Learning to Rank in Vector Spaces and Social Networks (WWW 2007 Tutorial)

Soumen Chakrabarti
IIT Bombay
http://www.cse.iitb.ac.in/~soumen

Motivation: Web search

- User query q, Web pages $\{v\}$
- (q, v) can be represented with a rich feature vector
- Text match score with title, anchor text, headings, bold text, body text, . . . , of v as a hypertext document
- Pagerank, topic-specific Pageranks, personalized Pageranks of v as a node in the Web graph
- Estimated location of user, commercial intent, . . .
- Must we guess the relative importance of these features?
- How to combine these into a single scoring function on (q, v) so as to induce a ranking on $\{v\}$?

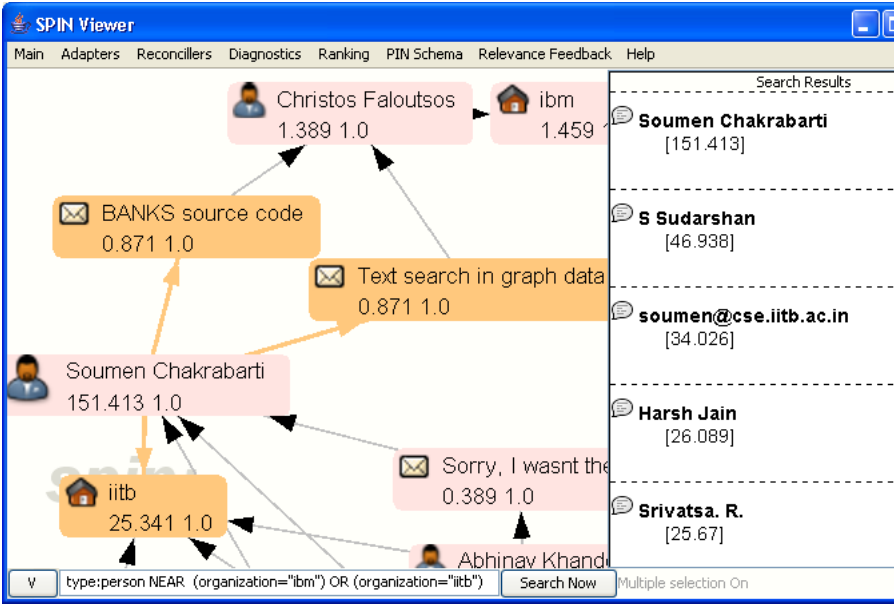
Motivation: Ad and link placement

- Here, the "query" is the surfer's contextual information
- More noisy than queries, which are noisy enough!
- Plus page and site contents
- A response is an ad to place, or a link to insert
- Must rank and select from a large pool of available ads or links
- (In this tutorial we will ignore issues of bidding and visibility pricing)

Motivation: Desktop search

- The Web has only a few kinds of hyperlinks: same-host subdirectory, same-host superdirectory, same-host across-path, different-host same-domain, different-domain etc.
- Often differentiated by hardwired policy, e.g, HITS completely ignores same-host links
- Entity-relationship (ER) graphs are richer
- E.g. A personal information management (PIM) system has many node/entity types (person, organization, email, paper, conference, phone number) and edge/relation types (works-for, sent, received, authored, published-in)
- Ranking needs to exploit the richer type system
- Don't want to guess the relative importance of edge types (may be dependent on queries)

Desktop search example



Relevance feedback

- Relevance feedback is well-explored in traditional IR
- User-assisted local modification of ranking function for vector-space models
- How to extend these to richer data representations that incorporate entities, relationship links, entity and relation types?
- Surprisingly unexplored area

Tutorial outline: Preliminaries

- Training and evaluation scenarios
- Measurements to evaluate quality of ranking
  - Label mismatch loss functions for ordinal regression
  - Preference pair violations
  - Area under (true positive, false positive) curve
  - Average precision
  - Rank-discounted reward for relevance
  - Rank correlations
- What's useful vs. what's easy to learn

Tutorial outline: Ranking in vector spaces

Instance v is represented by a feature vector $x_v \in \mathbb{R}^d$

- Discriminative max-margin ranking (RankSVM)
- Linear-time max-margin approximation
- Probabilistic ranking in vector spaces (RankNet)
- Sensitivity to absolute rank and cost of poor rankings

Tutorial outline: Ranking in graphs

Instance v is a node in a graph $G = (V, E)$

- The graph-Laplacian approach
  - Assign scores to nodes to induce ranking
  - G imposes a smoothness constraint on node scores
  - Large difference between neighboring node scores penalized
- The Markov walk approach
  - Random surfer, Pagerank and variants; by far most popular way to use graphs for scoring nodes
  - Walks constrained by preferences
  - How to incorporate node, edge types and query words
- Surprising connections between the two approaches

Tutorial outline: Stability and generalization

- Some notes on score- vs. rank-stability
- Stability and generalization of max-margin ranking in vector spaces
- Stability and generalization of graph-Laplacian ranking
- Stability and generalization of Markov walk based ranking

Preliminaries

- Motivation
- Training and evaluation setup
- Performance measures

Ranking in vector spaces

- Discriminative, max-margin algorithms
- Probabilistic models, gradient-descent algorithms

Ranking nodes in graphs

- Roughness penalty using graph Laplacian
- Constrained network flows

Stability and generalization

- Admissibility and stability
- Ranking loss and generalization bounds

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Forms of training input

Regression: For each entity x, an absolute real score y (unrealistic to expect users to assign absolute scores)

Ordinal regression: For each entity x, a score y from a discrete, ordered domain, such as a r-point scale (implemented in many sites like Amazon.COM)

Bipartite ranking: Ordinal regression with $r = 2$

Pairwise preferences: A (possibly inconsistent) partial order between entities, expressed as a collection of "$u \prec v$" meaning "u is less preferred than v" (low cognitive load on users, can be captured from click-logs and eye-tracking data)

Complete rank order: A total order on the entities but no scores (highly impractical for large entity sets)

Prefix of rank order: A total order on the top-k entities, meaning that all the other entities are worse (iffy)

Evaluation of ranking algorithms I

Error on score vectors: In case of standard regression, if $\hat{f}$ is the score assigned by the algorithm and f is the "true score", measure $\|\hat{f} - f\|_1$ or $\|\hat{f} - f\|_2$.

Ordinal reversals: If $y_u > y_v$ and $\hat{f}(u) < \hat{f}(v)$ then u and v have been reversed. Count the number of reversed pairs.

Precision at k: For a specific query q, let T_k^q and $\hat{T}_k^q$ be the top-k sets as per f and $\hat{f}$ scores. The precision at k for query q is defined as $|T_k^q \cap \hat{T}_k^q|/k \in [0, 1]$. Average over q.

Evaluation of ranking algorithms II

Relative aggregated goodness (RAG): For a specific query q,

$$\mathrm{RAG}(k, q) = \frac{\sum_{v \in \hat{T}_k^q} f(v)}{\sum_{v \in T_k^q} f(v)} \in [0, 1]$$

Note that $\hat{f}$ is not used! Average over q.

Mean reciprocal rank (MRR): For each query there is one or more correct responses. Suppose for specified query q, the first rank at which a correct response occurs is $R(q)$. Then MRR is

$$\frac{1}{|Q|} \sum_{q \in Q} \frac{1}{R(q)}$$

Evaluation of ranking algorithms III

Normalized discounted cumulative gain (NDCG): For a specific query q,

$$N_q \sum_{i=1}^{k} \frac{2^{\text{rating}(i)} - 1}{\log(1+i)}$$

Here N_q is a normalization factor so that a perfect ordering gets NDCG score of 1 for each query, k is the number of top responses considered, and rating(i) is the evaluator rating for the item returned at position i.

