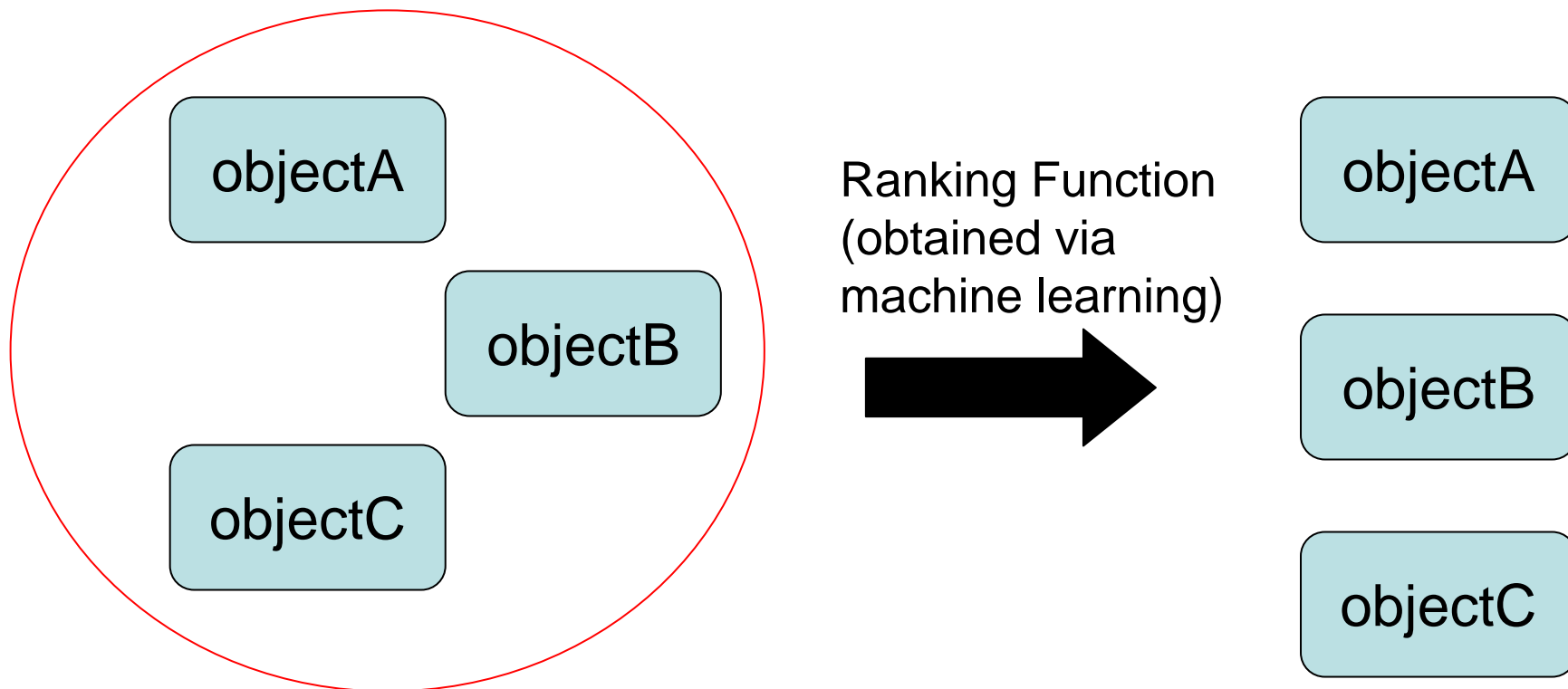

Learning to Rank with Partially-Labeled Data

Kevin Duh

University of Washington

The Ranking Problem

- Definition: Given a set of objects, sort them by preference.



Application: Web Search



You enter “uw” into the searchbox...

All webpages containing the term “uw”:

[University of Wyoming - New Thinking](#)

Official web site of the **University of Wyoming**, located in Laramie, Wyoming. Colleges, libraries, directories, faculty, student information and news.

[www.uwyo.edu/](#) - 15k - [Cached](#) - [Similar pages](#) - [Note this](#)

[UW Athletics - Official Site](#)

Badgers news, team links, tickets, and facilities information.

[www.uwbadgers.com/](#) - 14k - [Cached](#) - [Similar pages](#) - [Note this](#)

[University of Wisconsin-Madison](#)

Skip to menu for main topics about the **University of Wisconsin**; Skip to search; Skip to news ... 2008 Board of Regents of the **University of Wisconsin** System.

[www.wisc.edu/](#) - 14k - [Cached](#) - [Similar pages](#) - [Note this](#)

[refresh.uw.hu ::](#)

refresh.uw.hu - Gitáros Fórum. Gy.IK Gy.IK Keresés Keresés Taglista Taglista Csoportok Csoportok Regisztráció Regisztráció Profil ...

[refresh.uw.hu/viewtopic.php?p=120127](#) - 10k - [Cached](#) - [Similar pages](#) - [Note this](#)

[University of Washington](#)

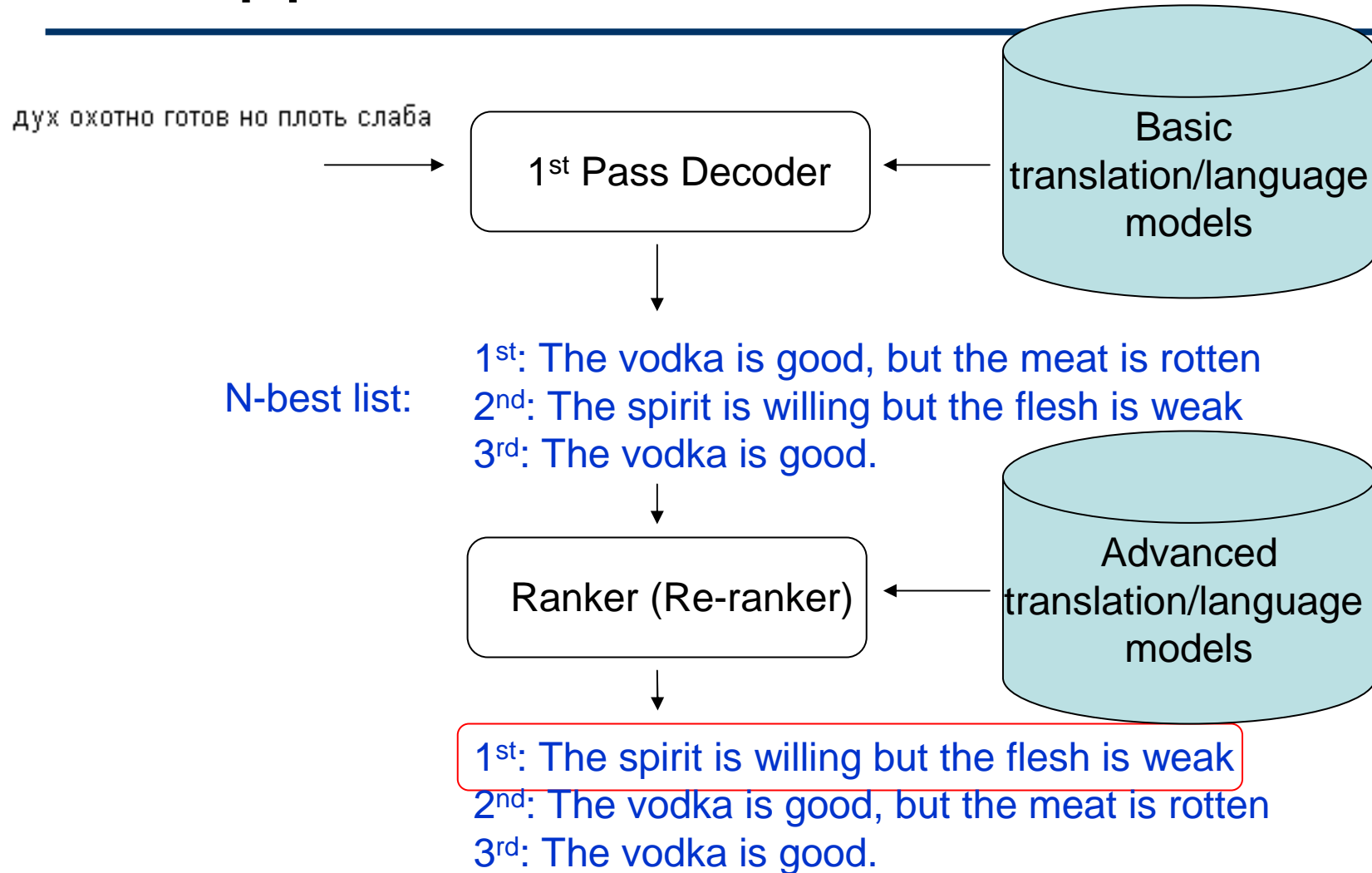
Offers information and news for prospective and current students, faculty, and staff. Highlights academic departments and athletics, serves as directory for ...

