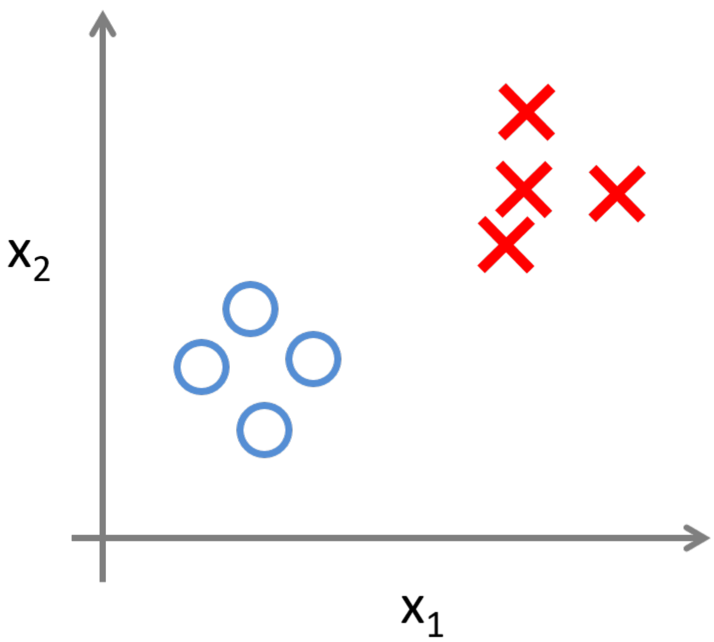
Semi-Supervised Learning

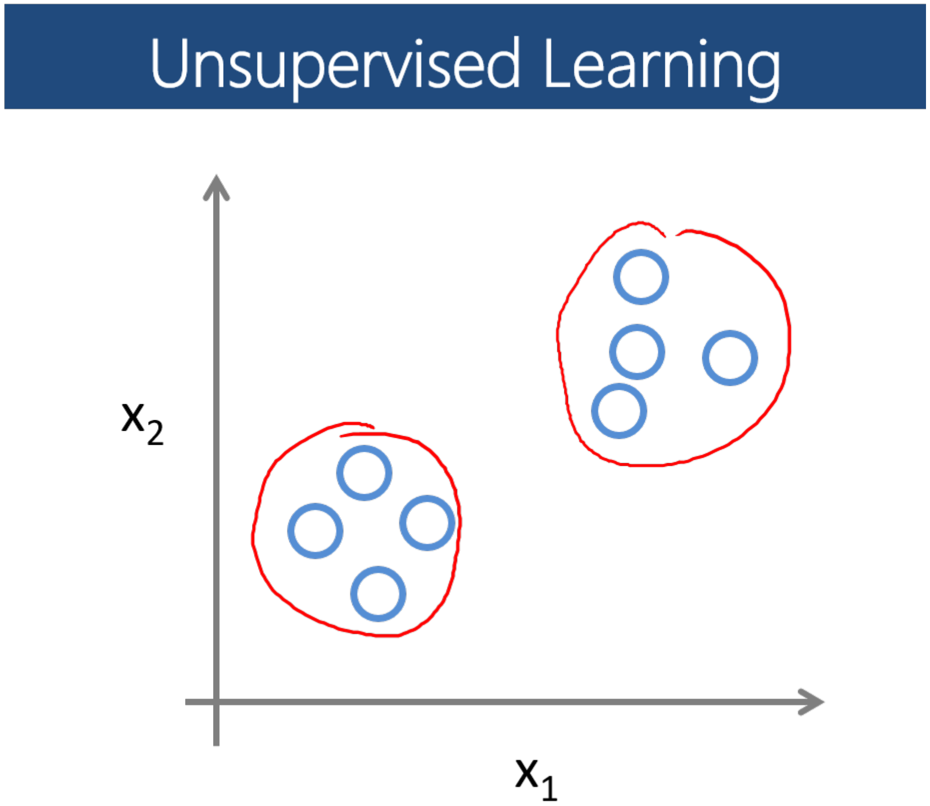
CSCI 4360/6360 Data Science II

Supervised learning

Supervised Learning



Unsupervised learning



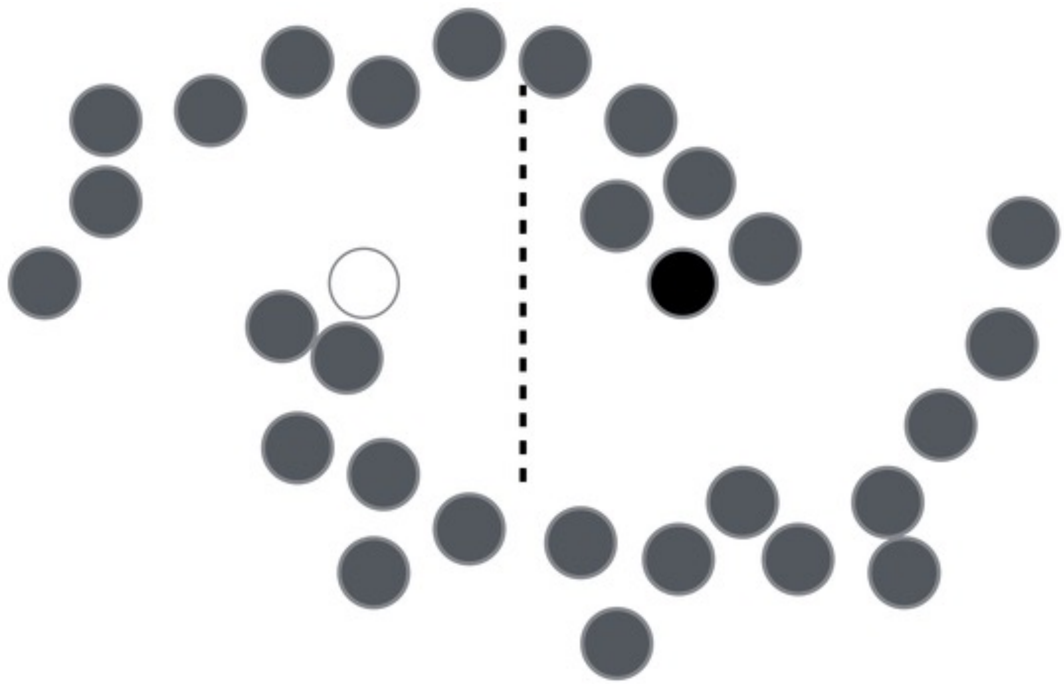
Semi-supervised learning

- Basically a hybrid!

- Given:
  - A pool of labeled examples L
  - A (usually larger) pool of unlabeled examples U

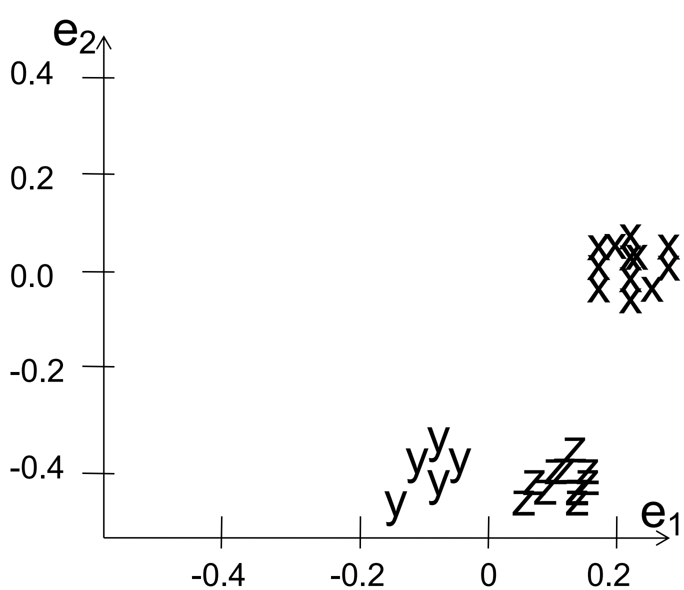
- **Can you improve accuracy somehow using U?**