Pair preference violation: If $u \prec v$ and $\hat{f}(u) > \hat{f}(v)$ a pair has been violated. Count the number of pair violations.

Evaluation of ranking algorithms IV

Rank correlation: Order entities by decreasing $f(u)$ and compute a rank correlation with the ground truth ranking. Impractical if a full ground truth ranking is expected.

Prefix rank correlation: Let exact and approximate scores be denoted by $S_q^k(v)$ and $\hat{S}_q^k(v)$ respectively for items v, where the scores are forced to zero if $v \notin T_k^q$ and $v \notin \hat{T}_k^q$. A node pair $v, w \in T_k^q \cup \hat{T}_k^q$ is *concordant* if $(S_q^k(v) - S_q^k(w))(\hat{S}_q^k(v) - \hat{S}_q^k(w))$ is strictly positive, and *discordant* if it is strictly negative. It is an *exact-tie* if $S_q^k(v) = S_q^k(w)$, and is an *approximate tie* if $\hat{S}_q^k(v) = \hat{S}_q^k(w)$. If there are c,

Evaluation of ranking algorithms V

d, e and a such pairs respectively, and m pairs overall in $T_k^q \cup \hat{T}_k^q$, then Kendall's τ is defined as

$$\tau(k,q) = \frac{c-d}{\sqrt{(m-e)(m-a)}} \in [-1,1].$$

Average over q.

- Theoretically sound and scalable rank learning techniques typically address simpler evaluation objectives
- Designing learning algorithms for the more complicated, non-additive evaluation objectives is very challenging
- Sometimes, we are lucky enough to establish a connection between the two classes of objectives

Bipartite ranking and area under curve (AUC)

- In bipartite ranking labeled data is of the form (x, y) where $y \in \{-1, 1\}$
- Algorithm orders instances by decreasing $f(x)$
- For $i = 0, 1, \ldots, n$
  - Assign label $+1$ to the first i instances
  - Assign label -1 to the rest
  - True positive rate at i

$$\frac{\text{number of positive instances labeled positive}}{\text{number of positive instances}}$$

  - False positive rate at i

$$\frac{\text{number of negative instances labeled positive}}{\text{number of negative instances}}$$

- Plot $x = \text{TruePosRate}, y = \text{FalsePosRate}$
- Measure area under curve

AUC and pair preference violations

- m positive and n negative examples
- Area under curve (AUC) using f for ranking can also be written as

$$\hat{A}(f, T) = \frac{1}{mn} \sum_{\substack{i:y_i=+1 \\ j:y_j=-1}} \left([\![f(i) > f(j)]\!] + \frac{1}{2}[\![f(i) = f(j)]\!] \right)$$

  where T is the training set
- The important part is the fraction of satisfied pair preferences between positive and negative instances
- Optimizing AUC is different from optimizing 0/1 error

y_i	-1	-1	-1	-1	$+1$	$+1$	$+1$	$+1$
$f_1(x_i)$	-2	-1	3	4	1	2	5	6
$f_2(x_i)$	-2	-1	5	6	1	2	3	4

Concordant and discordant instance pairs

- Suppose there are R relevant documents in response to a query
- The search engine creates a ranking r_{engine} which lists them at ranks $p_1 < p_2 < \cdots < p_R$
- An ideal system creates a ranking r_{ideal} that lists all relevant documents before any irrelevant document
- But keeps the relative ordering within the relevant and irrelevant subsets the same

$$\begin{aligned} r_{\text{engine}} &= d_1^+, d_2^-, d_3^+, d_4^+, d_5^-, d_6^-, d_7^+, d_8^- \\ r_{\text{ideal}} &= d_1^+, d_3^+, d_4^+, d_7^+; d_2^-, d_5^-, d_6^-, d_8^- \end{aligned}$$

- Let there be Q discordant pairs in r_{engine} compared to r_{ideal}

Relating ranks and discordant pairs

- Account for Q as follows: First consider the relevant document at position p_1 in r_{engine}. Because it has been pushed out from position 1 to position p_1, the number of inversions introduced is $p_1 - 1$.
- For the document at position p_2 in r_{engine}, the number of inversions introduced is $p_2 - 1 - 1$, the last "-1" thanks to having the first relevant document ahead of it.
- Summing up, we get

$$\sum_{i=1}^{R} p_i - 1 - (i-1) = Q, \quad \text{or}$$

$$\sum_{i=1}^{R} p_i \;=\; Q + \sum_{i=1}^{R} i = Q + \frac{R(R+1)}{2} \;=\; Q + \binom{R+1}{2}.$$

Average precision

- The average precision of r_{engine} wrt r_{ideal} is defined as

$$\text{AvgPrec}(r_{\text{engine}}, r_{\text{ideal}}) = \frac{1}{R} \sum_{i=1}^{R} \frac{i}{p_i}$$

- Like NDCG, average precision rewards the search engine if all p_i are as small as possible
- Intuitively, if Q is small, $\text{AvgPrec}(r_{\text{engine}}, r_{\text{ideal}})$ should be large.
- This can be formalized by framing an optimization problem that gives a lower bound to $\text{AvgPrec}(r_{\text{engine}}, r_{\text{ideal}})$ given a fixed Q (and R)

Bounding average precision given Q

- To lower bound average precision, optimize:

$$\min_{p_1,\ldots,p_R} \frac{1}{R}\sum_{i=1}^{R}\frac{i}{p_i} \quad \text{such that}$$

$$p_1+\cdots+p_R = Q + \binom{R+1}{2}$$

$$1 \le p_1 < p_2 < \cdots < p_R$$

$$p_1,\ldots,p_R \quad \text{are positive integers}$$

- Relaxing the last two constraints can only decrease the optimal objective, so we still get a lower bound
- The relaxed optimization is also convex because $1/p_i$ is convex in p_i, as far as p_i is concerned the numerator i is a "constant", and sum of convex functions is convex

Solving the relaxed optimization

- Using the Lagrangian method, we get

$$\mathcal{L}(p_1, \ldots, p_R; \lambda) = \frac{1}{R} \sum_{i=1}^{R} \frac{i}{p_i} + \lambda \left(\sum_{i=1}^{R} p_i - Q - \binom{R+1}{2} \right)$$

$$\therefore \frac{\partial \mathcal{L}}{\partial p_i} = -\frac{i}{R p_i^2} + \lambda \overset{\text{set}}{=} 0 \quad \text{to get} \quad p_i^* = \sqrt{\frac{i}{R\lambda}}.$$

- Replace back in the Lagrangian, set the derivative wrt λ to zero, and again substitute in the Lagrangian to get the optimal objective (in the relaxed optimization) as

$$\text{AvgPrec}(r_{\text{engine}}, r_{\text{ideal}}) \ge \frac{\left(\sum_{i=1}^{R} \sqrt{i} \right)^2}{R \left(Q + \binom{R+1}{2} \right)}$$

- Q and the lower bound on average precision are inversely related, which makes sense.

