THE UNIVERSITY OF TEXAS AT AUSTIN
Department of Statistics and Data Sciences
College of Natural Sciences

SDS 385: Stat Models for Big Data

Lecture 10: Pagerank and related methods

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Ranking and Pagerank

- Goal: obtain a ranking of webpages which are connected via hyperlinks
- Hope: webpages pointed to by other "important" webpages are also important.
- Developed by Brin and Page (1999)
- Many subsequent works:
    - HITS (Kleinberg, 1998)
    - Pagerank (Page and Brin, 1998)

Definitions

- $n \times n$ Adjacency matrix A
  - A_{ij} = weight on an edge from i to j
  - If graph is undirected $A(i,j) = A(j,i)$
- $n \times n$ Probability transition matrix P
  - P has rows summing to one, i.e. row stochastic
  - $P(i,j)$ is the probability that a random walker will step on j from i.
  - $P(i,j) = \frac{A(i,j)}{\sum_j A(i,j)}$
- $n \times n$ Laplacian matrix L
  - $L = D - A$, where D is the diagonal matrix of degrees
  - It is symmetric positive semidefinite for undirected graphs.
  - Singular, i.e. has a zero eigenvalue

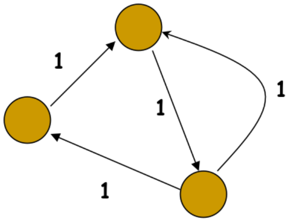
Definition

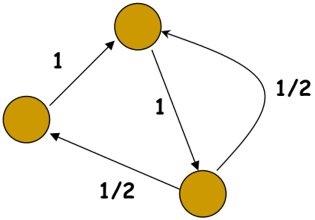
$$\begin{matrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{matrix}$$

$$\begin{matrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1/2 & 1/2 & 0 \end{matrix}$$

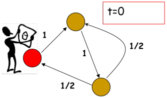
Adjacency matrix A

Transition matrix P





Random walks



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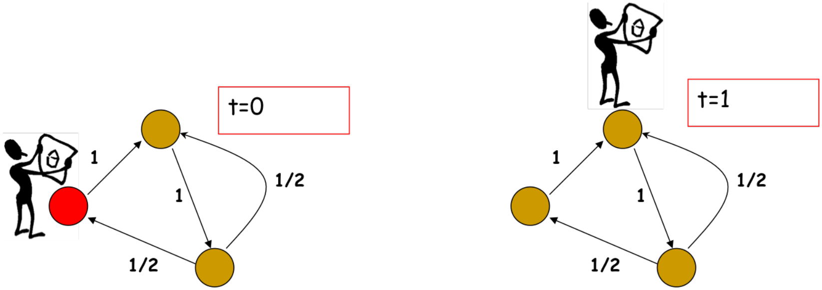

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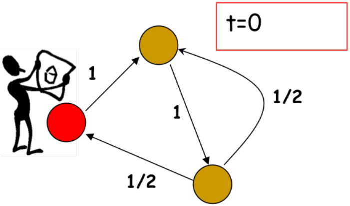
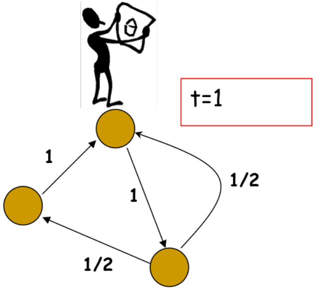
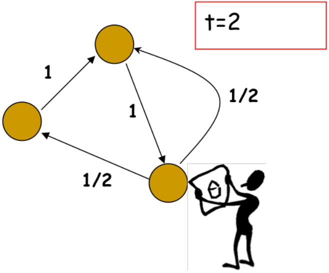
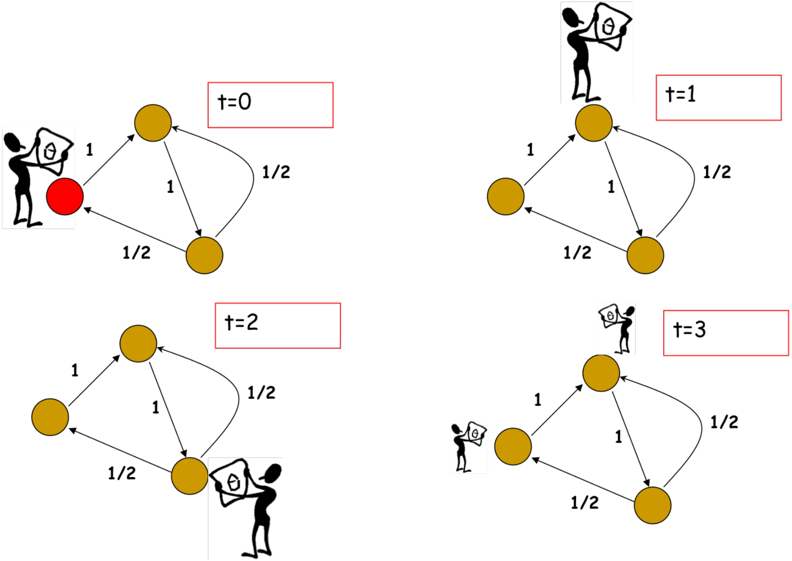