Semi-supervised Learning

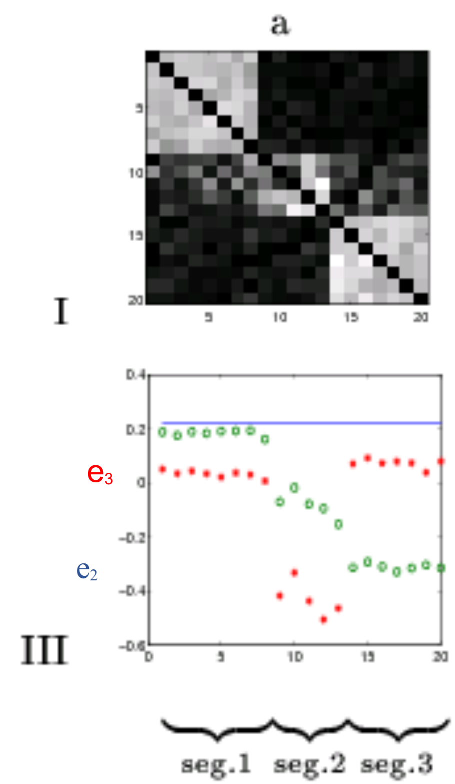


Spectral Clustering

- Graph = Matrix
  - $W^*v_1 = v_2$ “propogates weights from neighbors”

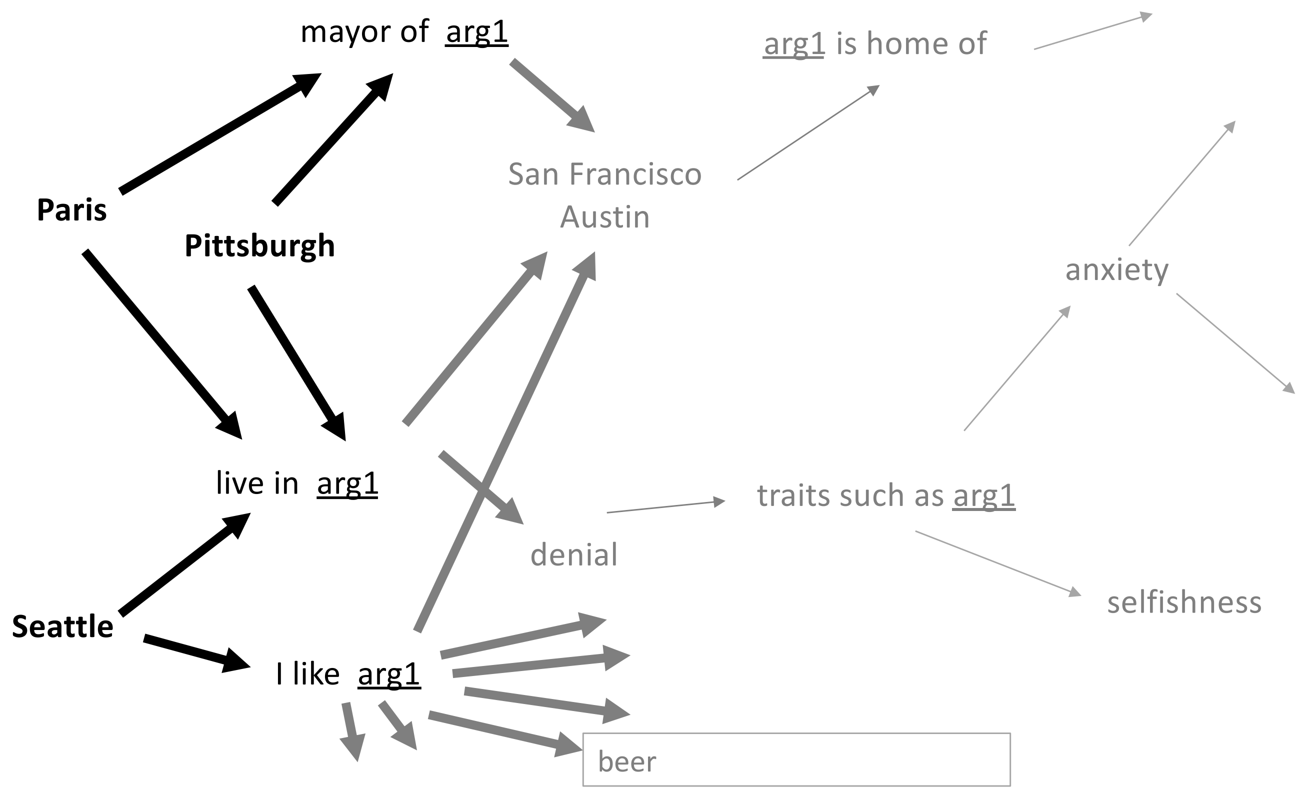


[Shi & Meila, 2002]



Semi-Supervised Learning as Label Propagation on a Graph

- Propagate label to "nearby" nodes
  - X is "near" Y if there is a high probability of reaching Y from X
- Propagation methods
  - Personalized PageRank
  - Random walk
- Rewards multiple paths
- Penalizes longer and "high fanout" paths



Semi-Supervised Classification of Network Data Using Very Few Labels

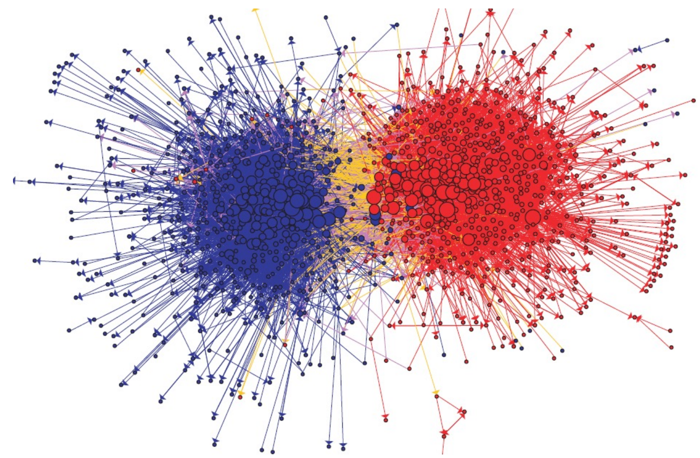
Frank Lin
Carnegie Mellon University, Pittsburgh, Pennsylvania
Email: frank@cs.cmu.edu

William W. Cohen
Carnegie Mellon University, Pittsburgh, Pennsylvania
Email: wcohen@cs.cmu.edu

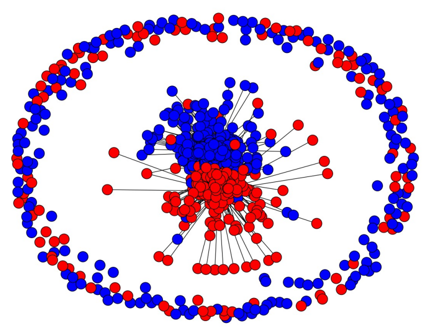
ASONAM-2010 (Advances in Social Networks Analysis and Mining)

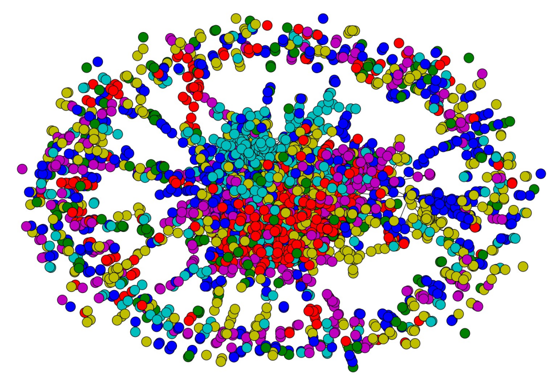
Network Datasets with Known Classes

- UBMCBlog
- AGBlog
- MSPBlog
- Cora
- Citeseer



	Nodes	Edges	Density
UMBCBlog	404	2725	0.01670
AGBlog	1222	19021	0.01274
MSPBlog	1031	9316	0.00876
Cora	2485	5209	0.00084
CiteSeer	2110	3757	0.00084





MultiRankWalk

- Seed Selection
  - Order by PageRank or degree, or even randomly
  - Traverse list until you have *k* examples/class

$$\vec{r} = (1-d)\vec{u} + dW\vec{r}$$

Given: A graph $G = (V, E)$, corresponding to nodes in G are instances X, composed of unlabeled instances X^U and labeled instances X^L with corresponding labels Y^L, and a damping factor d.
Returns: Labels Y^U for unlabeled nodes X^U.