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Ordinal regression

- Items assigned *ratings* on a discrete r-point scale, e.g., items for sale at `Amazon.COM`
- The task is to regress instance $x \in \mathcal{X}$ to label $y \in \mathcal{Y}$ where $\mathcal{Y}$ is typically small
- Bipartite ranking is a special case with $|\mathcal{Y}| = 2$ so we can write $\mathcal{Y} = \{-1, +1\}$

Ordinal regression is different from plain classification because

- Unlike in classification, where labels in $\mathcal{Y}$ are *incomparable*, here they have a total order imposed on them. (In standard regression, $\mathcal{Y} = \mathbb{R}$.)
- The accuracy measures of practical interest here are different from those ($0/1$ error, recall, precision, F_1) used in classification.

Max-margin ordinal regression I

- Apart from β, we will optimize over $r-1$ thresholds

$$-\infty = b_0 \le b_1 \le b_2 \le \cdots \le b_{r-2} \le b_{r-1} \le b_r = +\infty$$

- Let $j \in \{1, \ldots, r\}$ index score levels, and the ith instance in the j level be denoted x_i^j
- We wish to pick β such that, for any x_i^j,

$$b_{j-1} \; < \; \beta^\top x_i^j \; < \; b_j$$

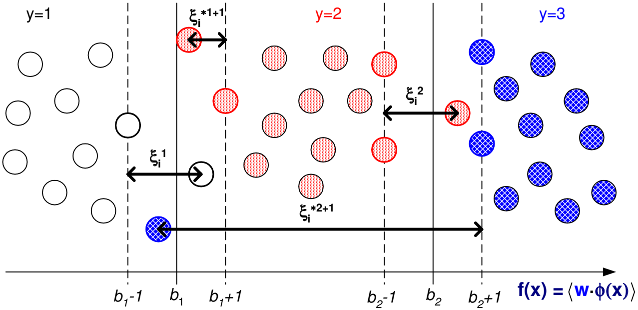
- Using the max-margin principle, we will insist that

$$b_{j-1} + 1 \; < \; \beta^\top x_i^j \; < \; b_j - 1$$

Max-margin ordinal regression II

- To avoid infeasibility, introduce lower slacks $\underline{s}_i^j \geq 0$ and upper slacks $\overline{s}_i^j \geq 0$, and relax the above inequalities to

$$b_{j-1} + 1 - \underline{s}_i^j \;\leq\; \beta^\top x_i^j \;\leq\; b_j - 1 + \overline{s}_i^j$$



Max-margin ordinal regression III

- The objective to minimize is modified to

$$\min_{\beta, b, \underline{s} \geq \vec{0}, \overline{s} \geq \vec{0}} \frac{1}{2}\beta^\top \beta + B \sum_{j,i} (\underline{s}_i^j + \overline{s}_i^j),$$

- Yet another quadratic program with linear inequalities
- Training time scales roughly as $n^{2.18\text{–}2.33}$ where n is the number of training instances
- More accurate than replacing ordinal regression with plain regression

Ranking to satisfy preference pairs

- Suppose $x \in X$ are instances and $\phi : X \to \mathbb{R}^d$ a feature vector generator
- E.g., x may be a document and ϕ maps x to the "vector space model" with one axis for each word
- The score of instance x is $\beta^\top \phi(x)$ where $\beta \in \mathbb{R}^d$ is a weight vector
- For simplicity of notation assume x is already a feature vector and drop ϕ
- We wish to learn β from training data $\prec$: "$i \prec j$" means the score of x_i should be less than the score of x_j, i.e.,

$$\beta^\top x_i \leq \beta^\top x_j$$

Soft constraints

- In practice, there may be no feasible β satisfying all preferences $\prec$
- For constraint $i \prec j$, introduce slack variable $s_{ij} \geq 0$

$$\beta^\top x_i \leq \beta^\top x_j + s_{ij}$$

- Charge a penalty for using $s_{ij} > 0$

$$\min_{s_{ij} \geq 0; \beta} \frac{1}{|\prec|} \sum_{i \prec j} s_{ij} \quad \text{subject to}$$
$$\beta^\top x_i \leq \beta^\top x_j + s_{ij} \quad \text{for all } i \prec j$$

A max-margin formulation

- Achieve "confident" separation of loser and winner:

$$\beta^\top x_i + 1 \leq \beta^\top x_j + s_{ij}$$

- Problem: Can achieve this by scaling β arbitrarily; must be prevented by penalizing $\|\beta\|$

$$\min_{s_{ij} \geq 0; \beta} \frac{1}{2}\beta^\top \beta + \frac{B}{|\prec|} \sum_{i \prec j} s_{ij} \quad \text{subject to}$$
$$\beta^\top x_i + 1 \leq \beta^\top x_j + s_{ij} \quad \text{for all } i \prec j$$

- B is a magic parameter that balances violations against model strength

Solving the optimization

- $\beta^\top x_i + 1 \le \beta^\top x_j + s_{ij}$ and $s_{ij} \ge 0$ together mean $s_{ij} = \max\{0, \beta^\top x_i - \beta^\top x_j + 1\}$ ("hinge loss")
- The optimization can be rewritten without using s_{ij}

$$\min_\beta \frac{1}{2}\beta^\top\beta + \frac{B}{|\prec|}\sum_{i\prec j} \max\{0, \beta^\top x_i - \beta^\top x_j + 1\}$$

- $\max\{0, t\}$ can be approximated by a number of smooth functions
  - e^t – growth at $t > 0$ too severe
  - $\log(1 + e^t)$ – much better, asymptotes to $y = 0$ as $t \to -\infty$ and to $y = t$ as $t \to \infty$

Approximating with a smooth objective

- Simple unconstrained optimization, can be solved by Newton method

$$\min_{\beta \in \mathbb{R}^d} \frac{1}{2}\beta^\top \beta + \frac{B}{|\prec|} \sum_{i \prec j} \log(1 + \exp(\beta^\top x_i - \beta^\top x_j + 1))$$

- If $\beta^\top x_i - \beta^\top x_j + 1 \ll 0$, i.e., $\beta^\top x_i \ll \beta^\top x_j$, then pay little penalty
- If $\beta^\top x_i - \beta^\top x_j + 1 \gg 0$, i.e., $\beta^\top x_i \gg \beta^\top x_j$, then pay large penalty

Performance issues

- Common SVM implementations will take time almost quadratic in the number of training pairs
- Consider a TREC-style relevance judgment: for each query, we are given, say, 10 relevant and (implicitly) $1\text{M} - 10$ irrelevant documents
- Don't really need to train RankSVM with 10M $x_i \prec x_j$ pairs
- E.g., if $\beta^\top x_0 \le \beta^\top x_1$ and $\beta^\top x_0 \le \beta^\top x_2$, then $\beta^\top x_0 \le \lambda\beta^\top x_1 + (1-\lambda)\beta^\top x_2$ for $\lambda \in [0,1]$
- Cannot, in general, say ahead of time which preferences will be redundant

A linear-time RankSVM approximation

- The primal optimization can be reformulated as

$$\min_{\beta, s \ge 0} \frac{1}{2}\beta^\top \beta + Bs \quad \text{such that} \qquad \text{(RankSVM2)}$$

$$\forall \vec{c} \in \{0,1\}^{|\prec|} : \frac{1}{|\prec|}\beta^\top \sum_{u \prec v} c_{uv}(x_v - x_u) \ge \frac{1}{|\prec|}\sum_{u \prec v} c_{uv} - s$$

- Only one slack variable s, but $2^{|\prec|}$ primal constraints and corresponding $2^{|\prec|}$ dual variables
- (But if most primal constraints are redundant, most dual variables will be inactive, i.e., 0)
- Compare with

$$\min_{\beta, \{s_{uv} \ge 0 : u \prec v\}} \frac{1}{2}\beta^\top \beta + \frac{B}{|\prec|}\sum_{u \prec v} s_{uv} \qquad \text{(RankSVM1)}$$

$$\text{such that } \forall u \prec v : \quad \beta^\top x_u + 1 \le \beta^\top x_v + s_{uv}$$