Random walks



Probability Distributions

- $x_t(i)$ denotes the probability that the surfer is at node i at time t.

$$x_{t+1}(i) = \sum_j x_t(j) P(j, i)$$

$$x_{t+1}^T = x_t^T P = x_{t-1}^T P^2 = \cdots = x_0^T P^t$$

- What happens if the surfer keeps walking for a long time?

Stationary Distribution

- When the surfer keeps walking for a long time
- When the distribution does not change anymore i.e. $x_{T+1} = x_T$
- For "well-behaved" graphs this does not depend on the start distribution!!

Stationary distribution

- The stationary distribution at a node is related to the amount of time a random walker spends visiting that node.

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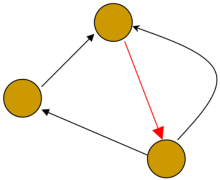
- Whoa! that's just the left eigenvectorof the transition matrix !

Stationary distribution

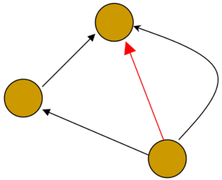
- Lot of theory hiding here.
- For example, what is the guarantee that there will be a unique left eigenvector, or the random walk will at all converge?
- Can't it just keep oscillating?

Well-behaved Markov chains

- Irreducible: There is a path from every node to every other node.



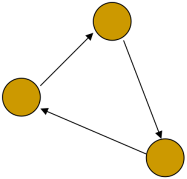
Irreducible



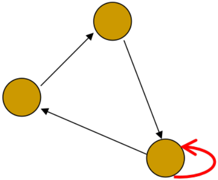
Not irreducible

Well-behaved Markov chains

- Aperiodic: The GCD of all cycle lengths is *1.* The GCD is also called period.



Periodicity is 3



Aperiodic

Well-behaved Markov chains

- If a markov chain is irreducible and aperiodic then the largest eigenvalue of the transition matrix will be equal to 1 and all the other eigenvalues will be strictly less than 1.
- These results imply that for a well behaved graph there exists an unique stationary distribution.

Pagerank and Perron Frobenius

- Perron Frobenius only holds if the graph is irreducible and aperiodic.
- But how can we guarantee that for the web graph? Do it with a small restart probability c.
- At any time-step the random surfer
  - jumps (teleport) to any other node with probability c
  - jumps to its direct neighbors with total probability $1 - c$.

$$\tilde{P} = (1 - c)P + c\mathbb{1}\mathbb{1}^T/n$$

Power iteration

- Power Iteration is an algorithm for computing the stationary distribution.
    - Start with any distribution x_0
    - Keep computing $x_{t+1}^T = x_t^T P$
    - Stop when x_{t+1} and x_t are almost the same

Power Iteration

- Why should this work?
- Write x_0 as a linear combination of the left eigenvectors $\{v_0, v_1, \ldots, v_{n-1}\}$ of P
- Remember that v_0 is the stationary distribution.