For each class c

1) Set $\mathbf{u}_i \leftarrow 1, \forall Y_i^L = c$
2) Normalize $\mathbf{u}$ such that $||\mathbf{u}||_1 = 1$
3) Set $R_c \leftarrow RandomWalk(G, \mathbf{u}, d)$

For each instance i

- Set $X_i^U \leftarrow argmax_c(R_{ci})$

Fig. 1. The MultiRankWalk algorithm.

Comparison: wvRN

- One definition [MacSkassy & Provost, JMLR 2007]:…

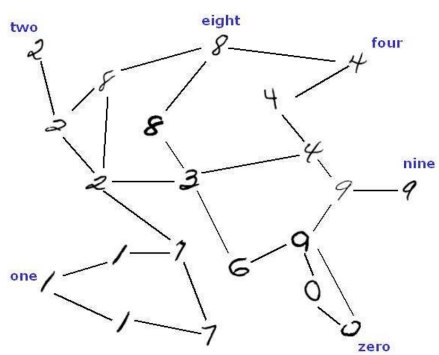
Definition. Given $v_i \in \mathbf{V}^U$, the weighted-vote relational-neighbor classifier (wvRN) estimates $P(x_i|\mathcal{N}_i)$ as the (weighted) mean of the class-membership probabilities of the entities in $\mathcal{N}_i$:

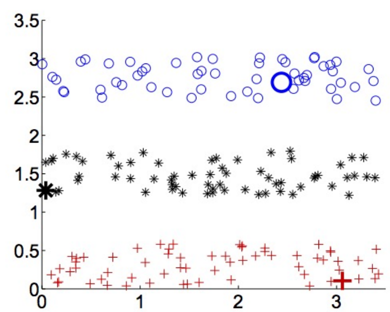
$$P(x_i = c|\mathcal{N}_i) = \frac{1}{Z} \sum_{v_j \in \mathcal{N}_i} w_{i,j} \cdot P(x_j = c|\mathcal{N}_j),$$

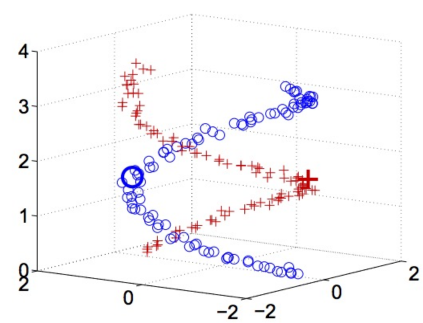
- Does this look familiar?
- **Homophily!**

Comparison: HF

- Another definition in [X. Zhu, Z. Ghahramani, and J. Lafferty, ICML 2003]
- A **harmonic field** – the score of each node in the graph is the harmonic, or linearly weighted, average of its neighbors' scores (harmonic field, HF)

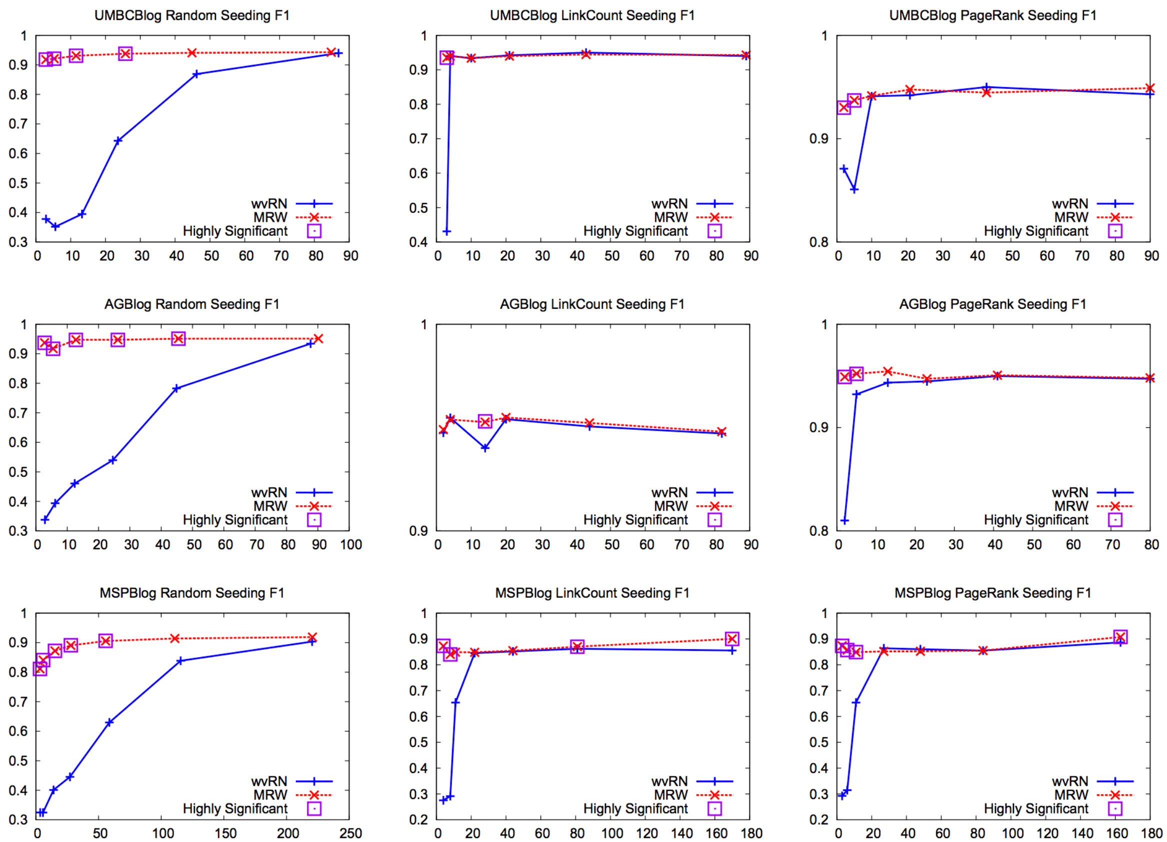






MRW versus wvRN

- MRW is easily the method to beat
- wvRN matches MRW **only** when seeding is **not** random
- Still takes a larger number of labeled instances compared to MRW



Why is MRW > wvRN?