[www.washington.edu/](#) - 15k - [Cached](#) - [Similar pages](#) - [Note this](#)

Results presented to user, after ranking:

- 1st** [University of Washington](#)
Offers information and news for prospective and current students, faculty, and staff. Highlights academic departments and athletics, serves as directory for ...
[www.washington.edu/](#) - 15k - [Cached](#) - [Similar pages](#) - [Note this](#)
- 2nd** [University of Wisconsin-Madison](#)
Skip to menu for main topics about the **University of Wisconsin**; Skip to search; Skip to news ... 2008 Board of Regents of the **University of Wisconsin** System.
[www.wisc.edu/](#) - 14k - [Cached](#) - [Similar pages](#) - [Note this](#)
- 3rd** [University of Wyoming - New Thinking](#)
Official web site of the **University of Wyoming**, located in Laramie, Wyoming. Colleges, libraries, directories, faculty, student information and news.
[www.uwyo.edu/](#) - 15k - [Cached](#) - [Similar pages](#) - [Note this](#)
- 4th** [UW Athletics - Official Site](#)
Badgers news, team links, tickets, and facilities information.
[www.uwbadgers.com/](#) - 14k - [Cached](#) - [Similar pages](#) - [Note this](#)
- 5th** [refresh.uw.hu ::](#)
refresh.uw.hu - Gitáros Fórum. Gy.IK Gy.IK Keresés Keresés Taglista Taglista Csoportok Csoportok Regisztráció Regisztráció Profil ...
[refresh.uw.hu/viewtopic.php?p=120127](#) - 10k - [Cached](#) - [Similar pages](#) - [Note this](#)

Application: Machine Translation



Application: Protein Structure Prediction

Amino Acid Sequence:

MMKLKSNQTRTYDGDGYKKRAACLCFSE

↓ *various protein folding simulations*

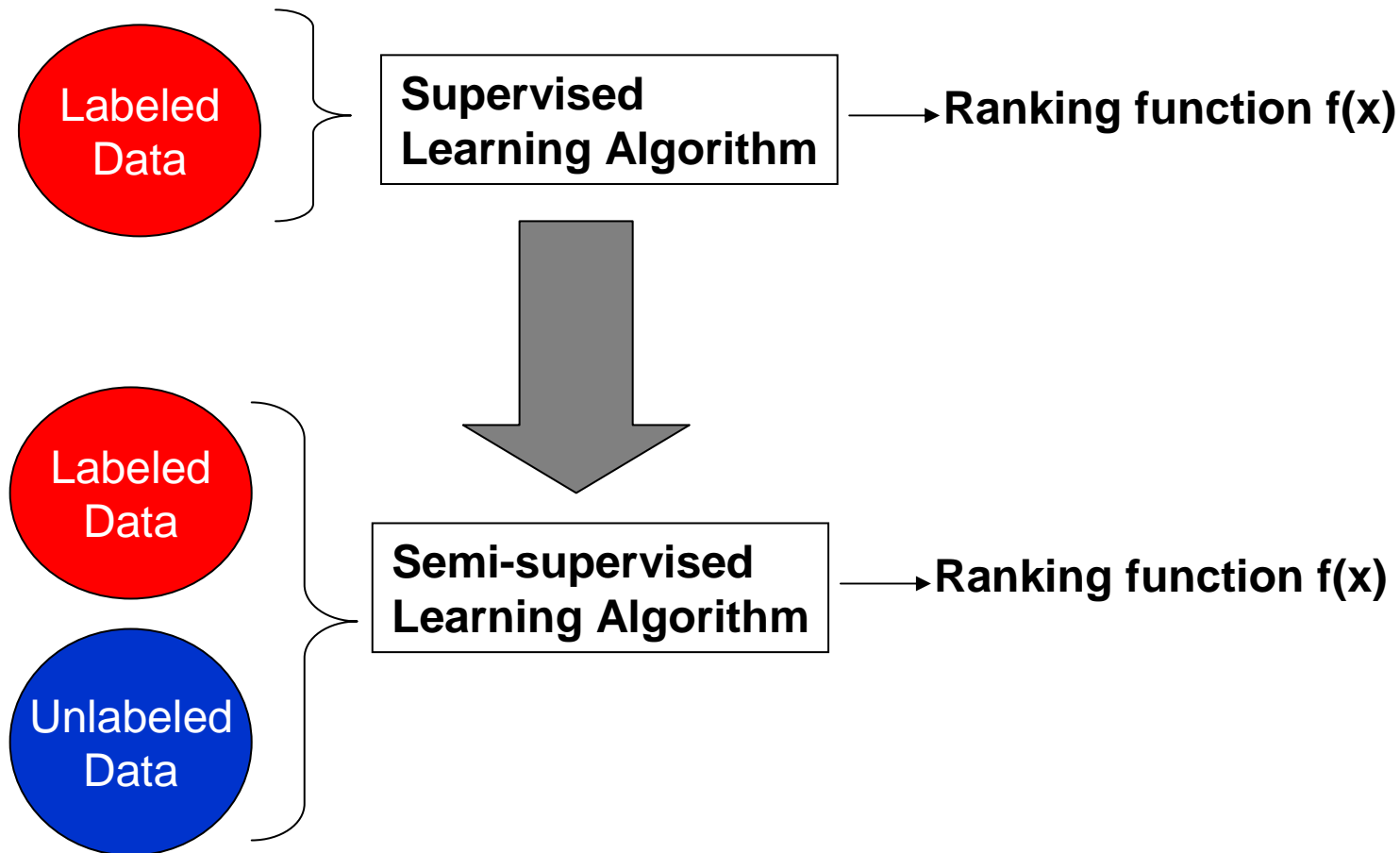


Candidate 3-D Structures

→ *Ranker*



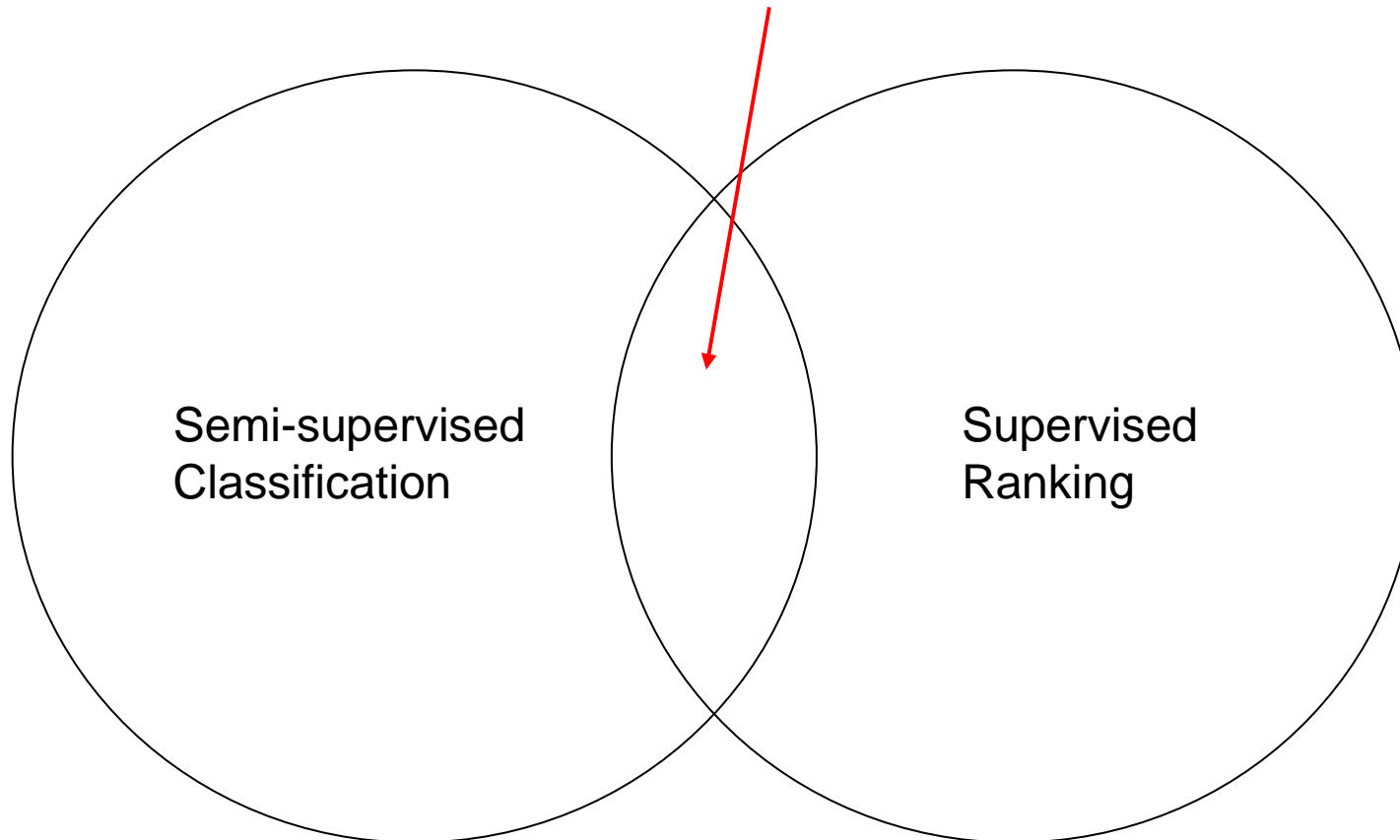
Goal of this thesis



Can we build a better ranker by adding cheap, unlabeled data?