$$x_0 = c_0 v_0 + c_1 v_1 + c_2 v_2 + \ldots + c_{n-1} v_{n-1}$$

Power Iteration

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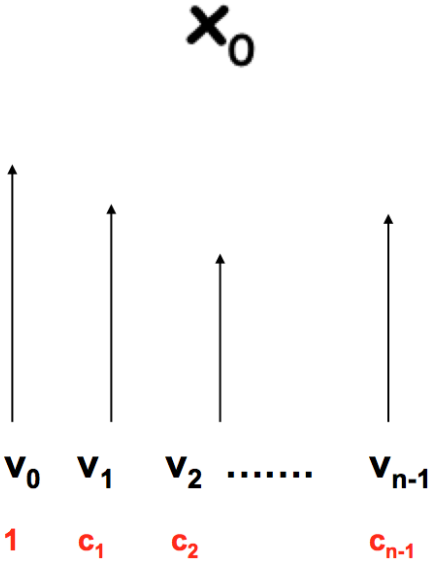
$$x_0 = c_0 v_0 + c_1 v_1 + c_2 v_2 + \ldots + c_{n-1} v_{n-1}$$

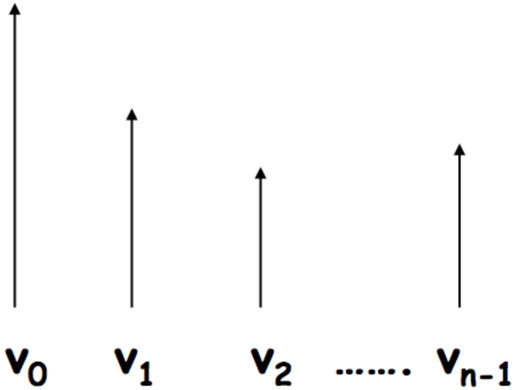
- $c_0 = 1$. Why?
    - First note that $1^T v_i = 0$ if $i \neq 1$
    - So $x_0^T 1 = c_0 = 1$, since both x_0 and v_0 are distributions.