- Start with wvRN & HF objectives

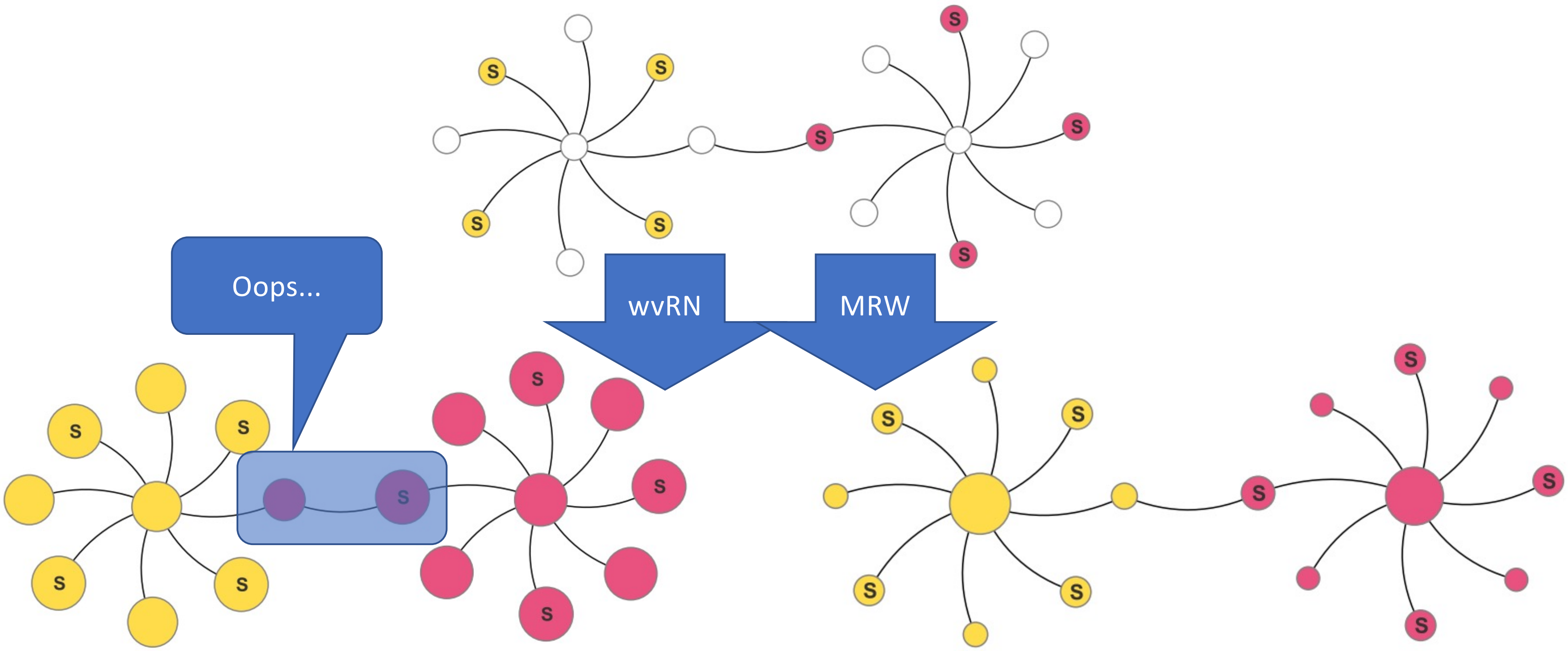
$$P(x_i = c|N_i) = \frac{1}{Z}\sum_{v_j \in N_i} w_{i,j}.P(x_j = c|N_j) \tag{6.2}$$

- Do not account for graph *structure*
  - Or location of seeds

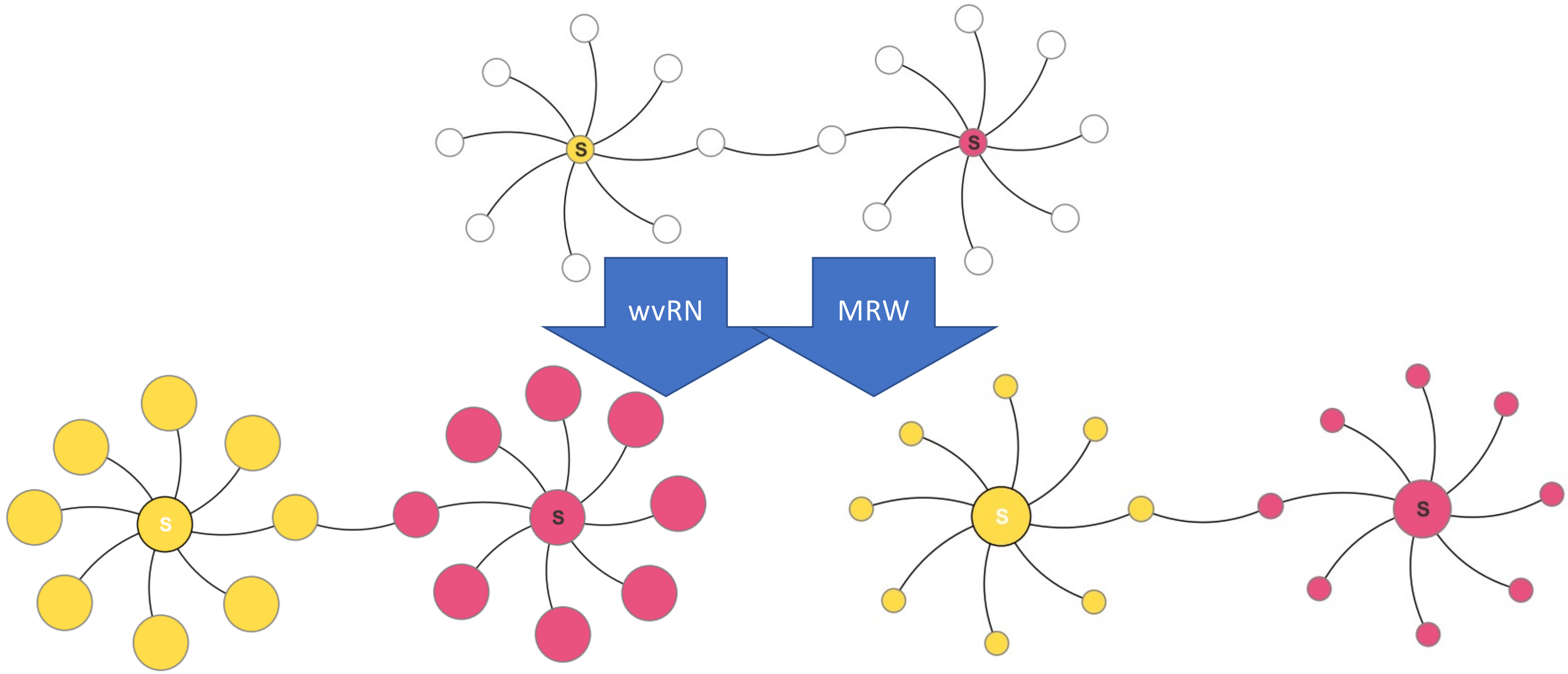
$$f(j) = \frac{1}{d_j}\sum_{i\ \ j} w_{i,j}.f(i) \tag{6.3}$$

- **Graph-walk methods do not have these constraints**
  - And directly account for graph structure

Why is MRW > wvRN?



Why is MRW > wvRN?



Modern SSL

- Graph Laplacians
  - Enforces graph structure
  - Imposes smoothness on labels
- Graph embeddings
  - "Embedding" ~ "context"
- Transductive -> Inductive
  - Transductive: learns the unlabeled data from the labeled data + structure
  - Inductive: generalizes to completely unobserved data

Graph Laplacians

- Reformulate SSL objective as two distinct terms:

$$f^T L f = \frac{1}{2} \sum_{i,j} W_{ij} \left(f(i) - f(j)\right)^2$$

Weighted sum of supervised loss over *labeled* instances

$$J(f) = f^T L f + \sum_{i=1}^{l} \lambda (f(i) - y_i)^2 = f^T L f + (f-y)^T \Lambda (f-y)$$

Graph Laplacian regularization term

Graph Embeddings

- Remember word embeddings with word2vec?
- **Context!**
- Estimate ”context” of each node with a random walk over neighborhood of a fixed window size
- Skipgram-based model, DeepWalk

$$-\sum_{(i,c)} \log p(c|i) = -\sum_{(i,c)} \left(\mathbf{w}_c^T \mathbf{e}_i - \log \sum_{c' \in \mathcal{C}} \exp(\mathbf{w}_{c'}^T \mathbf{e}_i) \right)$$

- C is set of all possible context
- w’s are parameters of Skipgram
- e_i is embedding of node *i*

Inductive SSL

- You start with X^l (labeled) and X^U (unlabeled), hoping their combination will result in a superior model
- Semi-supervised learning yields predictions on X^U
  - Transductive learning
- What if a *completely unobserved* data point shows up?
  - Inductive learning—a concept often left out in SSL literature
- **Convert your SSL framework to classification!**

Transductive learning (note embeddings)

$$p(y|\mathbf{x},\mathbf{e}) = \frac{\exp[\mathbf{h}^k(\mathbf{x})^T, \mathbf{h}^l(\mathbf{e})^T]\mathbf{w}_y}{\sum_{y'} \exp[\mathbf{h}^k(\mathbf{x})^T, \mathbf{h}^l(\mathbf{e})^T]\mathbf{w}_{y'}},$$