Emerging field

Semi-supervised Ranking



Outline

1. Problem Setup
 1. Background in Ranking
 2. Two types of partially-labeled data
 3. Methodology
2. Manifold Assumption
3. Local/Transductive Meta-Algorithm
4. Summary

Ranking as Supervised Learning Problem

Query: UW

University of Washington

Offers information and news for prospective and current students, faculty, and staff. Highlights academic departments and athletics, serves as directory for ...

www.washington.edu/ - 15k - [Cached](#) - [Similar pages](#) - [Note this](#)

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University of Wisconsin-Madison

Skip to menu for main topics about the **University of Wisconsin**; Skip to search; Skip to news ... 2008 Board of Regents of the **University of Wisconsin** System.

www.wisc.edu/ - 14k - [Cached](#) - [Similar pages](#) - [Note this](#)

Labels



3 $x_1^{(i)} = [tfidf, pagerank, \dots]$

1 $x_2^{(i)} = [tfidf, pagerank, \dots]$

2 $x_3^{(i)} = [tfidf, pagerank, \dots]$

Query: Seattle Traffic

WSDOT Seattle Area Traffic - Traffic Conditions and Travel Alerts

A map of current freeway **traffic** conditions for **Seattle** and surrounding areas; includes links to **traffic** cams, incident reports, mountain pass reports, ...

www.wsdot.wa.gov/Traffic/seattle/ - 38k - [Cached](#) - [Similar pages](#) - [Note this](#)

Seattle Praised for Traffic Efficiency: NPR

Seattle and Tacoma's program to ease **traffic** flows is cited as the nation's most effective by the Texas Transportation Institute.

www.npr.org/templates/story/story.php?storyId=3905008 - [Similar pages](#) - [Note this](#)

2 $x_1^{(j)} = [tfidf, pagerank, \dots]$

1 $x_2^{(j)} = [tfidf, pagerank, \dots]$

Ranking as Supervised Learning Problem

Query: UW

3 $x_1^{(i)} = [tfidf, pagerank, \dots]$

1 $x_2^{(i)} = [tfidf, pagerank, \dots]$

2 $x_3^{(i)} = [tfidf, pagerank, \dots]$

Train $F(x)$ such that

$$F(x_1^{(1)}) > F(x_3^{(1)}) > F(x_2^{(1)})$$

$$F(x_1^{(2)}) > F(x_2^{(2)})$$

Test Query: MSR

Query: Seattle Traffic

2 $x_1^{(j)} = [tfidf, pagerank, \dots]$

1 $x_2^{(j)} = [tfidf, pagerank, \dots]$

[MSR | MX Gear | One Brand Fits All...](#)

Motocross gear, off road gear, and hard parts.

[www.msrracing.com/ - 2k - Cached - Similar pages - Note this](#)

?

[Microsoft Research Home](#)

Corporate research division. Includes projects and publications, news and history, and job opportunities.

[research.microsoft.com/ - 25k - Cached - Similar pages - Note this](#)

?

[MSR Mountain Safety Research](#)

This is the home page for **Mountain Safety Research**®, manufacturers of the most reliable and functional backcountry gear in the world.

[www.msrgear.com/ - 11k - Cached - Similar pages - Note this](#)

?

Semi-supervised Data: Some labels are missing

Query: UW

[University of Washington](#)

Offers information and news for prospective and current students, faculty, and staff. Highlights academic departments and athletics, serves as directory for ...

[www.washington.edu/](#) - 15k - [Cached](#) - [Similar pages](#) - [Note this](#)

[University of Wyoming - New Thinking](#)

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[www.wisc.edu/](#) - 14k - [Cached](#) - [Similar pages](#) - [Note this](#)

Labels



$$3 x_1^{(i)} = [tfidf, pagerank, \dots]$$

$$1 x_2^{(i)} = [tfidf, pagerank, \dots]$$

$$\cancel{X} x_3^{(i)} = [tfidf, pagerank, \dots]$$

Query: Seattle Traffic

[WSDOT Seattle Area Traffic - Traffic Conditions and Travel Alerts](#)

A map of current freeway **traffic** conditions for **Seattle** and surrounding areas; includes links to **traffic** cams, incident reports, mountain pass reports, ...

[www.wsdot.wa.gov/Traffic/seattle/](#) - 38k - [Cached](#) - [Similar pages](#) - [Note this](#)

[Seattle Praised for Traffic Efficiency: NPR](#)

Seattle and Tacoma's program to ease **traffic** flows is cited as the nation's most effective by the Texas Transportation Institute.

[www.npr.org/templates/story/story.php?storyId=3905008](#) - [Similar pages](#) - [Note this](#)

$$\cancel{X} x_1^{(j)} = [tfidf, pagerank, \dots]$$

$$\cancel{X} x_2^{(j)} = [tfidf, pagerank, \dots]$$

Two kinds of Semi-supervised Data

1. Lack of labels for some documents (depth)

Query1
Doc1 Label
Doc2 Label
Doc3 ?

Query2
Doc1 Label
Doc2 Label
Doc3 ?

Query3
Doc1 Label
Doc2 Label
Doc3 ?

Some references:
Amini+, SIGIR'08
Agarwal, ICML'06
Wang+, MSRA TechRep'05
Zhou+, NIPS'04
He+, ACM Multimedia '04

2. Lack of labels for some queries (breadth)

Query1
Doc1 Label
Doc2 Label
Doc3 Label

Query2
Doc1 Label
Doc2 Label
Doc3 Label

Query3
Doc1 ?
Doc2 ?
Doc3 ?

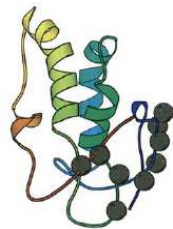
This thesis
Duh&Kirchhoff, SIGIR'08
Truong+, ICMIST'06

Why “Breadth” Scenario

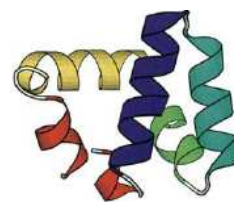
- Information Retrieval: Long tail of search queries
“20-25% of the queries we will see today, we have never seen before”

– Udi Manber (Google VP), May 2007

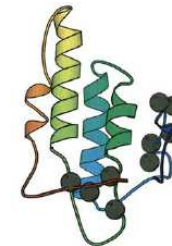
- Machine Translation and Protein Prediction:
 - **Given references (costly), computing labels is trivial**



reference



candidate 1
similarity=0.3



candidate 2
similarity=0.9

Methodology of this thesis

- 1. *Make an assumption*** about how can unlabeled lists be useful
 - Borrow ideas from semi-supervised classification
- 2. *Design a method*** to implement it
 - 4 unlabeled data assumptions & 4 methods
- 3. *Test on various datasets***
 - Analyze when a method works and doesn't work

Datasets

Information Retrieval datasets

- from LETOR distribution [Liu'07]
- TREC: Web search / OHSUMED: Medical search
- Evaluation: MAP (measures how high relevant documents are on list)

	TREC 2003	TREC 2004	OHSUMED	Arabic translation	Italian translation	Protein prediction
# lists	50	75	100	500	500	100
label type	2 level	2 level	3 levels	conti- nuous	conti- nuous	conti- nuous
avg # objects per list	1000	1000	150	260	360	120
# features	44	44	25	9	10	25

Datasets

Machine Translation datasets

- from IWSLT 2007 competition, UW system [Kirchhoff'07]
- translation in the travel domain
- Evaluation: BLEU (measures word match to reference)

	TREC 2003	TREC 2004	OHSUMED	Arabic translation	Italian translation	Protein prediction
# lists	50	75	100	500	500	100
label type	2 level	2 level	3 levels	continuous	continuous	continuous
avg # objects per list	1000	1000	150	260	360	120
# features	44	44	25	9	10	25

Datasets

Protein Prediction dataset

- from CASP competition [Qiu/Noble'07]
- Evaluation: GDT-TS (measures closeness to true 3-D structure)