Correctness

Any solution to (RankSVM2) corresponds to a solution to (RankSVM1), and vice versa

- Fix a β_0 in (RankSVM1)
- For optimality, must pick $s^*_{uv} = \max\{0, 1 + \beta_0^\top x_u - \beta_0^\top x_v\}$
- Fix the same β_0 for (RankSVM2)
- For optimality, must pick

$$s^* = \min_{\vec{c} \in \{0,1\}^{|\prec|}} \left\{ \frac{1}{|\prec|} \sum_{u \prec v} c_{uv} \left(1 + \beta_0^\top x_u - \beta_0^\top x_v\right) \right\}$$

- Pick $\vec{c}$ element-wise: $c^*_{uv} = [\![1 + \beta_0^\top x_u - \beta_0^\top x_v \leq 0]\!]$
- Can verify ▸ HW that objectives of (RankSVM1) and (RankSVM2) will be equal using $\beta_0, \{s^*_{uv}\}, s^*, \{c^*_{uv}\}$

Cutting plane method: General recipe

- Primal: $\min_x f(x)$ subject to $g(x) \leq \vec{0}$ (g is a vector-valued function)
- Dual:

$$\begin{aligned} \max_{z,u} \quad & z \\ \text{subject to} \quad & z \leq f(x) + u^\top g(x) \ \forall x \\ & u \geq 0 \end{aligned}$$

- "$\forall x$" is generally infinite
- Let z_k, u_k be a solution
- Find $\min_x f(x) + u_k^\top g(x)$, let solution be x_k
- If $z_k \leq f(x_k) + u_k^\top g(x_k)$, terminate
- Otherwise add kth constraint $z \leq f(x_k) + u^\top g(x_k)$
- To approximate and terminate faster, continue only if $z_k > f(x_k) + u_k^\top g(x_k) \quad + \quad \epsilon$

Gradual dual variable inclusion

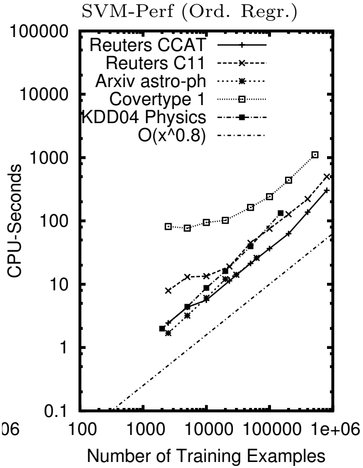
- Instead of all $\{0,1\}^{|\prec|}$, start with $\mathcal{W} \subset \{0,1\}^{|\prec|}$, typically $\mathcal{W} = \varnothing$
- Solve (RankSVM2) with $\mathcal{W}$ instead of $\{0,1\}^{|\prec|}$ to get the current β_0, s^*
- Look for a violator c^* such that

$$\frac{1}{|\prec|}\beta_0^\top \sum_{u \prec v} c^*_{uv}(x_v - x_u) \quad < \quad \frac{1}{|\prec|}\sum_{u \prec v} c^*_{uv} - s^* - \epsilon$$

- If no such c^* found, exit with an objective that is at most the optimal objective plus ϵ
- Otherwise add c^* to $\mathcal{W}$ and repeat
- For fixed (constant) ϵ, B and $\max \|x_v\|_2$, the number of inclusions into $\mathcal{W}$ before no further c^* is found is constant
- Each loop above can be implemented in $O(n \log n)$ vector operations in $\mathbb{R}^d$ where all $x_v \in \mathbb{R}^d$

Linear-time (RankSVM2) performance

- Almost linear scaling in practice too
- Dramatic improvement over (RankSVM1)
- (RankSVM1) scales roughly as $n^{3.4}$ (not shown)



A probabilistic interpretation of "ranking loss"

- Apart from $x_i \prec x_j$, trainer gives target probability $\bar{p}_{ij}$ with which trained system should rank i worse than j
- The score of x_i is $f(x_i) \in \mathbb{R}$; $f(x_i)$ induces a ranking on $\{x_i\}$
- The modeled posterior p_{ij} is assumed to have a familiar log-linear form

$$p_{ij} = \frac{\exp(f(x_j) - f(x_i))}{1 + \exp(f(x_j) - f(x_i))}$$

- If $f(x_j) \gg f(x_i)$, $p_{ij} \to 1$; if $f(x_j) \ll f(x_i)$, $p_{ij} \to 0$
- Goal is to design f to minimize divergence between trainer-specified $\bar{p}$ and modeled p, e.g.,

$$\ell(\bar{p}_{ij}, p_{ij}) = -\bar{p}_{ij} \log p_{ij} - (1 - \bar{p}_{ij}) \log(1 - p_{ij})$$

Consistency requirements on $\bar{p}_{ij}$

- Trainer cannot assign $\bar{p}_{ij}$ arbitrarily
- $\bar{p}_{ij}$ must be consistent with some ideal node-scoring function $\bar{f}$ such that

$$\bar{p}_{ij} = \frac{\exp(\bar{f}(x_j) - \bar{f}(x_i))}{1 + \exp(\bar{f}(x_j) - \bar{f}(x_i))}$$

- Using above, can show that

$$\bar{p}_{ik} = \frac{\bar{p}_{ij}\bar{p}_{jk}}{1 + 2\bar{p}_{ij}\bar{p}_{jk} - \bar{p}_{ij} - \bar{p}_{jk}}$$

- Consider $\bar{p}_{ik}$ if $\bar{p}_{ij} = \bar{p}_{kj} = p$, in particular $p = 0, .5, 1$
- Perfect uncertainty and perfect certainty propagate

Fitting f using gradient descent

- Model $f(x_i) = \beta^\top x_i$ for simplicity
- During training we are given ($i \prec j$ with) a target $\bar{p}_{ij}$
- We want to fit β so that

$$\bar{p}_{ij} = \frac{\exp(\beta^\top x_i - \beta^\top x_j)}{1 + \exp(\beta^\top x_i - \beta^\top x_j)}$$

- We can cast this as, say,

$$\min_\beta \sum_{i \prec j} \left(\bar{p}_{ij} - \frac{\exp(\beta^\top x_i - \beta^\top x_j)}{1 + \exp(\beta^\top x_i - \beta^\top x_j)} \right)^2$$

  and use gradient descent
- Or we can use more complex forms of $f(x)$, like a neural network

RankBoost

- Given partial orders with preference strengths $\phi(i, j) \geq 0$: if positive, $i \succ j$, otherwise impartial
- Input pair distribution $\mathcal{D}$ over $\mathcal{X} \times \mathcal{X}$
- Weak learner indexed by t gets input pairs as per a distribution $\mathcal{D}_t$ and outputs a weak ranking $h_t : \mathcal{X} \to \mathbb{R}$
- Initialize $\mathcal{D}_1 = \mathcal{D}$
- For $t = 1, \ldots, T$
  - Train tth weak learner using $\mathcal{D}_t$
  - Get weak ranking $h_t : \mathcal{X} \to \mathbb{R}$
  - Choose $\alpha_t \in \mathbb{R}$
  - Update

$$\mathcal{D}_{t+1}(x_i, x_j) \propto \mathcal{D}_t(x_i, x_j) \exp\big(\alpha_t(h_t(x_i) - h_t(x_j))\big)$$