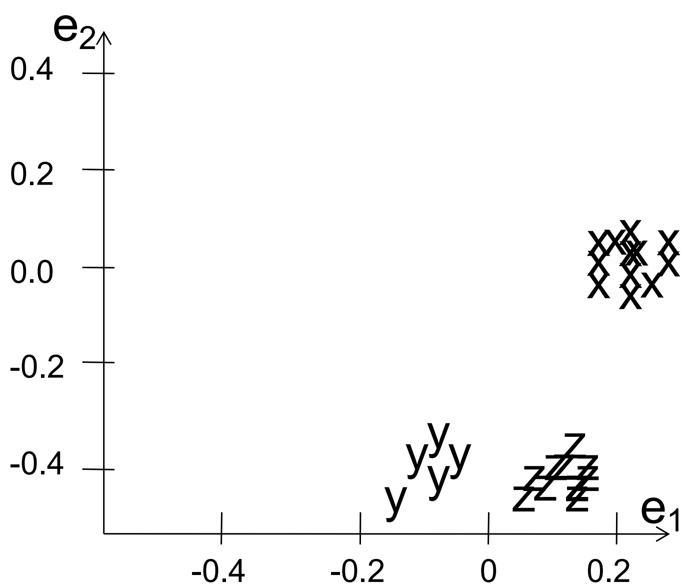
Inductive learning (dependent only on *x*)

$$p(y|\mathbf{x}) = \frac{\exp[\mathbf{h}^k(\mathbf{x})^T, \mathbf{h}^l(\mathbf{x})^T]\mathbf{w}_y}{\sum_{y'} \exp[\mathbf{h}^k(\mathbf{x})^T, \mathbf{h}^l(\mathbf{x})^T]\mathbf{w}_{y'}}$$

Quick digression to unsupervised learning…

Spectral Clustering

- Graph = Matrix
  - $W^*v_1 = v_2$ “propogates weights from neighbors”



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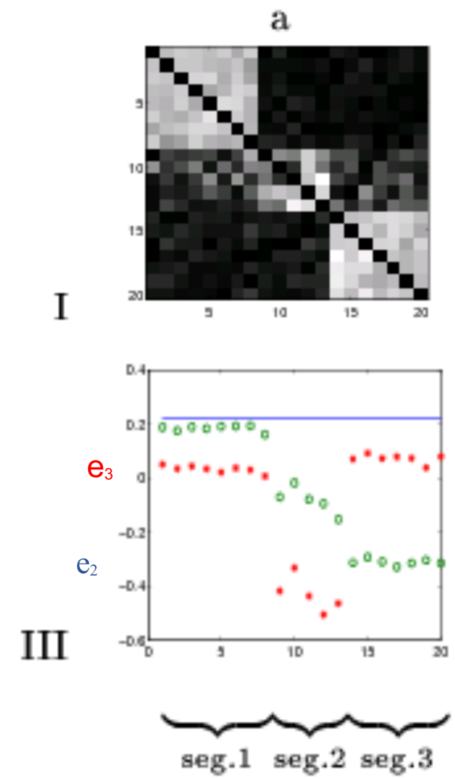
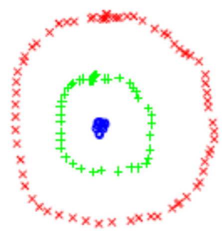


Repeated averaging with neighbors as a clustering method

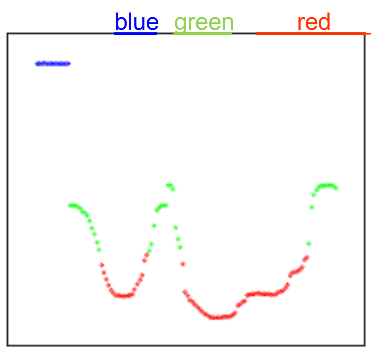
- Pick a vector v^0 (maybe at random)
- Compute $v^1 = Wv^0$
  - i.e., replace $v^0[x]$ with *weighted average* of $v^0[y]$ for the neighbors y of x
- Plot $v^1[x]$ for each x
- Repeat for v^2, v^3, …

- Variants widely used for *semi-supervised* learning
  - clamping of labels for nodes with known labels
- Without clamping, will converge to constant v^t
- What are the *dynamics* of this process?

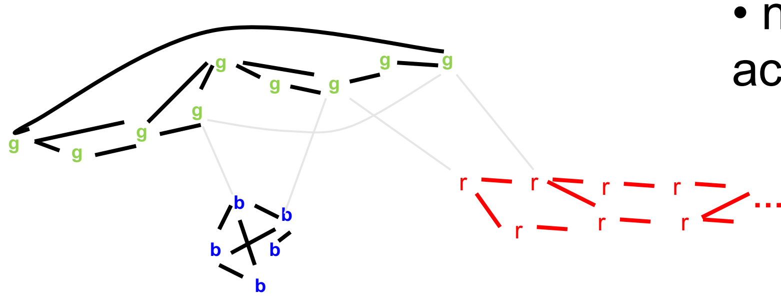
Repeated averaging with neighbors on a sample problem…



(a) 3Circles PIC result

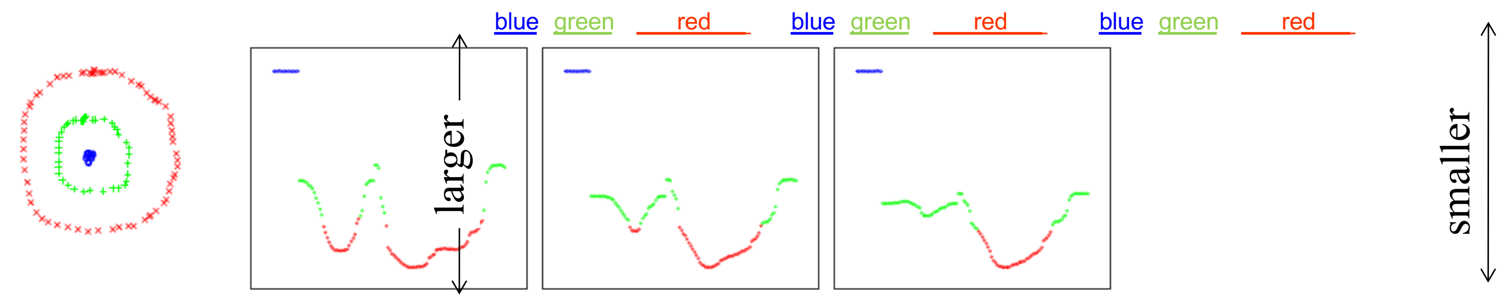


(b) Embedding at $t = 10$



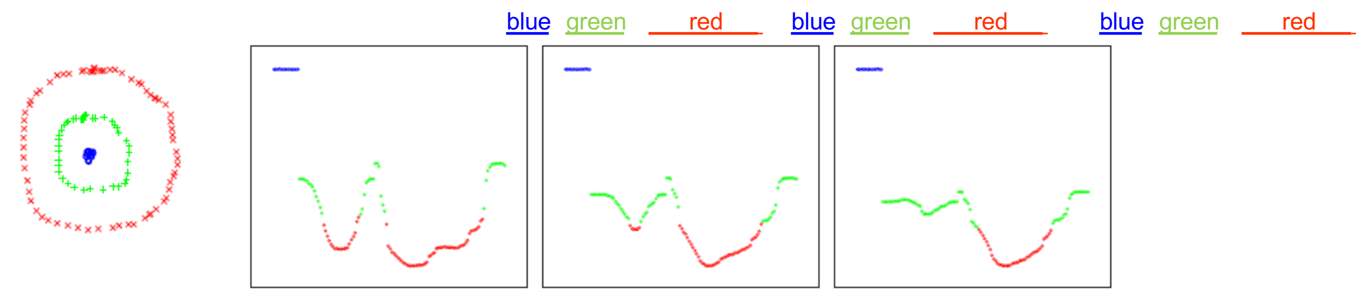
- Create a graph, connecting all points in the 2-D initial space to all other points
    - Weighted by distance
- Run power iteration for 10 steps
- Plot node id x vs $v^{10}(x)$
    - nodes are ordered by actual cluster number

Repeated averaging with neighbors on a sample problem…



(a) 3Circles PIC result (b) Embedding at $t = 10$ (c) Embedding at $t = 50$ (d) Embedding at $t = 100$