	TREC 2003	TREC 2004	OHSUMED	Arabic translation	Italian translation	Protein prediction
# lists	50	75	100	500	500	100
label type	2 level	2 level	3 levels	conti- nuous	conti- nuous	conti- nuous
avg # objects per list	1000	1000	150	260	360	120
# features	44	44	25	9	10	25

Outline

1. Problem Setup

2. Manifold Assumption

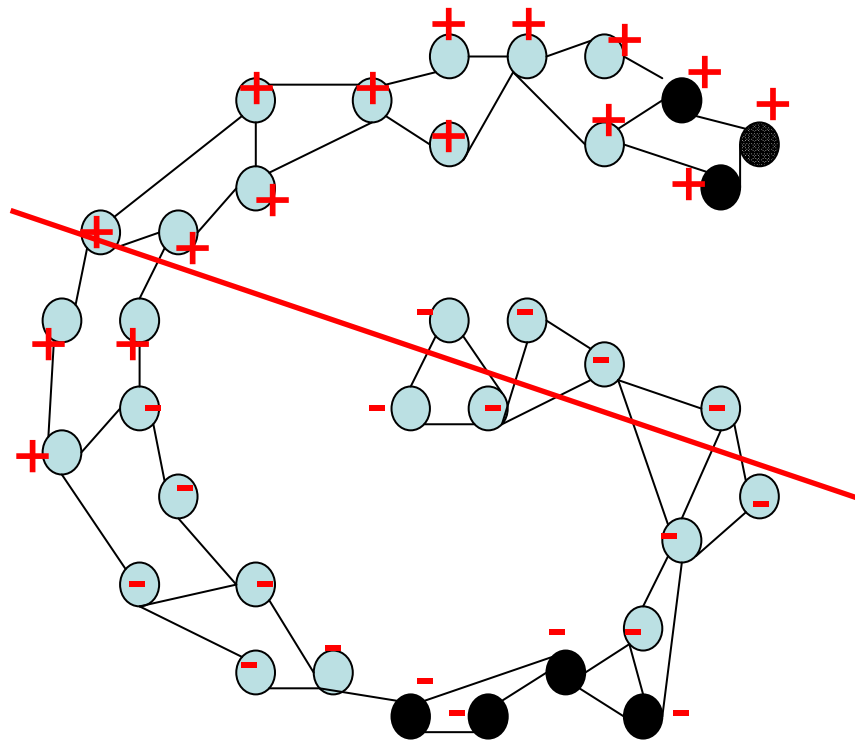
- Definition
- Ranker Propagation Method
- List Kernel similarity

3. Local/Transductive Meta-Algorithm

4. Summary

Manifold Assumption in Classification

- Unlabeled data can help discover underlying data manifold
- Labels vary smoothly over this manifold



Prior work:

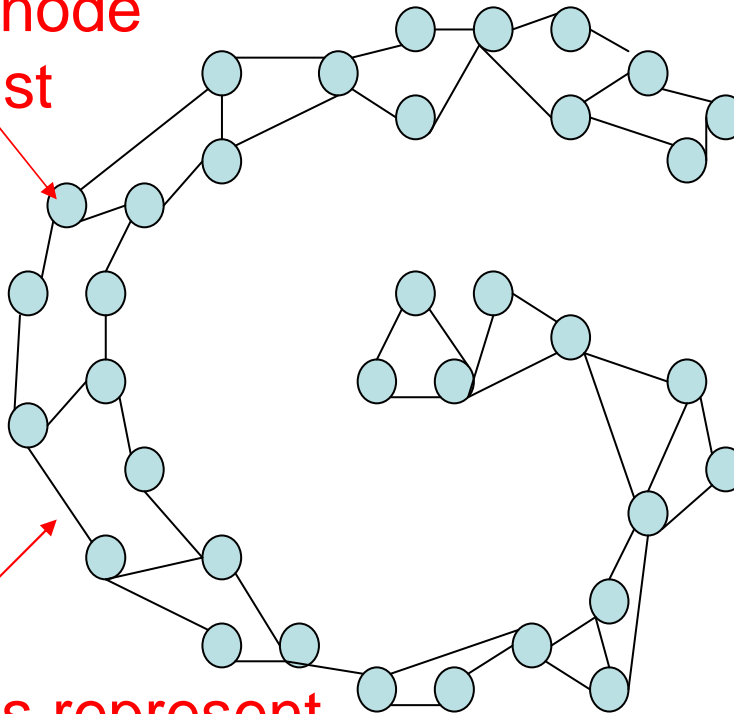
1. How to give labels to test samples?
 - Mincut [Blum01]
 - Label Propagation [Zhu03]
 - Regularizer+Optimization [Belkin03]
2. How to construct graph?
 - k-nearest neighbors, eps-ball
 - data-driven methods [Argyriou05,Alexandrescu07]

Manifold Assumption in Ranking

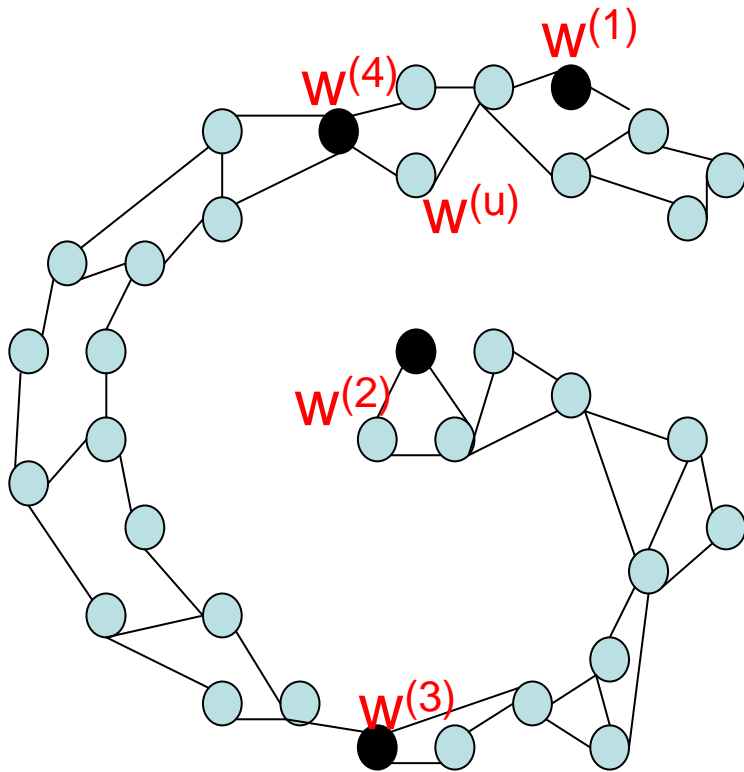
Ranking functions vary smoothly over the manifold

Each node
is a List

Edges represent
“similarity” between two lists



Ranker Propagation



Algorithm:

1. For each train list, fit a ranker

$$F(x) = w^T x \quad w \in R^d, x \in R^d$$

2. Minimize objective:

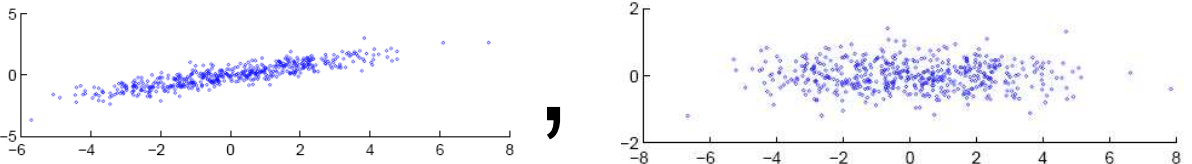
$$\sum_{ij \in \text{edges}} K^{(ij)} \|w^{(i)} - w^{(j)}\|^2$$

↑ ↑
Similarity between list i,j Ranker for list i

$$W^{(u)} = -\text{inv}(L^{(uu)})L^{(ul)}W^{(l)}$$

Similarity between lists: Desirable properties

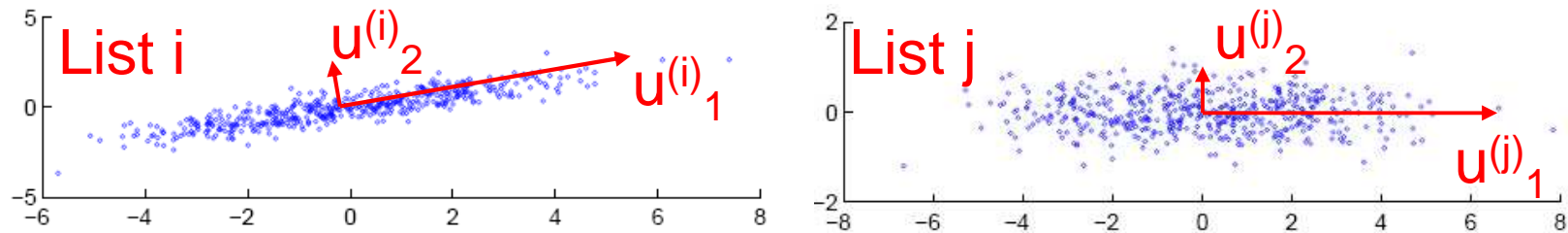
- Maps two lists of feature vectors to scalar

$$K\left(\begin{array}{c} \text{Scatter plot 1} \\ \text{Scatter plot 2} \end{array}\right) = 0.7$$