Power Iteration



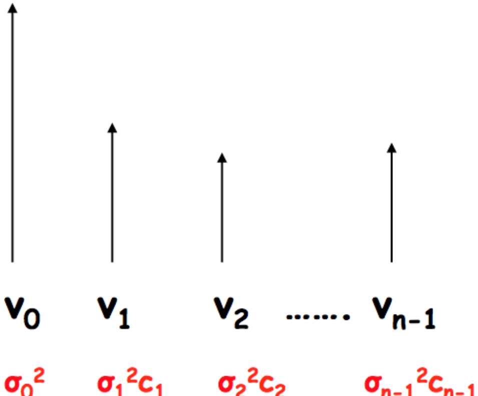
Power Iteration

$$x_1 = x_0 \tilde{P}$$



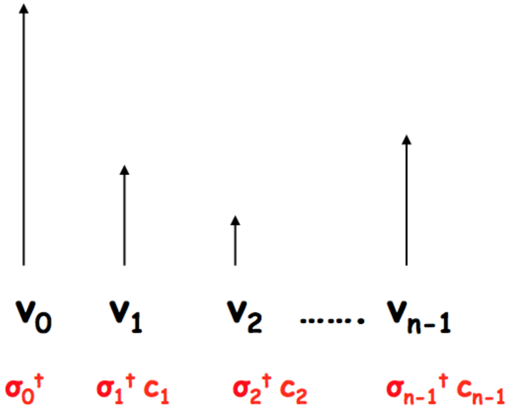
Power Iteration

$$x_2 = x_1 \tilde{P} = x_0 \tilde{P}^2$$



Power Iteration

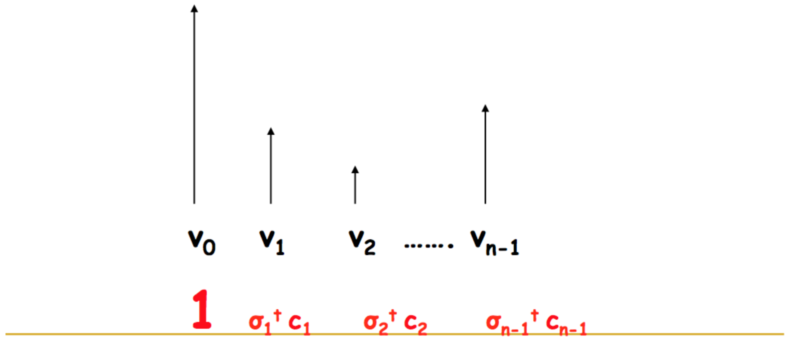
$$x_t = x_0 \tilde{P}^t$$



Power Iteration

$$x_t = x_0 \tilde{P}^t$$

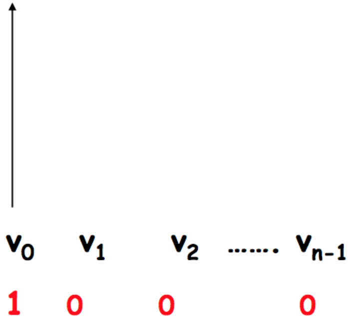
$\boxed{\sigma_0 = 1 > \sigma_1 \geq \ldots \geq \sigma_n}$



Power Iteration

$$X_\infty$$

$$\boxed{\sigma_0 = 1 > \sigma_1 \geq \ldots \geq \sigma_n}$$



Second eigenvalue

- Smaller σ_2 is faster the chain mixes.
- For pagerank, we wonder what the second largest eigenvalue is of $\tilde{P} = (1-c)P + cU$
- The largest eigenvalue is 1
- The second largest is less than $1-c$ in magnitude.
- So pagerank computation converges fast.

Pagerank

- We are looking for the vector v s.t.

$$v^T = (1 - c)v^T P + cr^T$$

- r is a distribution over web-pages.
- If r is the uniform distribution we get pagerank.
- What happens if r is non-uniform?

Pagerank

- We are looking for the vector v s.t.

$$v^T = (1 - c)v^T P + cr^T$$

- r is a distribution over web-pages.
- If r is the uniform distribution we get pagerank.
- What happens if r is non-uniform?
- Personalization

Personalized Pagerank

- The only difference is that we use a non-uniform teleportation distribution, i.e. at any time step teleport to a set of webpages.
- In other words we are looking for the vector v s.t.

$$v^T = (1 - c)v^T P + cr^T$$

- r is a non-uniform preference vector specific to an user.
- v gives "personalized views" of the web.

Personalized Pagerank

- Pre-computation: r is not known from before
- Computing during query time takes too long
- A crucial observation1 is that the personalized pagerank vector is linear w.r.t r

$$\mathbf{r} = \begin{pmatrix} \alpha \\ 0 \\ 1-\alpha \end{pmatrix} \Rightarrow v(r) = \alpha v(r_0) + (1-\alpha) v(r_2)$$

$$\mathbf{r}_0 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \mathbf{r}_2 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

- Lots of literature for computing personalized pagerank fast, and on the go.

Rank Stability

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- Computing during query time takes too long
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- Lots of literature for computing personalized pagerank fast, and on the go.

Rank Stability

- How does the ranking change when the link structure changes?
- The web-graph is changing continuously.
- How does that affect page-rank?

Rank Stability

Rank on the entire database.

Rank on 5 perturbed datasets by deleting 30% of the papers

1	"Genetic Algorithms in Search, Optimization and...", Goldberg	1	1	1	1	1
2	"Learning internal representations by error...", Rumelhart+al	2	2	2	2	2
3	"Adaptation in Natural and Artificial Systems", Holland	3	5	6	4	5
4	"Classification and Regression Trees", Breiman+al	4	3	5	5	4
5	"Probabilistic Reasoning in Intelligent Systems", Pearl	5	6	3	6	3
6	"Genetic Programming: On the Programming of ...", Koza	6	4	4	3	6
7	"Learning to Predict by the Methods of Temporal ...", Sutton	7	7	7	7	7
8	"Pattern classification and scene analysis", Duda+Hart	8	8	8	8	9
9	"Maximum likelihood from incomplete data via...", Dempster+al	10	9	9	11	8
10	"UCI repository of machine learning databases", Murphy+Aha	9	11	10	9	10
11	"Parallel Distributed Processing", Rumelhart+McClelland	-	-	-	10	-
12	"Introduction to the Theory of Neural Computation", Hertz+al	-	10	-	-	-

1. **Link analysis, eigenvectors, and stability,** Andrew Y. Ng, Alice X. Zheng and Michael Jordan, IJCAI-01
2. **Automating the contruction of Internet portals with machine learning,** A. Mc Callum, K. Nigam, J. Rennie, K. Seymore, In Information Retrieval Journel, 2000

Rank Stability

Rank on the entire database.