Repeated averaging with neighbors on a sample problem…



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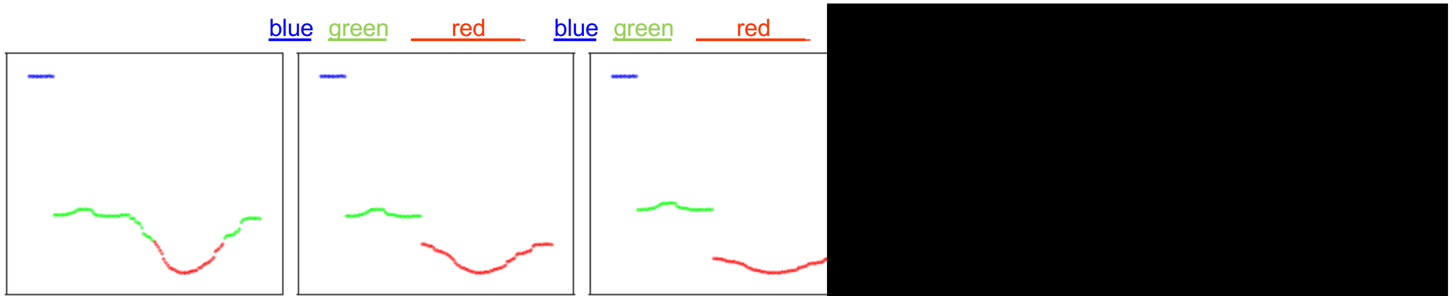
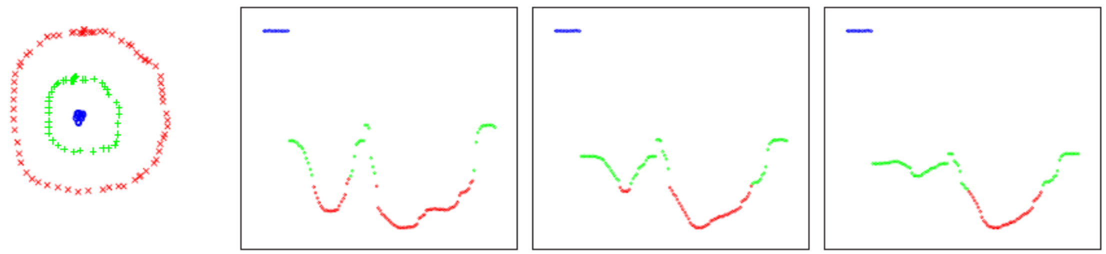


(e) Embedding at $t = 200$ (f) Embedding at $t = 400$ (g) Embedding at $t = 60$[redacted]

Repeated averaging with neighbors on a sample problem…



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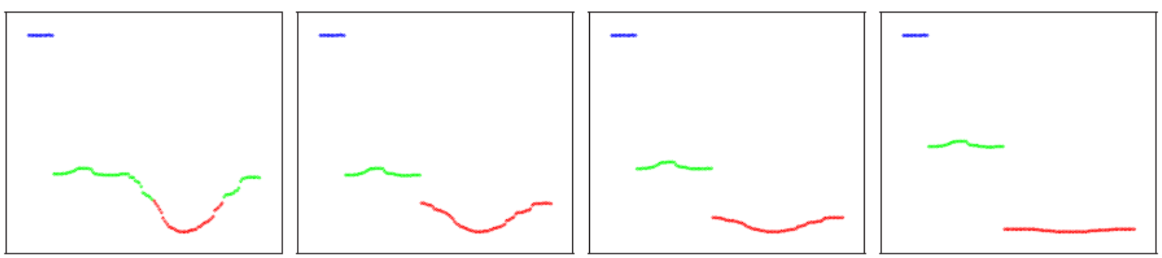
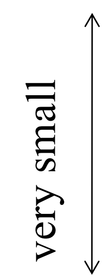


(e) Embedding at $t = 200$ (f) Embedding at $t = 400$ (g) Embedding at $t = 600$ (h) Embedding at $t = 1000$



PIC: Power Iteration Clustering

- Run power iteration (repeated averaging w/ neighbors) with early stopping

1. Pick an initial vector $\mathbf{v^0}$.
2. Set $\mathbf{v^{t+1}} \leftarrow \frac{W\mathbf{v^t}}{\|W\mathbf{v^t}\|_1}$ and $\boldsymbol{\delta}^{t+1} \leftarrow |\mathbf{v^{t+1}} - \mathbf{v^t}|$.
3. Increment t and repeat above step until $|\boldsymbol{\delta}^t - \boldsymbol{\delta}^{t-1}| \simeq \mathbf{0}$.
4. Use k-means to cluster points on $\mathbf{v^t}$ and return clusters $C_1, C_2, ..., C_k$.

- v^0: random start, or "degree matrix" D, or others
- Easy to implement, and relatively efficient (& easily parallelized!)
- Empirically, often **better** than traditional spectral methods
  - Surprising given embedded space is 1-dimensional!

References

- "Semi-Supervised Classification of Network Data Using Very Few Labels", https://lti.cs.cmu.edu/sites/default/files/research/reports/2009/cmulti09017.pdf
- "New Regularized Algorithms for Transductive Learning", http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.220.42&rep=rep1&type=pdf
- "Semi-supervised Learning in Gigantic Image Collections", http://papers.nips.cc/paper/3633-semi-supervised-learning-in-gigantic-image-collections.pdf
- "Revisiting Semi-Supervised Learning with Graph Embeddings", http://proceedings.mlr.press/v48/yanga16.pdf

Notations

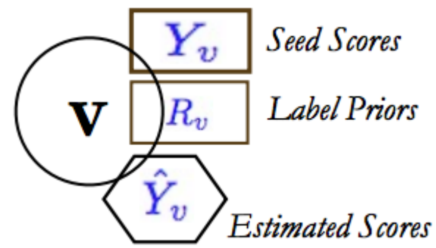
$\hat{Y}_{v,l}$: score of estimated label l on node v

$Y_{v,l}$: score of seed label l on node v

$R_{v,l}$: regularization target for label l on node v

S : seed node indicator (diagonal matrix)

W_{uv} : weight of edge (u, v) in the graph



LP-ZGL (Zhu et al., ICML 2003)

Smooth

$$\arg\min_{\hat{Y}} \boxed{\sum_{l=1}^{m} W_{uv}(\hat{Y}_{ul} - \hat{Y}_{vl})^2} = \sum_{l=1}^{m} \hat{Y}_l^T L \hat{Y}_l$$

Graph Laplacian
L = D - W (PSD)

such that $\boxed{Y_{ul} = \hat{Y}_{ul}, \ \forall S_{uu} = 1}$

Match Seeds (hard)

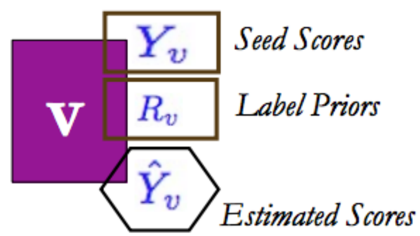
- Smoothness
  - two nodes connected by an edge with high weight should be assigned similar labels
- Solution satisfies harmonic property

Modified Adsorption (MAD)

[Talukdar and Crammer, ECML 2009]

$$\arg\min_{\hat{\mathbf{Y}}} \sum_{l=1}^{m+1} \left[\|\boldsymbol{S}\hat{\mathbf{Y}}_l - \boldsymbol{S}\mathbf{Y}_l\|^2 + \mu_1 \sum_{u,v} \boldsymbol{M}_{uv} (\hat{\mathbf{Y}}_{ul} - \hat{\mathbf{Y}}_{vl})^2 + \mu_2 \|\hat{\mathbf{Y}}_l - \boldsymbol{R}_l\|^2 \right]$$

- m labels, +1 dummy label
- $\boldsymbol{M} = \boldsymbol{W}^{\dagger} + \boldsymbol{W}'$ is the symmetrized weight matrix
- $\hat{\mathbf{Y}}_{vl}$: weight of label l on node v
- $\mathbf{Y}_{vl}$: seed weight for label l on node v
- $\boldsymbol{S}$: diagonal matrix, nonzero for seed nodes
- $\boldsymbol{R}_{vl}$: regularization target for label l on node v