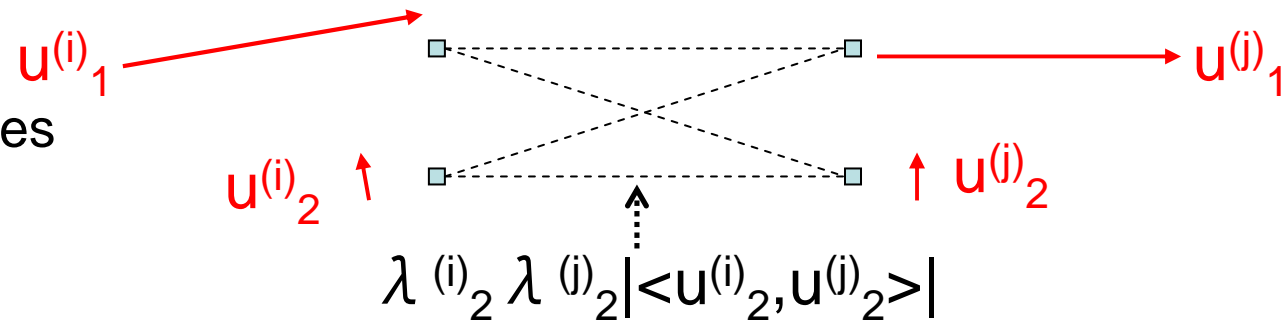
- Work on variable length lists (different N in N-best)
- Satisfy symmetric, positive semi-definite properties
- Measure rotation/shape differences

List Kernel

Step 1:
PCA



Step 2: Compute
similarity between axes

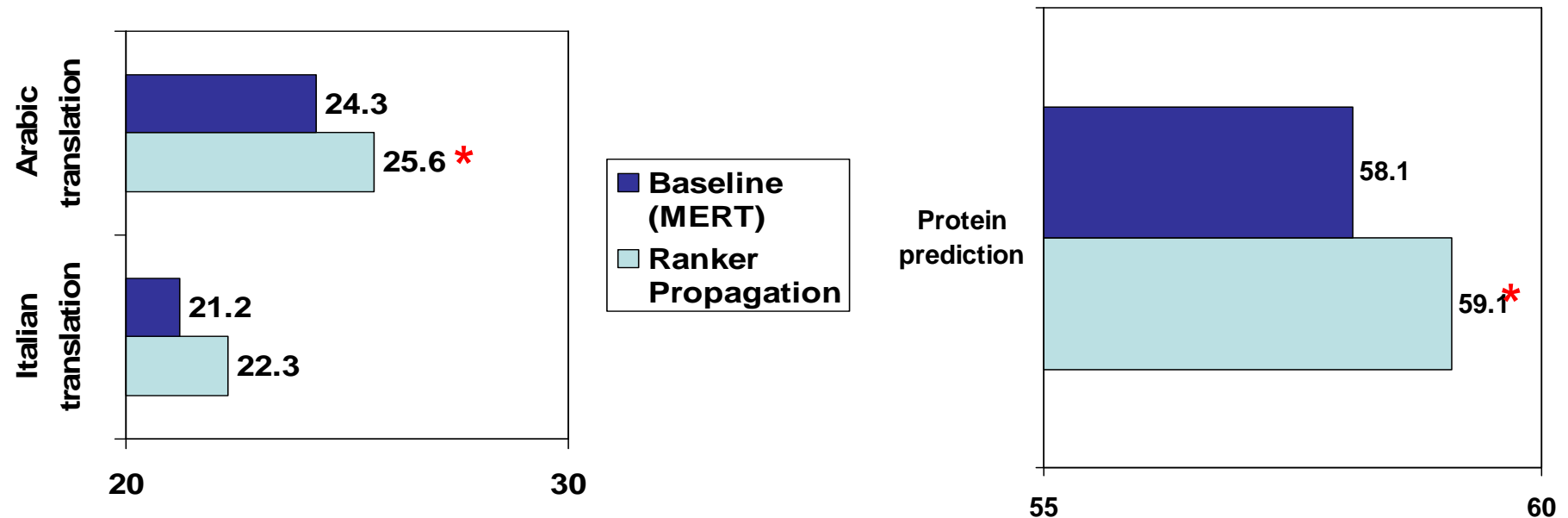


Step 3: Maximum
Bipartite Matching

$$K^{(ij)} = \sum_{m=1}^M \lambda_m^{(i)} \lambda_{a(m)}^{(j)} |\langle u_m^{(i)}, u_{a(m)}^{(j)} \rangle| / \|\lambda^{(i)}\| \cdot \|\lambda^{(j)}\|$$

Evaluation in Machine Translation & Protein Prediction

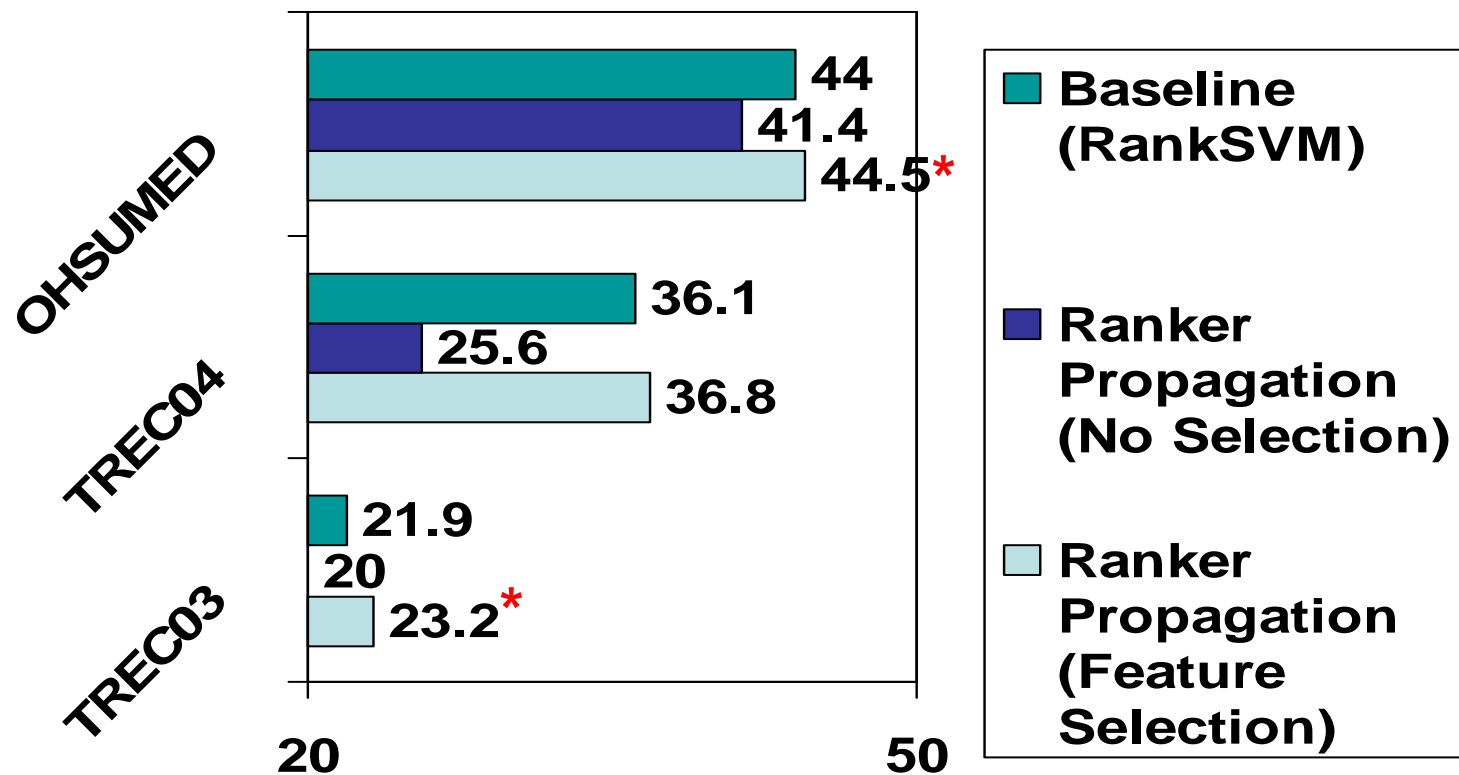
Ranker Propagation (with List Kernel)
outperforms Supervised Baseline (MERT linear ranker)