Rank on 5 perturbed datasets by deleting 30% of the papers

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Rank Stability

- Ng et al 2001: $\tilde{P} = (1-c)P + cU$
- Theorem: if v is the left eigenvector of . Let the pages $i_1, i_2, \ldots, i_k$ be changed in any way, and let v' be the new pagerank. Then

$$\|v - v'\|_1 \leq \frac{\sum_{j=1}^{k} v(i_j)}{c}$$

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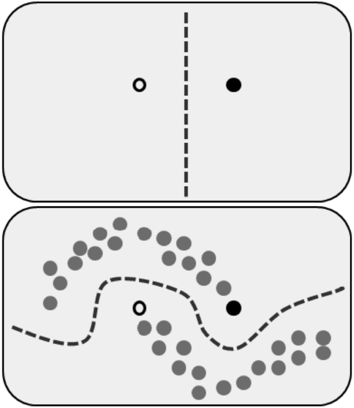
$$\|v - v'\|_1 \leq \frac{\sum_{j=1}^{k} v(i_j)}{c}$$

- So if c is not too close to 0, the system would be rank stable and also converge fast!

Semi-supervised learning

- You are given a lot of unlabeled data.
- Only a few points are labeled.
- Is this useful?



Semi-supervised learning

- Two broad ways
  - Label propagation:
    - Graph Based algorithm
    - Does not generalize to unseen data, i.e. Transductive
  - Manifold regularization
    - Graph Based regularization
    - Does generalize to unseen data, i.e. Inductive

Semi-supervised learning

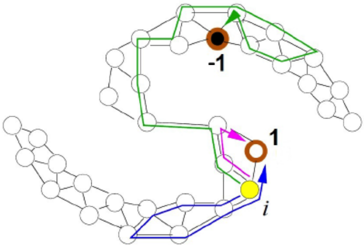
- Input n data points $x_1, \ldots, x_n$
- Define similarity matrix $S \in \mathbb{R}^{n \times n}$

$$S_{ij} = \exp(-\|x_i - x_j\|^2 / 2\sigma^2)$$

- Since S is dense, often k nearest neighbor graphs are also used. (Your homework!)

Label propagation [Zhu et al, 2003]

- Input:
  - ℓ labeled datapoints $(x_1, y_1), \ldots, (x_\ell, y_\ell)$
  - u unlabeled datapoints $x_{\ell+1}, \ldots, x_{\ell+u}$
- Predict: labels $y_{\ell+1}, \ldots, y_{\ell+u}$



Label propagation algorithm

- Compute $P \in [0,1]^{(\ell+u)\times(\ell+u)}$
- $P_{ij} = \dfrac{S_{ij}}{\sum_j S_{ij}}$
- Harmonic function:
  - Function value at an unlabeled node is an average of function values at its neighbors
  - For $j = \ell+1 : \ell+u$,

$$f(j) = \frac{\sum_i S_{ji} f(i)}{\sum_i S_{ji}} = \underbrace{\sum_i P_{ji} f(i)}_{\text{convex combination of values of neighbors}}$$

  - In other words, for the unlabeled nodes, this fixed point equation is satisfied

$$f[U] = Pf[U] \qquad f[L] = y[L]$$

  - For a vector v and set S, we denote by $v[S]$ the subset of values in S
  - U and L denote the set of unlabeled and labeled points respectively.