Modified Adsorption (MAD)

[Talukdar and Crammer, ECML 2009]

$$\arg\min_{\hat{\mathbf{Y}}} \sum_{l=1}^{m+1} \left[\|\boldsymbol{S}\hat{\boldsymbol{Y}}_l - \boldsymbol{S}\boldsymbol{Y}_l\|^2 + \mu_1 \sum_{u,v} \boldsymbol{M}_{uv}(\hat{\boldsymbol{Y}}_{ul} - \hat{\boldsymbol{Y}}_{vl})^2 + \mu_2 \|\hat{\boldsymbol{Y}}_l - \boldsymbol{R}_l\|^2 \right]$$

How to do this minimization?
First, differentiate to find min is at

$$\left(\mu_1 \mathbf{S} + \mu_2 \mathbf{L} + \mu_3 \mathbf{I}\right) \hat{\mathbf{Y}}_l = \left(\mu_1 \mathbf{S}\mathbf{Y}_l + \mu_3 \mathbf{R}_l\right) .$$

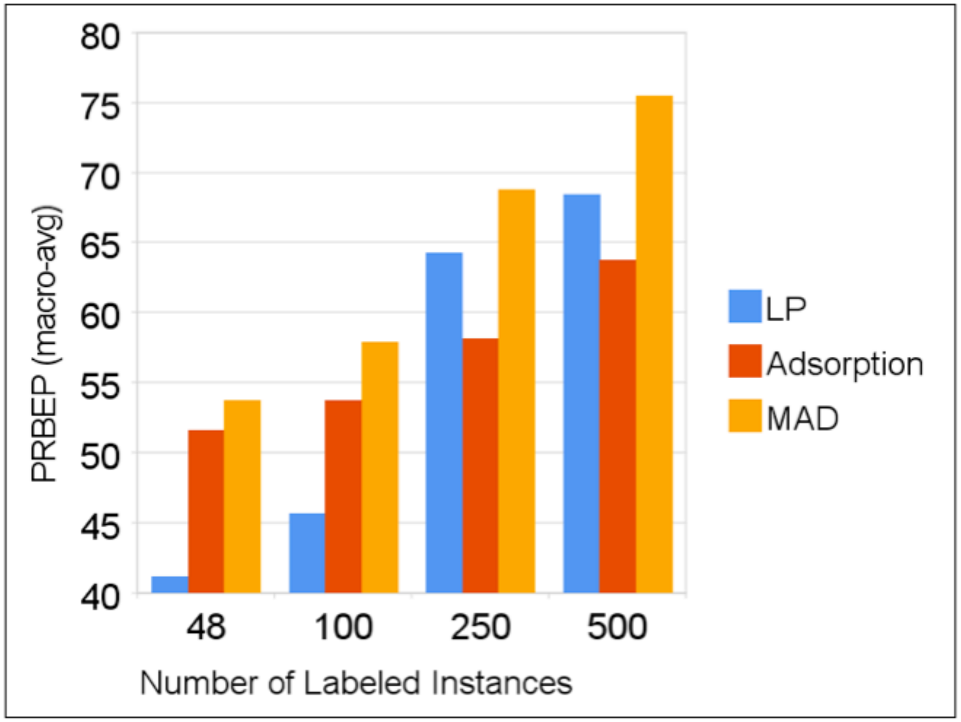
Jacobi method:

- To solve Ax=b for x
- Iterate: $$\mathbf{x}^{(k+1)} = D^{-1}(\mathbf{b} - R\mathbf{x}^{(k)}).$$
- … or: $$x_i^{(k+1)} = \frac{1}{a_{ii}} \left(b_i - \sum_{j \neq i} a_{ij} x_j^{(k)} \right), \quad i = 1, 2, \ldots, n.$$

Inputs $\boldsymbol{Y}, \boldsymbol{R} : |V| \times (|L|+1)$, $\boldsymbol{W} : |V| \times |V|$, $\boldsymbol{S} : |V| \times |V|$ diagonal
$\hat{\boldsymbol{Y}} \leftarrow \boldsymbol{Y}$
$\boldsymbol{M} = \boldsymbol{W}' + \boldsymbol{W}^{\dagger}$
$Z_v \leftarrow \boldsymbol{S}_{vv} + \mu_1 \sum_{u \neq v} \boldsymbol{M}_{vu} + \mu_2 \quad \forall v \in V$
repeat
  for all $v \in V$ **do**
    $\hat{\boldsymbol{Y}}_v \leftarrow \frac{1}{Z_v} \left((\boldsymbol{SY})_v + \mu_1 \boldsymbol{M}_{v\cdot} \hat{\boldsymbol{Y}} + \mu_2 \boldsymbol{R}_v \right)$
  end for
until convergence

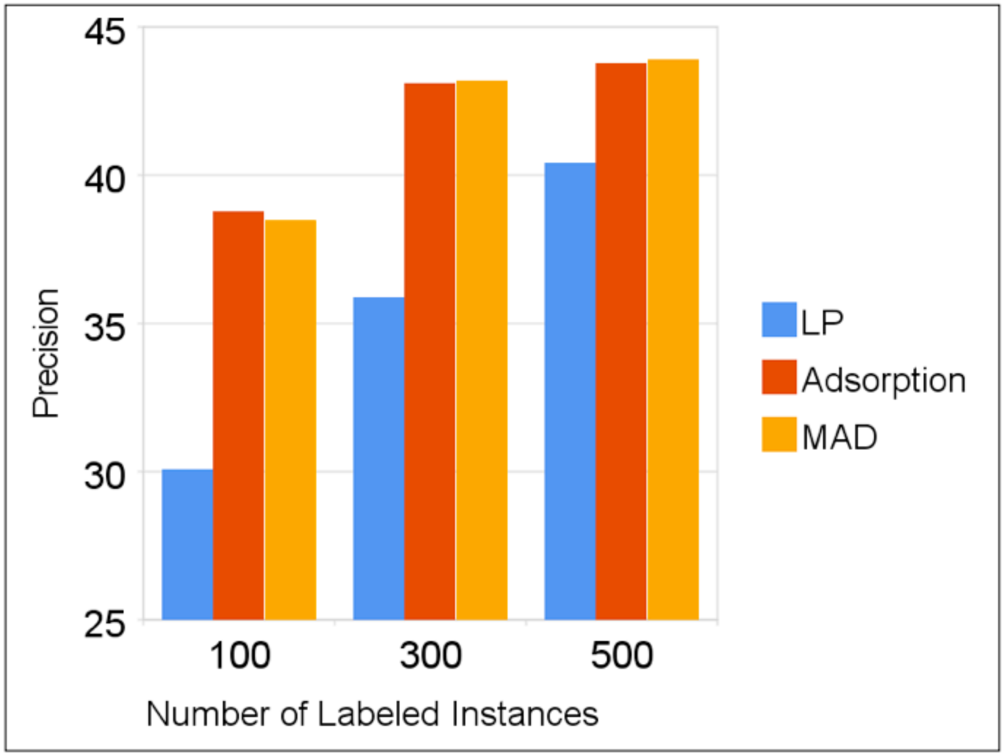
- Extends Adsorption with well-defined optimization
- Importance of a node can be discounted
- Easily Parallelizable: Scalable