- Final scoring function $H(x) = \sum_{t=1}^{T} \alpha_t h_t(x)$

Some properties of RankBoost

- The ranking loss $R_{\mathcal{D}}(H)$ is defined as

$$\sum_{x_i,x_j} \mathcal{D}(x_i,x_j)[\![H(x_i) \le H(x_j)]\!] = \Pr_{(x_i,x_j)\sim\mathcal{D}}[\![H(x_i) \le H(x_j)]\!]$$

- $R_{\mathcal{D}}(H) \le \prod_{t=1}^{T} Z_t$
- By suitably choosing α_t we can ensure $Z_t \le 1$
- E.g., if $h : \mathcal{X} \to \{0,1\}$, we can minimize Z_t analytically:
  - For $b \in \{-1,0,+1\}$, define

$$W_b = \sum_{x_i,x_j} \mathcal{D}(x_i,x_j)[\![h(x_i) - h(x_j)]\!]$$

  - Z_t is minimized when $\alpha = \frac{1}{2}\ln(W_{-1}/W_{+1})$ HW

Preliminaries

- Motivation
- Training and evaluation setup
- Performance measures

Ranking in vector spaces

- Discriminative, max-margin algorithms
- Probabilistic models, gradient-descent algorithms

Ranking nodes in graphs

- Roughness penalty using graph Laplacian
- Constrained network flows

Stability and generalization

- Admissibility and stability
- Ranking loss and generalization bounds

Undirected graph Laplacian

- Simple unweighted undirected graph $G = (V, E)$ with $|V| = n$, $|E| = m$, no self-loops or parallel edges
- Node-node adjacency matrix $A \in \{0, 1\}^{n \times n}$ with $A(u, v) = 1$ if $(u, v) \in E$ and 0 otherwise
- Node-edge incidence matrix $N \in \{-1, 0, 1\}^{n \times m}$ with

$$N(v, e) = \begin{cases} -1 & \text{if } e = (v, \cdot) \\ 1 & \text{if } e = (\cdot, v) \\ 0 & \text{if } v \text{ is not either endpoint of } e \end{cases}$$

- Consider the graph Laplacian matrix $L_G = NN^\top \in \mathbb{R}^{n \times n}$
- $(NN^\top)(u, u)$ is the degree of node u
- $(NN^\top)(u, v)$ is -1 if $(u, v) \in E$, 0 otherwise
- Let D be a diagonal matrix with $D(u, u) =$ degree of u
- $NN^\top = D - A$ ▸ HW is a symmetric positive semidefinite matrix

Extending to weighted undirected graphs

- A is not boolean; $A(u, v)$ is the weight of edge (u, v) if any, 0 otherwise
- Modify N to

$$N(v, e) = \begin{cases} -\sqrt{A(e)} & \text{if } e = (v, \cdot) \\ \sqrt{A(e)} & \text{if } e = (\cdot, v) \\ 0 & \text{if } v \text{ is not either endpoint of } e \end{cases}$$

- Modify L_G to

$$L_G(u, v) = \begin{cases} \sum_w A(u, w), & u = v \\ -A(u, v), & u \neq v, (u, v) \in E \\ 0 & \text{otherwise} \end{cases}$$

- Modify "degree" matrix D to $D(u, u) = \sum_v A(u, v)$
- Still have $L_G = NN^\top = D - A$

Laplacian and node score smoothness

- For any vector $x \in \mathbb{R}^n$, ▸ HW

$$x^\top L x = \sum_{(u,v)\in E} A(u,v)\big(x_u - x_v\big)^2$$

- $x^\top L x$ penalizes node scores that are very different across "heavy" edges
- If $u \prec v$, we want $x_u + 1 \le x_v$
- Therefore define the ranking loss of score vector x as $\max\{0, 1 + x_u - x_v\}$
- The complete optimization problem is to $\min_x x^\top L x + B \sum_{u \prec v} \max\{0, 1 + x_u - x_v\}$
- B balances between roughness and data fit
- Because L is positive semidefinite, this is a convex quadratic program with linear constraints ▸ HW

Directed graph Laplacian

- Assume each row of A has at least one nonzero element
- Let $D(u,u)$ be the sum of the uth row of A
- Define Markovian transition probability matrix $Q \in [0,1]^{n \times n}$ with $Q(u,v) = \Pr(v|u) = A(u,v)/D(u,u)$
- Assume the Markov random walk is irreducible and aperiodic
- Let $\pi \in \mathbb{R}^n$ be the steady-state probability vector for the random walk, and $\Pi = \mathrm{diag}(\pi)$
- The directed graph Laplacian is defined as

$$L = \mathbb{I} - \frac{\Pi^{1/2} Q \Pi^{-1/2} + \Pi^{-1/2} Q \Pi^{1/2}}{2}$$

- Use in optimization in place of undirected graph Laplacian

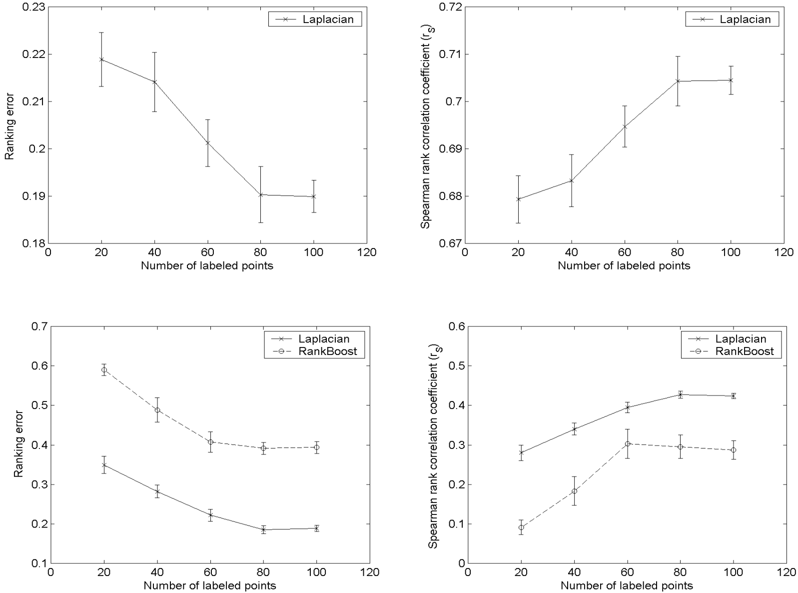
Smoothing properties

- We can show that

$$x^\top L x = \sum_{(u,v)\in E} \pi(u) Q(u,v) \left(\frac{x_u}{\sqrt{\pi(u)}} - \frac{x_v}{\sqrt{\pi(v)}} \right)^2$$

- In $\min_x x^\top L x + B \sum_{u \prec v} \max\{0, 1 + x_u - x_v\}$, suppose we set $B = 0$ (i.e., only smoothness matters)
- Clearly, $x_u \propto \sqrt{\pi(u)}$ will minimize $x^\top L x$
- I.e., in the absence of training preferences, a directed Laplacian smoother will lead to ordering nodes by decreasing Pagerank

Laplacian smoothing results



Limitations of the graph Laplacian approach

- The "link as hint of score smoothness" view is not universally applicable: millions of obscure pages u link to $v =$`http://yahoo.com`, with $x_u \ll x_v$
- While $\pi(u)$ is a probability, $x_u \in \mathbb{R}$ is an arbitrary score that need not satisfy Markov balance constraints (coming soon) and may even be negative
- Dual optimization involves computing the pseudoinverse L^+ of the Laplacian matrix
- Unlike L, L^+ is usually not sparse, and most packages need to hold it in RAM
- The generalization power of the learner (defined later) depends on $\kappa = \max_{u \in V} L^+(u, u)$, a quantity hard to interpret

Pagerank as network circulation

- Can use Q and π to define a reference circulation $\{q_{uv} : (u, v) \in E\}$ as follows:

$$q_{uv} = \pi(u)Q(u, v)$$

- Idea: directly search for a circulation $\{p_{uv} : (u, v) \in E\}$
- Pagerank of node v will fall out naturally as $\sum_{(u,v)\in E} p_{uv}$

What properties must $\{p_{uv}\}$ satisfy?