Closed form

- Assume there are just two classes. Set $y[L] \in \{0,1\}^\ell$ accordingly.
- We have:

$$\begin{bmatrix} P_{LL} & P_{LU} \\ P_{UL} & P_{UU} \end{bmatrix} \begin{bmatrix} Y_L \\ Y_U \end{bmatrix} = \begin{bmatrix} Y_L \\ Y_U \end{bmatrix}$$

- Expanding, we get:

$$P_{UL} Y_L + P_{UU} Y_U = Y_U$$

- Moving things around:

$$Y_U = (I - P_{UU})^{-1} P_{UL} Y_L$$

- Can use a linear system solver

Label propagation - Random walk interpretation

- Think of the labeled nodes as absorbing states
- Use

$$
\begin{aligned}
Y_U &= \sum_{t=0}^{\infty} P_{UU}^t P_{UL} Y_L \\
&= \underbrace{P_{UL} Y_L}_{\text{Probability of reaching ``1''s in one step}} + \underbrace{P_{UU} P_{UL} Y_L}_{\text{Probability of reaching in two steps}} + \\
&= \text{Probability of reaching a label ``1'' in a long random walk}
\end{aligned}
$$

- Why is this useful?
  - If the labels are all reachable, a long walk must hit a "0" or a "1"
  - So if $Y_i > 1/2$, that means from i, its more likely to reach a "1" than a "0"

Graph Laplacian interpretation

- Graph Laplacian: $L = D - S$, where $D_{ii} = \sum_j S_{ij}$ is a diagonal matrix
- L is positive semi-definite (we are assuming $S_{ij} > 0$)
- Why?
  - For any vector v,
    $$v^T L v = \sum_{ij} S_{ij}(v_i - v_j)^2$$
  - So this measures how unsmooth v is w.r.t S
  - L is also singular, why?

Label propagation algorithm

- We can also frame label propagation as

$$\arg\min_{v} v^T L v \qquad s.t. v[L] = y_L$$

- Why?

Label propagation algorithm

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$$\arg\min_{v} v^{T} L v \qquad s.t. v[L] = y_L$$

- Why?
- Write $v = \begin{bmatrix} y_L & v_U \end{bmatrix}$

Label propagation algorithm

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$$\arg\min_{v} v^T L v \qquad s.t. v[L] = y_L$$

- Why?
- Write $v = \begin{bmatrix} y_L & v_U \end{bmatrix}$
- Now set the derivative to zero.
    - $Lv = 0$ such that $v[L] = y_L$
    - $$\begin{bmatrix} D_{LL} - S_{LL} & -S_{LU} \\ -S_{UL} & D_{UU} - S_{UU} \end{bmatrix} \begin{bmatrix} y_L \\ v_U \end{bmatrix} = 0$$
    - Solving:

$$-S_{UL} y_L + (D_{UU} - S_{UU}) v_U = 0$$

Label propagation algorithm

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$$\arg\min_v v^T L v \qquad s.t. v[L] = y_L$$

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  - Solving:

$$-S_{UL} y_L + (D_{UU} - S_{UU}) v_U = 0$$

  - rearranging: $v_U = (D_{UU} - S_{UU})^{-1} S_{UL} y_L = (I - P_{UU})^{-1} P_{UL} y_L$

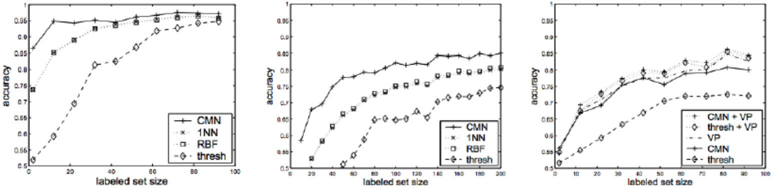

Figure 3. Harmonic energy minimization on digits "1" vs. '2" (left) and on all 10 digits (middle) and combining voted-perceptron with harmonic energy minimization on odd vs. even digits (right)

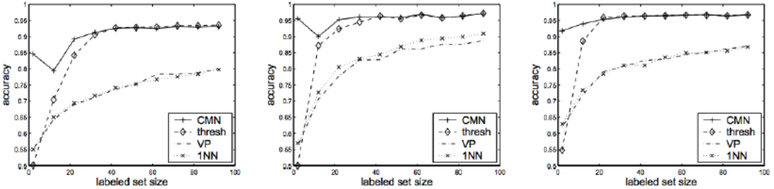

Figure 4. Harmonic energy minimization on PC vs. MAC (left), baseball vs. hockey (middle), and MS-Windows vs. MAC (right)