** Indicates statistically significant improvement ($p < 0.05$) over baseline*

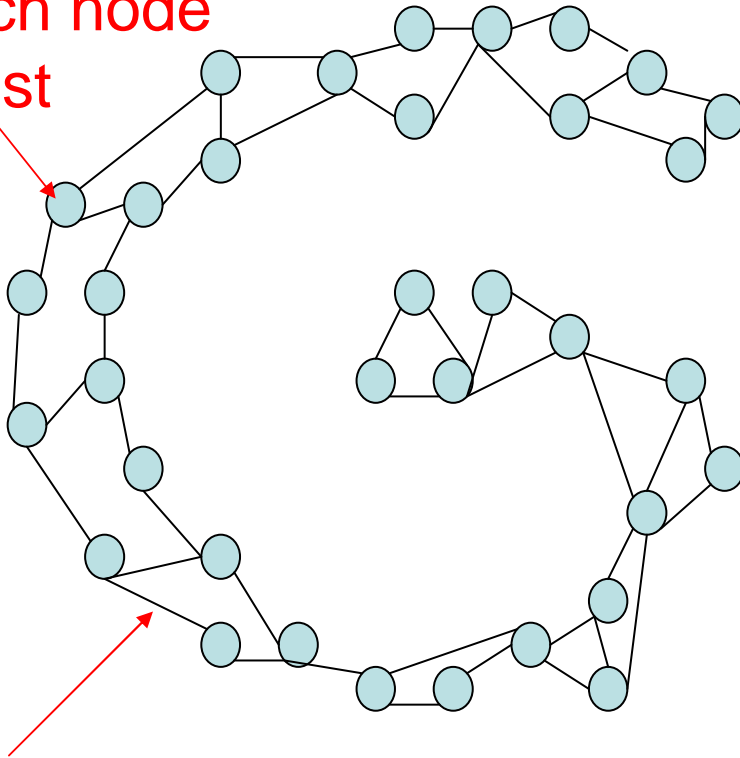
Evaluation in Information Retrieval

1. List Kernel did not give good similarity
2. Feature selection is needed



Summary

1. Each node
is a List



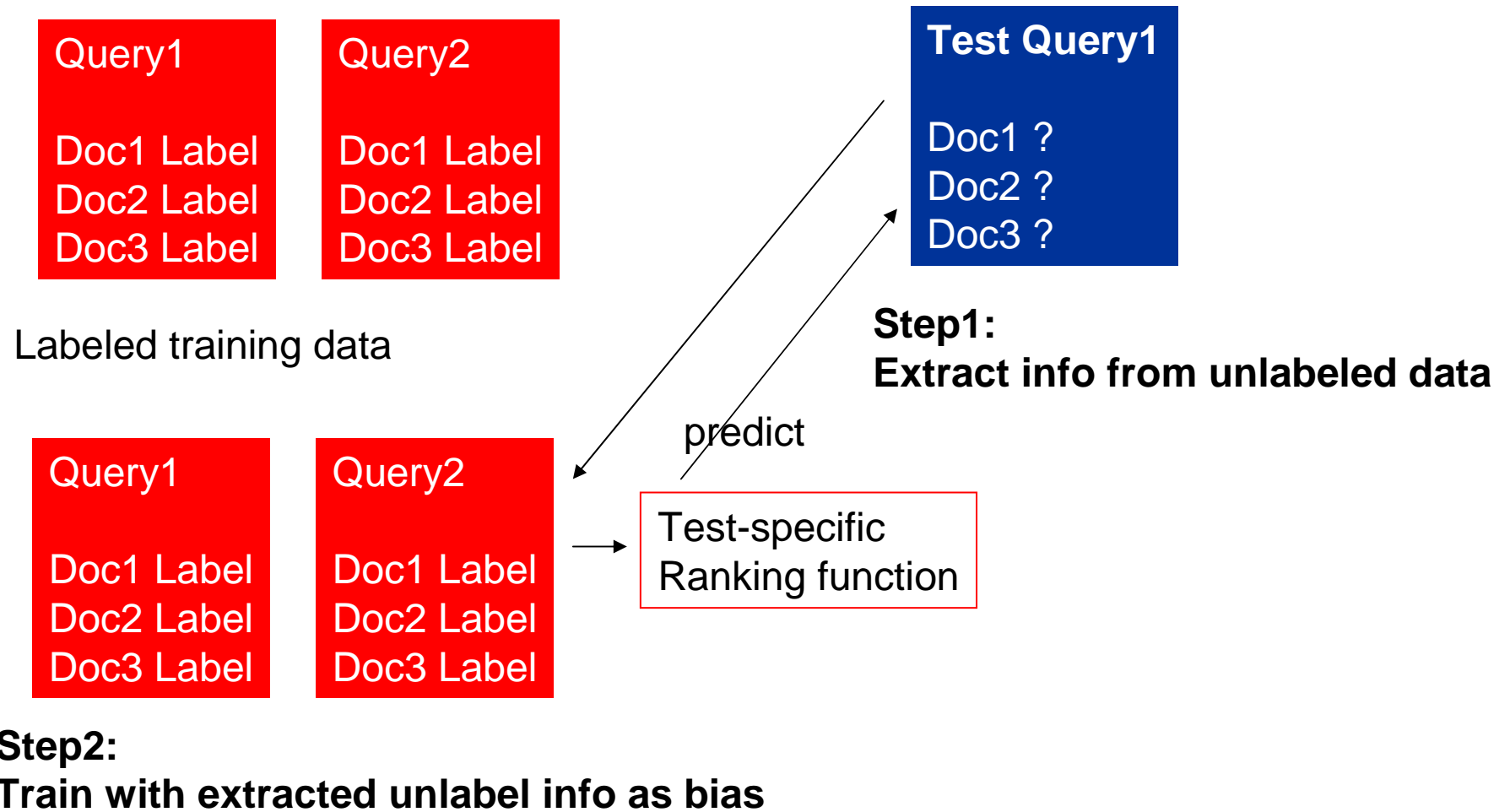
2. Edge similarity = List Kernel

3. Ranker Propagation
computes rankers
that are smooth over manifold

Outline

1. Problem Setup
2. Manifold Assumption
3. Local/Transductive Meta-Algorithm
 1. Change of Representation Assumption
 2. Covariate Shift Assumption
 3. Low Density Separation Assumption
4. Summary

Local/Transductive Meta-Algorithm



Local/Transductive Meta-Algorithm

- **Rationale: Focus only on one unlabeled (test) list each time**
 - Ensure that the information extracted from unlabeled data is directly applicable
- **The name:**
 - Local = ranker is targeted at a single test list
 - Transductive = training doesn't start until test data is seen
- **Modularity:**
 - We will plug-in 3 different unlabeled data assumptions

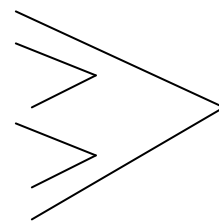
RankBoost [Freund03]

Query: UW

3 $x_1^{(i)} = [tfidf, pagerank, \dots]$

2 $x_2^{(i)} = [tfidf, pagerank, \dots]$

1 $x_3^{(i)} = [tfidf, pagerank, \dots]$



Objective: maximize pairwise accuracy

$$F(x_1^{(i)}) > F(x_2^{(i)})$$

$$F(x_2^{(i)}) > F(x_3^{(i)})$$

$$F(x_1^{(i)}) > F(x_3^{(i)})$$

Initialize distribution over pairs $D_0(p, q) \forall x_p$ ranked-above x_q

For $t=1..T$

Train weak ranker h_t to maximize $D_t(p, q) \cdot \mathbf{I}_{\{F(x_p) > F(x_q)\}}$