- $p_{uv} \geq 0$ for all $(u, v) \in E$
- $\sum_{(u,v) \in E} p_{uv} = 1$
- Flow balance at each node v:

$$\sum_{u \in V} p_{uv} = \sum_{w \in V} p_{vw}$$

What roughness penalty should we assess?

- May want to maximize the entropy of $\{p_{uv} : (u, v) \in E\}$, i.e., $-\sum_{u,v} p_{uv} \log p_{uv}$
- May want to propose flow $\{q_{uv} : (u, v) \in E\}$ as a parsimonious belief and minimize $\mathrm{KL}(p||q) = \sum_{u,v} p_{uv} \log \frac{p_{uv}}{q_{uv}}$
- Can show that staying close to q is good for learning

Unconstrained maximum entropy flows

- Associate dual variable β_v for every flow balance constraint

$$\sum_{u \in V} p_{uv} = \sum_{w \in V} p_{vw}$$

- By dualizing the optimization, we see that ▸ HW flows have the form

$$p_{uv} \propto q_{uv} \exp(\beta_v - \beta_u)$$

- Dual objective is $\min_\beta Z$ where $Z = \sum_{(u,v) \in E} q_{uv} \exp(\beta_v - \beta_u)$

Optimizing $\{p_{uv}\}$ with teleports

- The Markov walk specified by Q need not be irreducible and aperiodic
- As in Pagerank, we can make it so using teleports
- Walk probability $\alpha \in (0, 1)$, teleport probability $1 - \alpha$
- Implement teleport using transition from every v to dummy node d and back
- This leads to additional primal constraints

$$\frac{p_{vd}}{1-\alpha} = \frac{\sum_{(v,w)\in E} p_{vw}}{\alpha} \qquad \forall v \in V$$

- And dual variables τ_v, leading to the solution

$$\begin{aligned}
p_{dv} &\propto q_{dv} \exp(\beta_v - \beta_d) \\
p_{vd} &\propto q_{dv} \exp(\beta_d - \beta_v + \alpha\tau_v) \\
p_{uv} &\propto q_{uv} \exp(\beta_v - \beta_u - (1-\alpha)\tau_u)
\end{aligned}$$

Preference constraints

- Preference $u \prec v$ leads to constraint

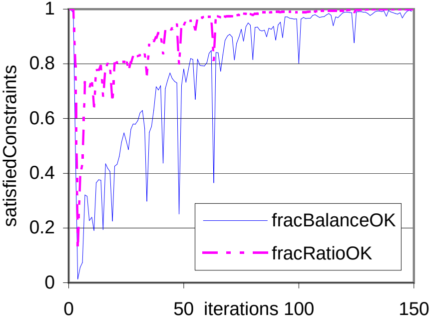
$$\sum_{(w,u)\in\hat{E}} p_{wu} \le \sum_{(w,v)\in\hat{E}} p_{wv},$$

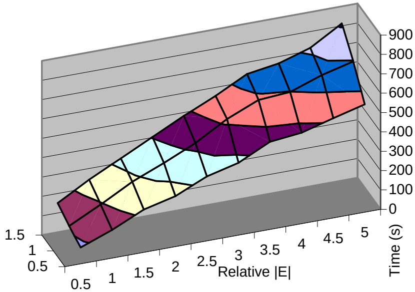
where $\hat{E} = E \cup \{(v,d) : v \in V\} \cup \{(d,v) : v \in V\}$

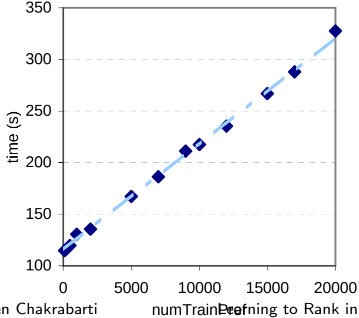
- Note, no margin (yet)
- Corresponding dual variables $\{\pi_{uv} : u \prec v\}$
- Define $\text{bias}(v) = \sum_{r \prec v} \pi_{rv} - \sum_{v \prec s} \pi_{vs}$
- Modified solution has form

$$p_{dv} \propto q_{dv} \exp(\beta_v - \beta_d + \text{bias}(v))$$
$$p_{vd} \propto q_{dv} \exp(\beta_d - \beta_v + \alpha\tau_v)$$
$$p_{uv} \propto q_{uv} \exp(\beta_v - \beta_u - (1-\alpha)\tau_u + \text{bias}(v))$$

Performance of constrained circulation approach







- Must check primal constraints before terminating dual
- Scales linearly with $|V|$, $|E|$ and $|\prec|$

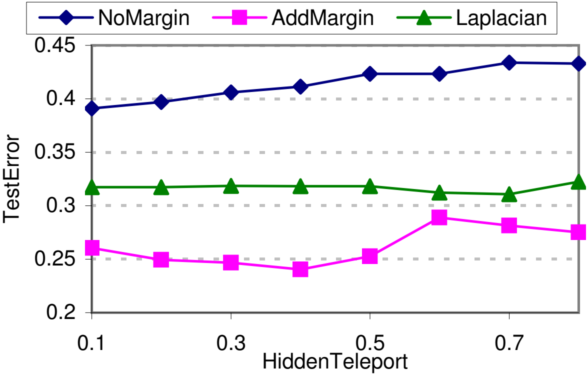
Incorporating an additive margin

- Preference constraints were expressed as $\sum_{(w,u)\in\hat{E}} p_{wu} \le \sum_{(w,v)\in\hat{E}} p_{wv}$, not $1 + \sum_{(w,u)\in\hat{E}} p_{wu} \le s_{uv} + \sum_{(w,v)\in\hat{E}} p_{wv}$
- $s_{uv} \ge 0$ is a primal slack variable
- Because $\sum_{u,v} p_{uv} = 1$, 1 is "too aggressive" as a margin
- …unless we scale up $\{p_{uv}\}$
- Let q be a probability distribution and p an unnormalized distribution such that $\sum_x p(x) = F$
  - $\mathrm{KL}(p\|q) \ge 0$ if $F \ge 1$
  - For a fixed $F \ge 1$, $\arg\min_p \mathrm{KL}(p\|q) = Fq$
- New objective

$$\min_{\{p_{uv}\},\{s_{uv}\ge 0\},F\ge 1} \mathrm{KL}(p\|q) + C\sum_{u\prec v} s_{uv} + C_1 F^2$$

- New constraint $\sum_{u,v} p_{uv} = F$ replaces $\sum_{u,v} p_{uv} = 1$

Comparing Laplace vs. circulation



- In Laplace score smoothing, node scores can induce all possible permutations
- In case of network circulation, many node permutations may not be achievable for a given graph
- Smaller hypothesis space, more bias, more stable
- Seems to actually help; even better with additive margin