Manifold regularization

- Input:
  - ℓ labeled datapoints $(x_1, y_1), \ldots, (x_\ell, y_\ell)$
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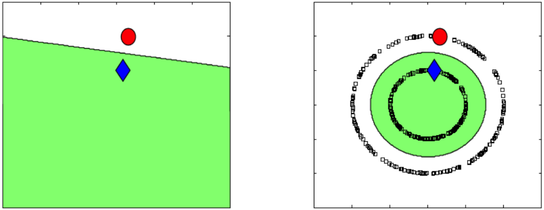

Figure 1: Unlabeled data and prior beliefs

Manifold regularization

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  - u unlabeled datapoints $x_{\ell+1}, \ldots, x_{\ell+u}$
- Predict: labels $y_{\ell+1}, \ldots, y_{\ell+u}$
- Before the constraint was $v[L] = y_L$, now instead we will use a loss function and learn a classifier on the labeled data

$$\min_w \underbrace{\sum_{i=1}^{\ell} \text{loss}(y_i, w^T x_i)}_{\textit{loss}} + \lambda \underbrace{R(w)}_{\textit{regularization}}$$

Manifold regularization

- Input:
  - ℓ labeled datapoints $(x_1, y_1), \ldots, (x_\ell, y_\ell)$
  - u unlabeled datapoints $x_{\ell+1}, \ldots, x_{\ell+u}$
- Predict: labels $y_{\ell+1}, \ldots, y_{\ell+u}$
- Before the constraint was $v[L] = y_L$, now instead we will use a loss function and learn a classifier on the labeled data

$$\min_w \underbrace{\sum_{i=1}^{\ell} \text{loss}(y_i, w^T x_i)}_{\textit{loss}} + \lambda \underbrace{R(w)}_{\textit{regularization}}$$

- How about the unlabeled data?

Manifold regularization: Belkin et al 2006

$$\min_{w} \underbrace{\sum_{i=1}^{\ell} \text{loss}(y_i, w^T x_i)}_{loss} + \lambda \underbrace{R(w)}_{regularization} + \beta (Xw)^T L(Xw)$$

- Assume a linear predictor $w^T x$
- Idea: close/similar points have similar predicted labels.
- LapSVM:

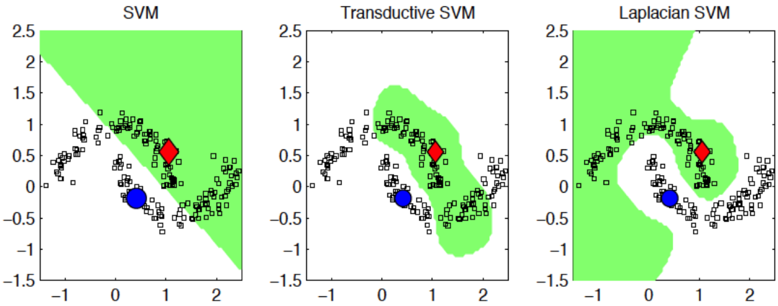
$$\min_{w} \sum_{i=1}^{\ell} (1 - y_i f(x_i))_+ + \lambda \underbrace{\|f\|_K^2}_{regularization} + \beta f^T L f$$

Transductive SVM: Joachims et al 1999

$$\min_{w, y_{\ell+1}, \ldots, y_{\ell+u}} \sum_{i=1}^{\ell} (1 - y_i f(x_i))_+ + C' \sum_{i=\ell+1}^{n} (1 - y_i f(x_i))_+ + \lambda \underbrace{\|f\|_K^2}_{regularization}$$

- Iteratively solves SVM quadratic programs
- Switches labels to improve objective function
- Suffers from local optima, inherently combinatorial problem

Transductive SVM VS LapSVM



Acknowledgments

- Cho-Jui Hsieh's lecture notes from UC Davis
- Zhu et al's paper in ICML "Semi-Supervised Learning Using Gaussian Fields and Harmonic Functions"
- Ng et al's paper on ranking Stability "Link Analysis, Eigenvectors and Stability", IJCAI 2001
- Belkin, Niyogi and Sindhwani's paper "Manifold Regularization: A Geometric Framework for Learning from Labeled and Unlabeled Examples" in JMLR 2006
- My old talk on Random walks.