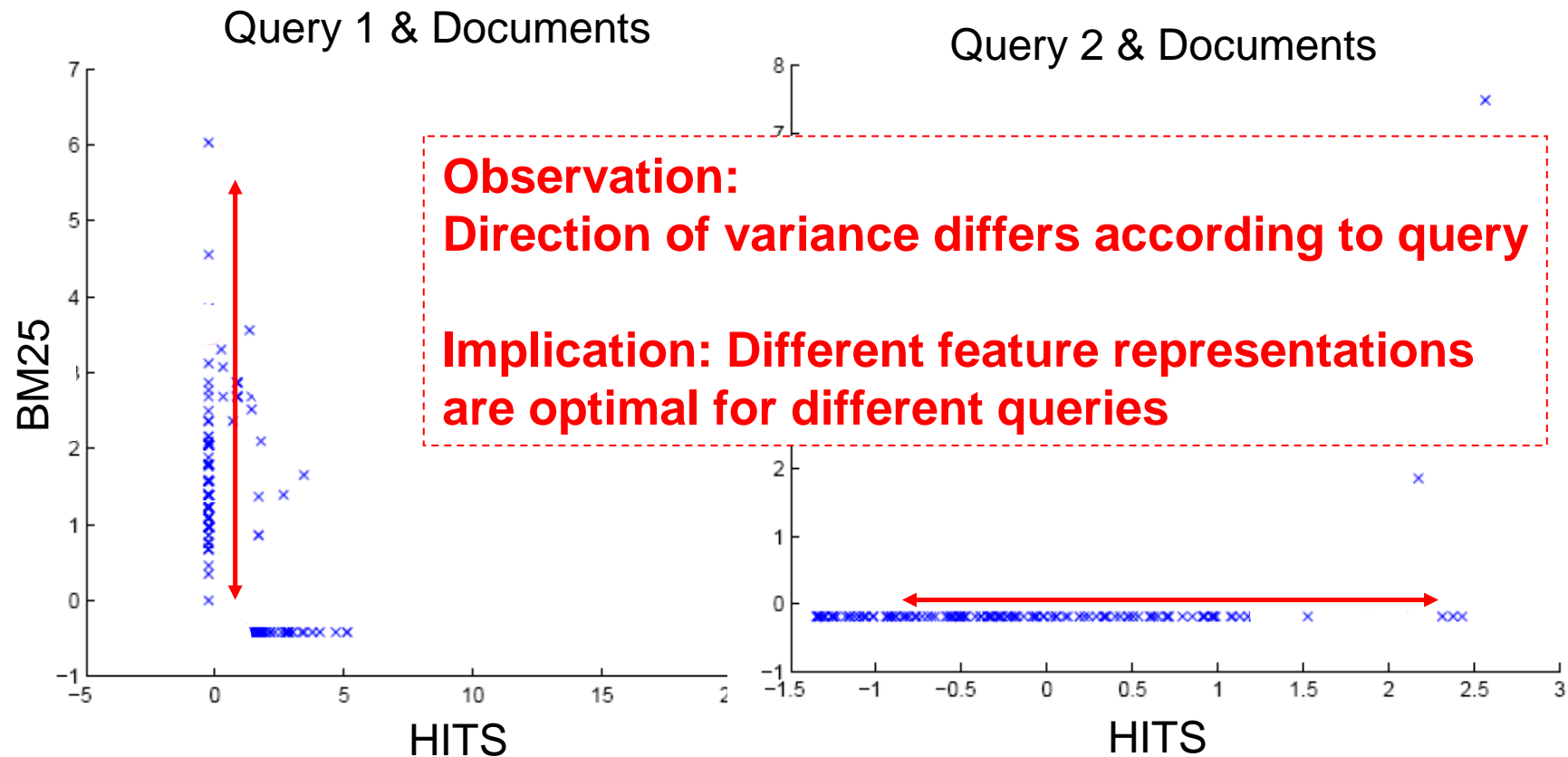
Update distribution $D_{t+1}(p, q) = D_t(p, q) \exp\{\alpha_t (h_t(x_p) - h_t(x_q))\}$