Typed edge conductance

- In the constrained circulation formulation, training input has very local effect owing to teleport
- Beyond a distance of about $1/(1-\alpha)$, training preferences cannot generalize
- A different, very common setting associates a type $t(u,v) \in \{1,\ldots,T\}$ with each edge (u,v)
- The weight of edge (u,v) is $\beta(t(u,v))$
- Given $\prec$ we want to estimate $\beta_1,\ldots,\beta_T$
- Assuming no dead-end nodes,

$$C(j,i) = \begin{cases} \alpha \frac{\beta(t(i,j))}{\sum_{(i,k)\in E} \beta(t(i,k))}, & i \neq d, j \neq d \\ 1-\alpha, & i \neq d, j = d \\ r_j, & i = d, j \neq d \\ 0, & i = j = d \end{cases}$$

- Here r_j is the teleport into node j, implemented using dummy node d

Constrained design of conductance

- Scaling all β by any positive factor keeps all $C(\cdot, \cdot)$ unchanged
- So we can arbitrarily scale $\beta_t \geq 1$
- C is a function of β, therefore sometimes written as $C(\beta)$
- Goal is to find $\beta \geq \vec{1}$ such that
  - $p = C(\beta)p$
  - $p_i \leq p_j$ for all $i \prec j$
- As before, we can change the constraint $p_i \leq p_j$ into a loss function $\text{loss}(p_i - p_j)$
- Two problems to solve
  - Break recursion $p = C(\beta)p$ and express p directly in terms of β, so we can use a numerical optimizer
  - If there are many solutions β, which one should we prefer?

Choice of loss function

- Standard hinge $\text{hinge}(y) = \max\{0, 1 + y\}$
- As before, enforcing additive margin 1 is tricky
- Scaling β has no effect on satisfying margin
- In practice, no margin or very small arbitrary margin makes no difference, both work well
- To make loss smooth and differentiable, could have picked $\text{loss}(y) = \ln(1 + e^y)$
- But this does not work, experiments suggest that $\text{loss}(0) = 0$ is essential
- Approximation of hinge with zero margin ($\text{hinge}(y) = \max\{0, y\}$) with Huber loss:

$$\text{huber}(y) = \begin{cases} 0, & y \le 0 \\ y^2/(2W), & y \in (0, W] \\ y - W/2, & W < y \end{cases}$$

Parsimonious choice of β

- If $\beta = \vec{1}$, we get unweighted Pagerank
- Therefore the model cost can be taken as $\sum_t (\beta(t) - 1)^2$
- In fact, we get unweighted Pagerank if all $\beta(t)$ are equal, not necessarily all equal to one
- Model cost $\sum_{t,t'} (\beta(t) - \beta(t'))^2$ is another possibility
- Discourages large multiplicative factors . . .
  $\text{ModelCost}(K\beta) = K^2 \text{ModelCost}(\beta)$
- . . . but not additive terms:
  $\text{ModelCost}(\beta + K\vec{1}) = \text{ModelCost}(\beta)$
- In practice these work about equally well

Breaking the $p = C(\beta)p$ recursion I

- Pagerank usually approximated using the Power Method $p \approx C^H p^0$ where
  - p^0 is an initial distribution over nodes, usually uniform
  - H is a suitably large horizon for convergence
- Overall optimization problem:

$$\min_{\beta \geq \vec{1}} \sum_t (\beta(t) - 1)^2 + B \sum_{i \prec j} \text{huber}\big((C^H p^0)_i - (C^H p^0)_j\big)$$

- Unfortunately, not a convex optimization; need some grid plus local gradient search
- Next: computing gradient

Breaking the $p = C(\beta)p$ recursion II

- Compute alongsize Pagerank (using Chain Rule):

$$\forall i \forall t: \quad \frac{\partial}{\partial \beta(t)}(C^0 p^0)_i = 0$$

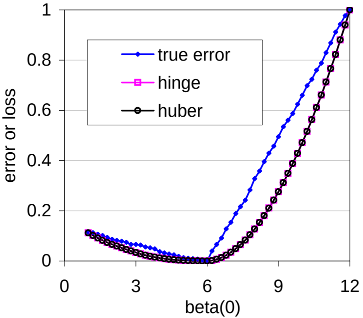
$$(C^h p^0)_i = \sum_j C(i,j)(C^{h-1}p^0)_j$$

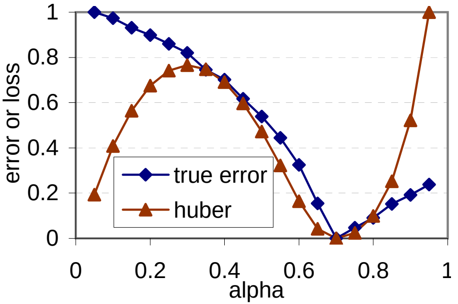
$$\frac{\partial (C^h p^0)_i}{\partial \beta(t)} = \sum_j \left[\frac{\partial C(i,j)}{\partial \beta(t)} (C^{h-1}p^0)_j + C(i,j) \frac{\partial}{\partial \beta(t)} (C^{h-1}p^0)_j \right]$$

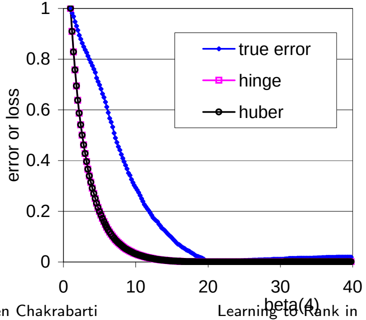
- Finally,

$$\frac{\partial C(i,j)}{\partial \beta(\tau)} = \begin{cases} -\alpha \frac{\beta(t(i,j)) \sum_w [\![\tau = t(i,w)]\!]}{(\sum_w \beta(t(i,w)))^2} & \tau \neq t(i,j) \\ \alpha \frac{\sum_w \beta(t(i,w)) - \beta(t(i,j)) \sum_w [\![\tau = t(i,w)]\!]}{(\sum_w \beta(t(i,w)))^2}, & \tau = t(i,j) \end{cases}$$

Exact loss and the approximations

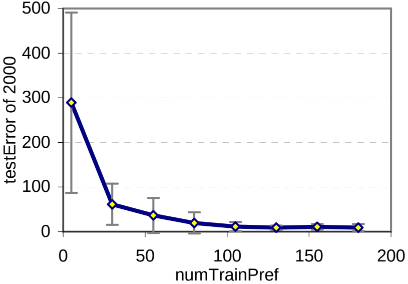


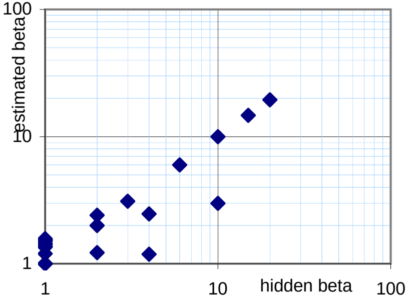


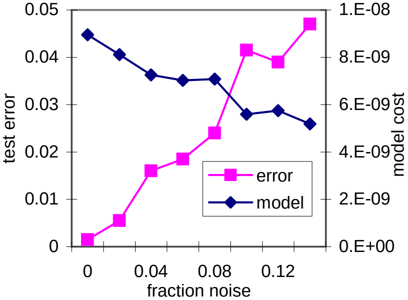


- Theoretically, the optimization surface has local minima
- Wrt β, the surface is very benign in practice
- If one also wanted to search for α, a little more care is needed

