_{uu}} f_u = r$$

Laplacian on graph then index on unlabeled nodes

M = Laplacian on graph induced by U

+ extra degrees from connections to labeled nodes

$$= \underbrace{\hat{L}}_{\geq 0} + \bar{D}$$

null space is span $\{\mathbb{1}\}$

$$\mathbb{1}^T(\hat{L} + \bar{D})\mathbb{1}$$

$$= \mathbb{1}^T \bar{D} \mathbb{1} > 0$$

$\hat{L} + \bar{D}$ is positive definite

(we can actually solve the system)

Random walk interpretation

1. Start a random walk from some unlabeled node $u \in U$
2. Solution f_u is the probability you end up at label 1 before label 0

$(f_v \in [0, 1]$ for all $v \in V)$

ZGL
Zhu, Ghahramani, Lafferty
2003

Clustering interpretation

$$\min_f \; f^T L f$$

s.t. $f[H] = \ell$

$\cancel{f \in \{0,1\}^n}$ soft clustering

s-t min-cut

solution is real-valued

- replacing L with N,
- normalized Laplacian
- $\langle f, \Delta_p f \rangle = \sum_{(i,j) \in E} |f_i - f_j|^p$

What about multiple labels?

$F \in \mathbb{R}^{n \times k}$

k labels

if $i \in \mathbb{L}$ with

$\ell = f_i \in \{1, \dots, k\}$

set. $F_{i\ell} = 1$

$F_{ij} = 0 \quad j \neq \ell$

Smoothness constraint:

$$\mathrm{tr}(F^T L F) = \sum_{\ell=1}^{k} F_{:,\ell}^T L F_{:,\ell}$$

$$\min \ \mathrm{tr}(F^T L F)$$

s.t. labeling

Solution:

$$(I - P_{uu}) F_{u,l} = P_{uH} F_{H,l}$$

for $l \in \{1, \dots, k\}$

Learning with local and global consistency (Zhou et al. 2004)

Idea: do not fix labels at the labeled nodes, but still use the information

① Normalized adjacency:

$$S = D^{-1/2} A D^{-1/2}$$

② $$F(t+1) = \underbrace{\alpha S F(t)}_{\text{global consistency}} + \underbrace{(1-\alpha) Y}_{\text{local}}$$

given labels

$$Y_{ij} = \begin{cases} 1 & \text{if } i \text{ labeled } j \\ 0 & \text{o/w} \end{cases}$$

③ $$F^* = \lim_{t \to \infty} F(t)$$

label node i with

$$\arg\max_k F^*_{ik}$$

limit is given by

$$(I - \alpha S) F^* = (1-\alpha) Y$$

$I - S = N$ normalized laplacian

$\alpha \in [0,1)$

$I - \alpha S$ is nonsingular

Spectral graph transducer

(Joachims 2003)

basic idea: penalize differences with true labeling while forcing RCUT-like objective

RCUT relaxation

$$\min_x \; x^T L x$$

$$\text{s.t.} \quad \mathbb{1}^T x = 0 \qquad x^T x = n$$

now some points are labeled, say ± 1

Add penalty

labels

$$(x - \ell)^T C (x - \ell) \qquad \ell_i \in \left\{\begin{array}{l} +1 \\ -1 \end{array}\right\} \text{labeled}, \quad 0 \ \text{unlabeled}$$

$$C_{ii} = \begin{cases} 1 & i \in H \\ 0 & i \in U \end{cases}$$

Opt. problem

$$\min_x \; x^T L x + \lambda (x-\ell)^T C (x-\ell)$$

$$\text{s.t.} \quad x^T \mathbb{1} = 0$$

convex objective

linear constraints

(also closed form)