Text Classification



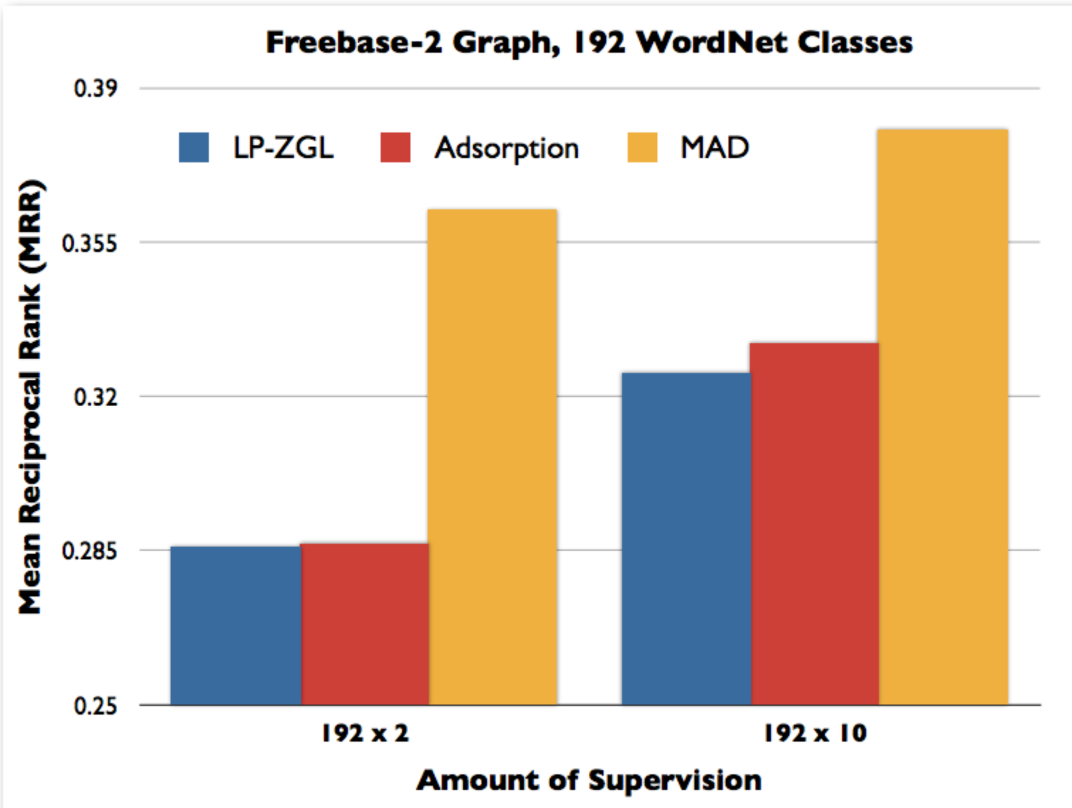
PRBEP (macro-averaged) on WebKB Dataset, 3148 test instances

Sentiment Classification



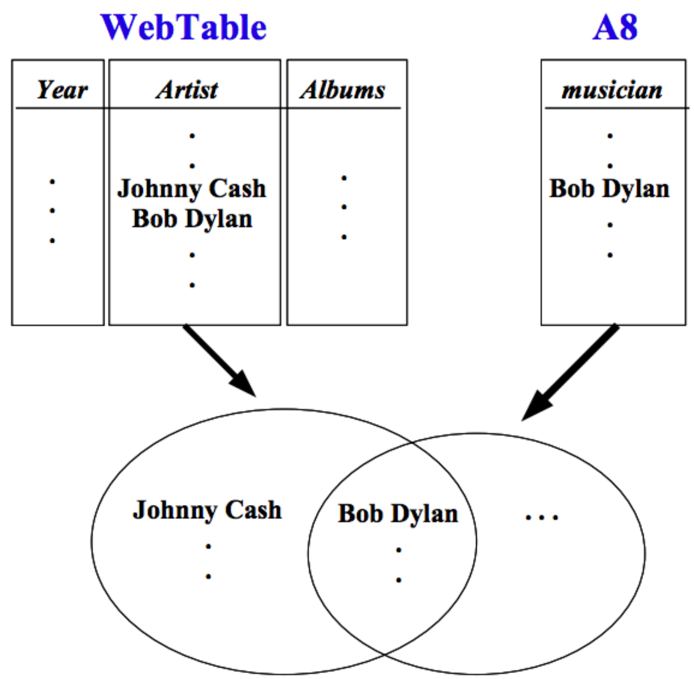
Precision on 3568 Sentiment test instances

Class-Instance Acquisition

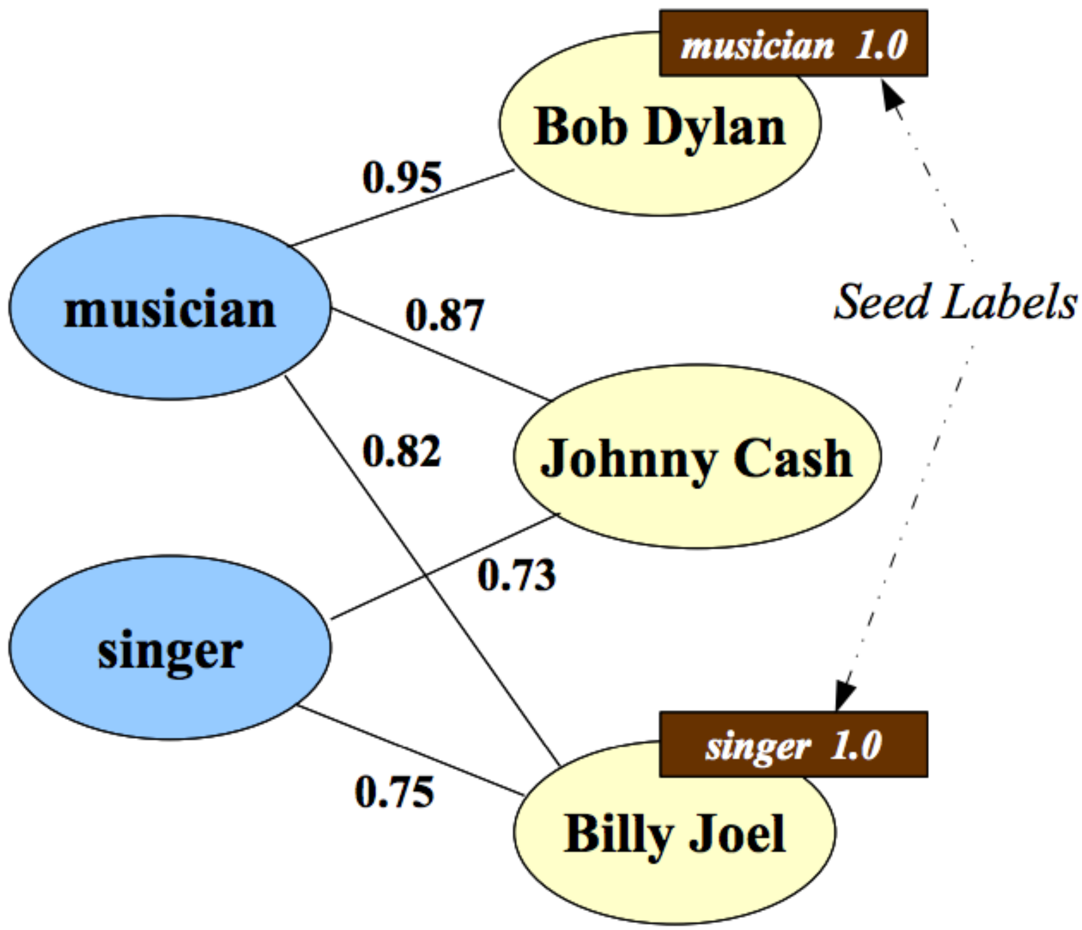


Graph with 303k nodes, 2.3m edges.

Assigning class labels to WebTable instances



Score (musician, Johnny Cash) = 0.87



musician 1.0
Bob Dylan
0.95
musician
0.87
Seed Labels
0.82
Johnny Cash
0.73
singer
singer 1.0
0.75
Billy Joel

New (Class, Instance) Pairs Found

Class	**A few non-seed Instances found by Adsorption**
Scientific Journals	Journal of Physics, Nature, Structural and Molecular Biology, Sciences Sociales et sante, Kidney and Blood Pressure Research, American Journal of Physiology-Cell Physiology, …
NFL Players	Tony Gonzales, Thabiti Davis, Taylor Stubblefield, Ron Dixon, Rodney Hannan, …
Book Publishers	Small Night Shade Books, House of Ansari Press, Highwater Books, Distributed Art Publishers, Cooper Canyon Press, …

Total classes: **9081**