β estimation and learning performance







- Fast training rate
- Robust to training noise
- Reconstructs β reasonably

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Stability and generalization

- Admissibility and stability
- Ranking loss and generalization bounds

Some sample results

- Pagerank is score-stable but not rank-stable
- (HITS is not score-stable and not rank-stable)
- More notions of stability, connections with generalization
- Max-margin vector-space ranking is stable
- Ranking based on Laplace smoothing is stable
- Ranking based on constrained circulation is stable

Pagerank is score-stable when G is perturbed

- V kept fixed
- Nodes in $P \subset V$ get incident links changed in any way (additions and deletions)
- Thus G perturbed to $\tilde{G}$
- Let the random surfer visit (random) node sequence $X_0, X_1, \ldots$ in G, and $Y_0, Y_1, \ldots$ in $\tilde{G}$
- Coupling argument: instead of two random walks, we will design one joint walk on (X_i, Y_i) such that the marginals apply to G and $\tilde{G}$

Coupled random walks on G and $\tilde{G}$

- Pick $X_0 = Y_0 \sim \text{Multi}(r)$
- At any step t, with probability $1-\alpha$, reset both chains to a common node using teleport r: $X_t = Y_t \in_r V$
- With the remaining probability of α
  - If $x_{t-1} = y_{t-1} = u$, say, and u remained unperturbed from G to $\tilde{G}$, then pick one out-neighbor v of u uniformly at random from all out-neighbors of u, and set $X_t = Y_t = v$.
  - Otherwise, i.e., if $x_{t-1} \neq y_{t-1}$ or x_{t-1} was perturbed from G to $\tilde{G}$, pick out-neighbors X_t and Y_t independently for the two walks.

Analysis of coupled walks I

Let $\delta_t = \Pr(X_t \neq Y_t)$; by design, $\delta_0 = 0$.

$$\begin{aligned}
\delta_{t+1} &= \Pr(\text{reset at } t+1)\, \Pr(X_{t+1} \neq Y_{t+1} | \text{reset at } t+1) + \\
&\qquad \Pr(\text{no reset at } t+1)\, \Pr(X_{t+1} \neq Y_{t+1} | \text{no reset at } t+1) \\
&= \Pr(\text{reset at } t+1)\, 0 + \alpha \Pr(X_{t+1} \neq Y_{t+1} | \text{no reset at } t+1) \\
&= \alpha \Big(\Pr(\underline{X_{t+1} \neq Y_{t+1}}, X_t \neq Y_t | \text{no reset at } t+1) + \\
&\qquad \Pr(X_{t+1} \neq Y_{t+1}, X_t = Y_t | \text{no reset at } t+1) \Big)
\end{aligned}$$

Analysis of coupled walks II

The event $X_{t+1} \neq Y_{t+1}, X_t = Y_t$ can happen only if $X_t \in P$. Therefore we can continue the above derivation as follows:

$$
\begin{aligned}
\delta_{t+1} &= \dots \\
&\le \alpha\Big(\Pr(X_t \neq Y_t | \underline{\text{no reset at } t+1}) + \\
&\qquad \Pr(X_{t+1} \neq Y_{t+1}, X_t = Y_t, \underline{X_t \in P} | \text{no reset at } t+1)\Big) \\
&= \alpha\Big(\Pr(X_t \neq Y_t) + \\
&\quad \Pr(X_{t+1} \neq Y_{t+1}, X_t = Y_t, \underline{X_t \in P} | \text{no reset at } t+1)\Big) \\
&\le \alpha\Big(\Pr(X_t \neq Y_t) + \Pr(X_t \in P)\Big) \\
&= \alpha\left(\delta_t + \textstyle\sum_{u \in P} p_u\right),
\end{aligned}
$$

(using $\Pr(H, J|K) \le \Pr(H|K)$, and that events at time t are independent of a potential reset at time $t+1$)

Analysis of coupled walks III

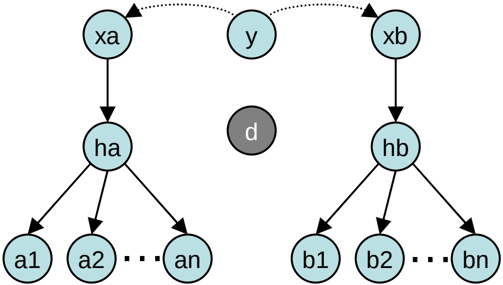
Unrolling the recursion,
$\delta_\infty = \lim_{t\to\infty} \delta_t \le \left(\sum_{u\in P} p_u\right) / (1-\alpha)$ HW

- Standard result: If the probability of a state disagreement between the two walks is bounded, then their Pagerank vectors must also have small L_1 distance to each other. In particular,

$$\|p - \tilde{p}\|_1 \le \frac{2\sum_{u\in P} p_u}{1-\alpha}$$

- Lower the value of α, the more the random surfer teleports and more stable is the system
- Gives no direct guidance why α should not be set to exactly zero!

Pagerank is not rank-stable when G is perturbed



- Adversarial setting
- G formed by connecting y to x_a, $\tilde{G}$ by connecting y to x_b
- $\Omega(n^2)$ node pairs flip Pagerank order HW
- I.e., L_1 score stability does not guarantee rank stability
- Can "natural" social networks lead often to such tie-breaking?

Generalization of bipartite ranking

- $f : \mathcal{X} \to \mathbb{R}$ is a fixed ranking function
- The ("true") ranking accuracy of f is

$$A(f) = \mathbb{E}_{X \in \mathcal{D}_{+1}, X' \in \mathcal{D}_{-1}} \left([\![f(X) > f(X')]\!] + \frac{1}{2} [\![f(X) = f(X')]\!] \right)$$

- Recall that the empirical ranking accuracy of f over training set T is denoted $\hat{A}(f, T)$
- We are interested in upper-bounding

$$\Pr(|\hat{A}(f, T) - A(f)| > \epsilon)$$

- Recall that $T = \{(x_i, y_i \in \{-1, 1\})\}$ in bipartite ranking; projections on $\mathcal{X}$ and $\mathcal{Y}$ are called $T_{\mathcal{X}}$ and $T_{\mathcal{Y}}$
- Let there be m positive and n negative instances, and $\underline{y}$ the sequence of labels

$$\Pr_{T_{\mathcal{X}} | T_{\mathcal{Y}} = \underline{y}} (\hat{A}(f, T) - A(f) \geq \epsilon) \leq 2e^{-2mn\epsilon^2/(m+n)}$$

Generalization of circulation-based ranking

- Given graph $G = (V, E)$
- Rewrite regularized optimization objective in the form

$$R_{\text{reg}}(p) = \frac{1}{m}\sum_{j=1}^{m} \underbrace{\max\left\{0, \sum_{(w,u)\in\hat{E}} p_{wu} - \sum_{(w,v)\in\hat{E}} p_{wv}\right\}}_{\text{ranking loss}} + \lambda\,\mathrm{KL}(p\|q)$$

- $\prec$ is sampled randomly from $V \times V$ according to some unknown fixed distribution
- Over random draws of $\prec$ with $|\prec| = m$, with probability at least $1-\delta$,

$$R \leq R_{\text{emp}} + \frac{4\ln 2}{\lambda m} + \left(\frac{8\ln 2}{\lambda} + 1\right)\sqrt{\frac{\ln(1/\delta)}{2m}}$$

- Here R is the true ranking loss and R_{emp} is the empirical ranking loss over training data

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