Final ranker

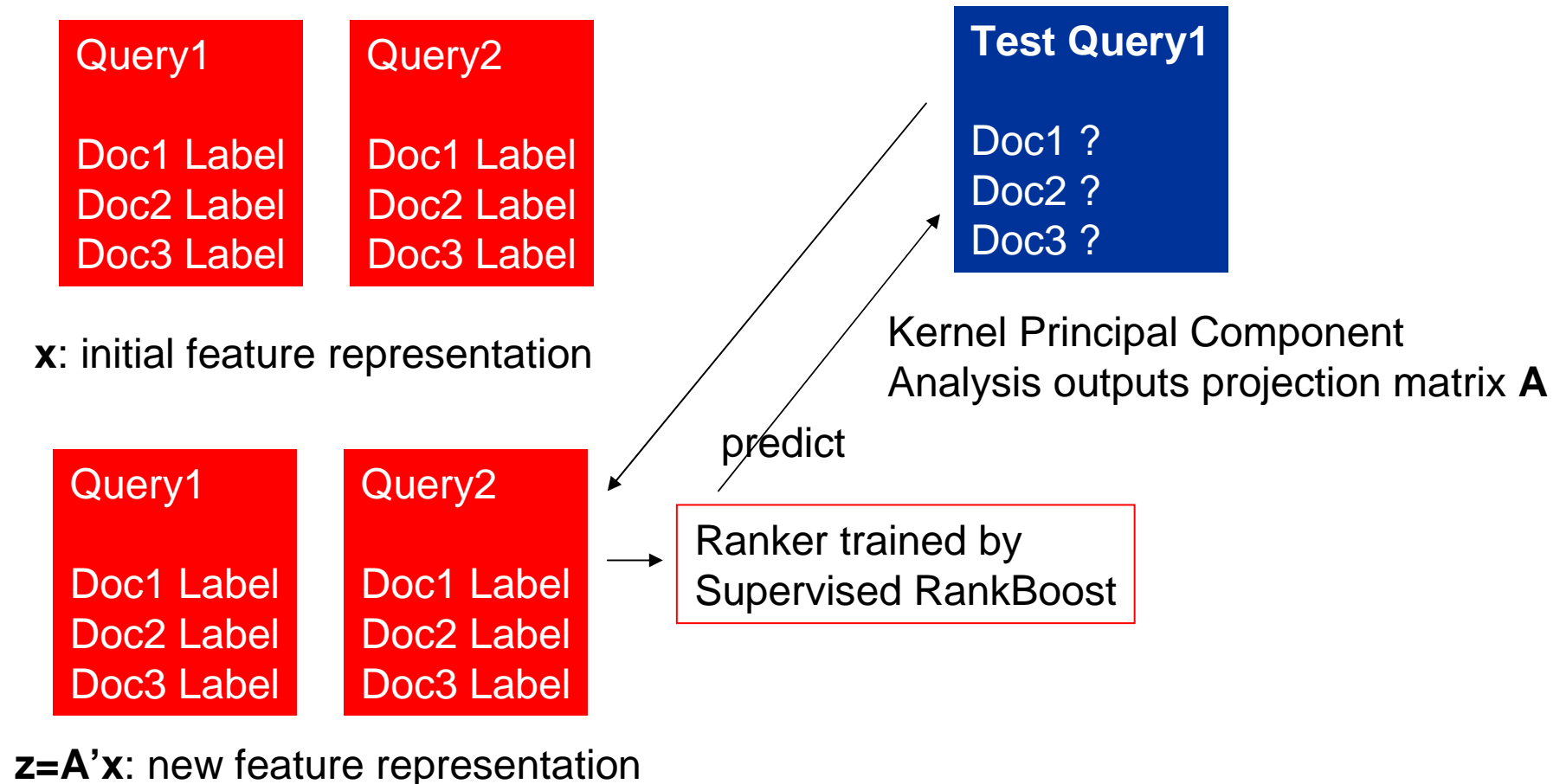
$$F(x) = \sum_{t=1}^T \alpha_t h_t(x)$$

Change of Representation Assumption

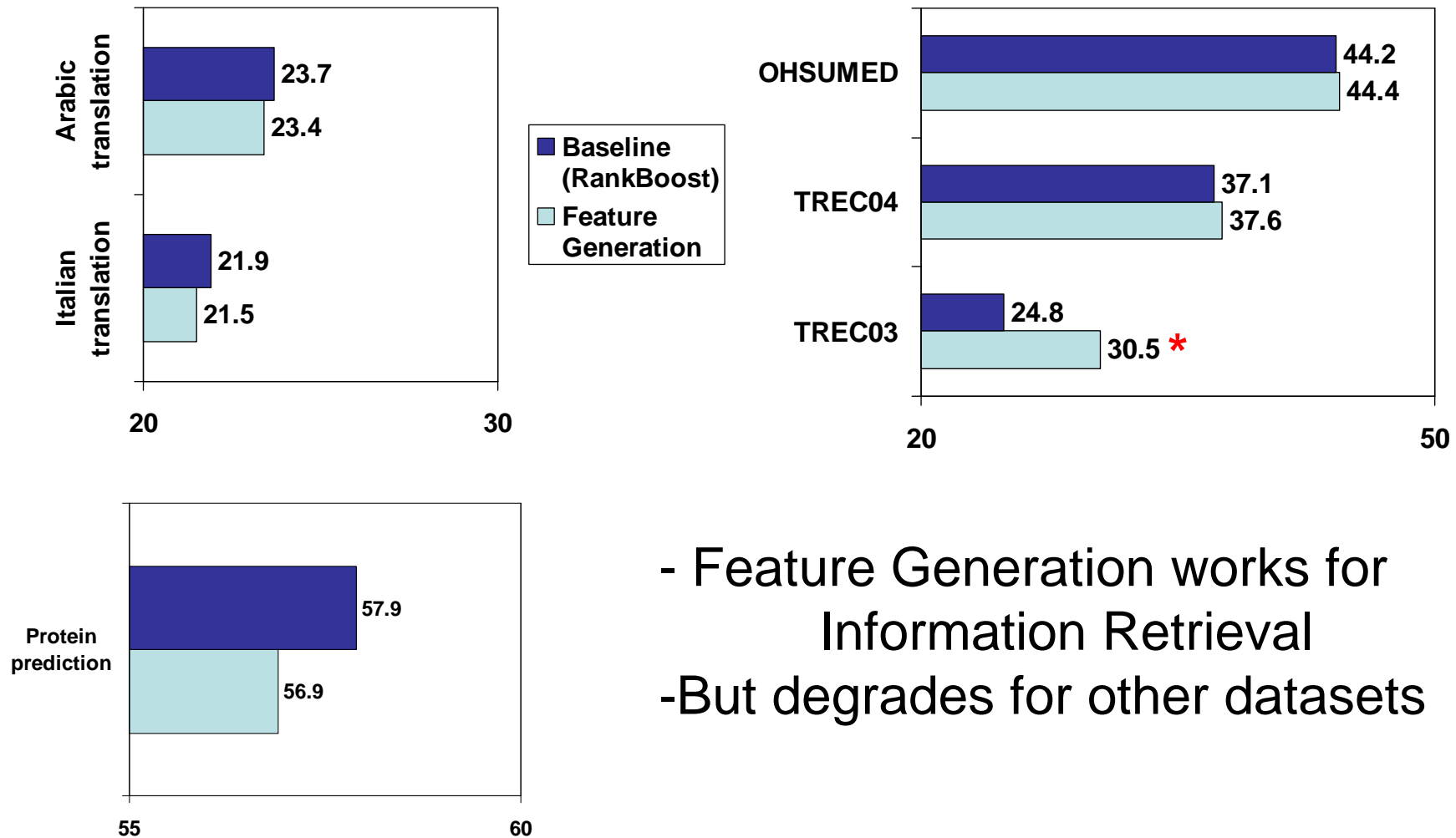
“Unlabeled data can help discover better feature representation”



Feature Generation Method



Evaluation (Feature Generation)



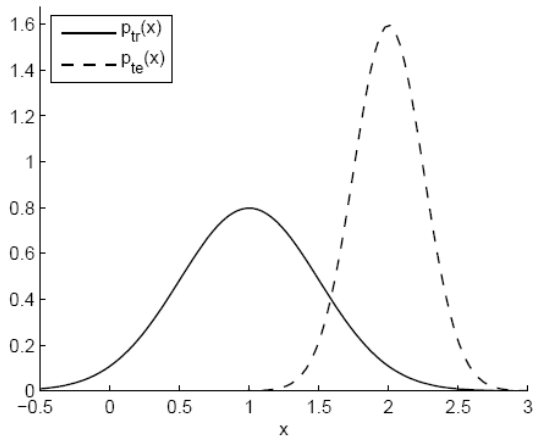
- Feature Generation works for Information Retrieval
-But degrades for other datasets

Analysis: Why didn't it work for Machine Translation?

- 40% of weights are for Kernel PCA features
 - Pairwise Training accuracy actually improves:
 - 82% (baseline) → 85% (Feature Generation)
- We're increasing the model space *and* optimizing on the wrong loss function
- Feature Generation more appropriate if pairwise accuracy correlates with evaluation metric

Covariate Shift Assumption in Classification (Domain Adaptation)

If training & test distributions differ in marginals $p(x)$,
optimize on weighted data to reduce bias



$$F_{ERM} = \arg \min_F \frac{1}{n} \sum_{i=1}^n Loss(F, x_i, y_i)$$

$$F_{IW} = \arg \min_F \frac{1}{n} \sum_{i=1}^n \frac{p_{test}(x_i)}{p_{train}(x_i)} Loss(F, x_i, y_i)$$

KLIEP method [Sugiyama08] for generating importance weights r

$$\min_r KL(p_{test}(x) || r(x)p_{train}(x))$$

Covariate Shift Assumption in Ranking

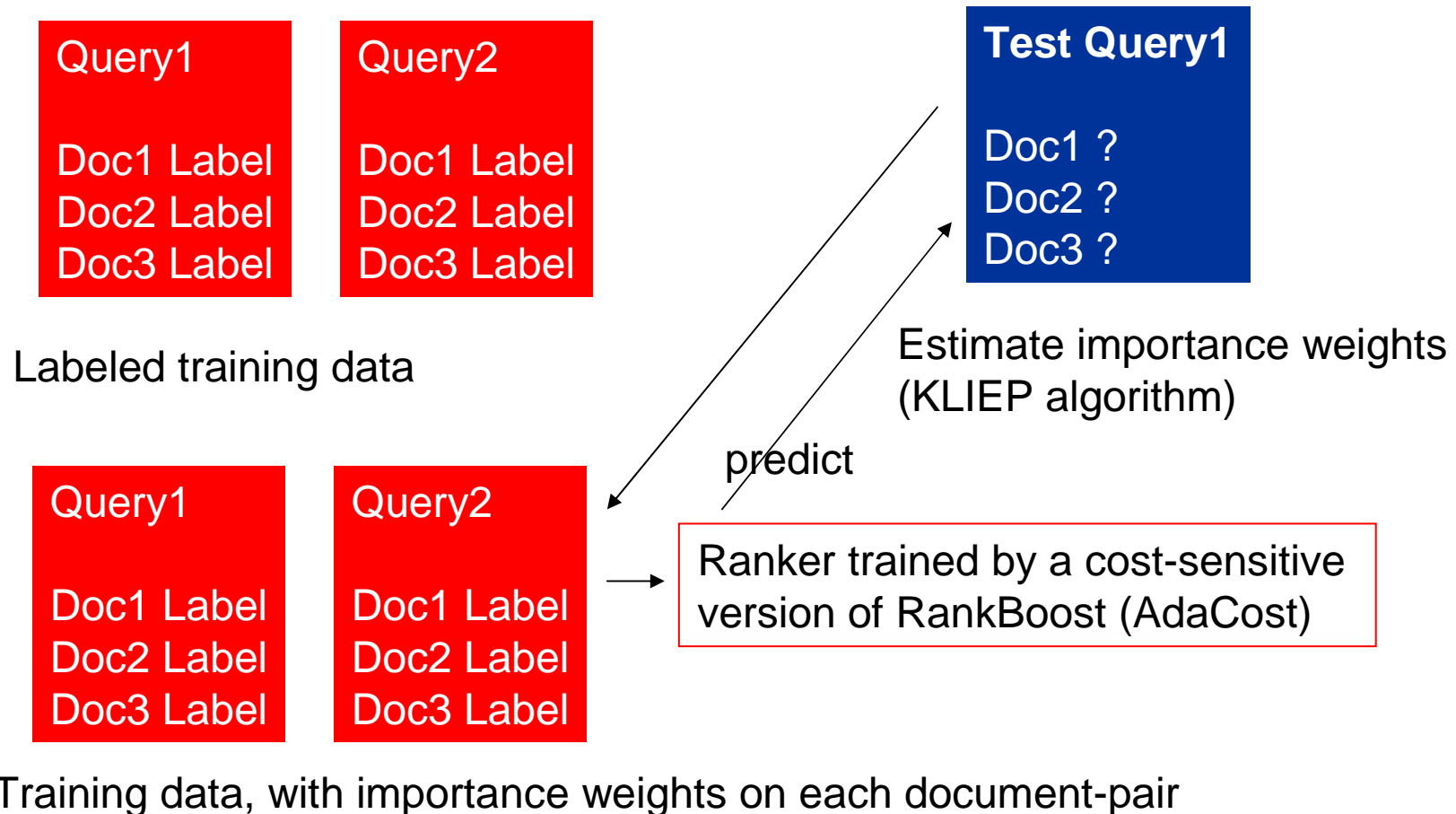
- Each test list is a “different domain”
- Optimize **weighted** pairwise accuracy

$$\begin{array}{l} \mathbf{3} \quad x_1^{(i)} = [\text{tfidf}, \text{pagerank}, \dots] \\ \mathbf{2} \quad x_2^{(i)} = [\text{tfidf}, \text{pagerank}, \dots] \\ \mathbf{1} \quad x_3^{(i)} = [\text{tfidf}, \text{pagerank}, \dots] \end{array} \begin{array}{c} \diagup \\ \diagdown \\ \diagup \\ \diagdown \\ \diagup \\ \diagdown \end{array} \begin{array}{l} F(x_1^{(i)}) > F(x_2^{(i)}) \\ F(x_2^{(i)}) > F(x_3^{(i)}) \\ F(x_1^{(i)}) > F(x_3^{(i)}) \end{array}$$

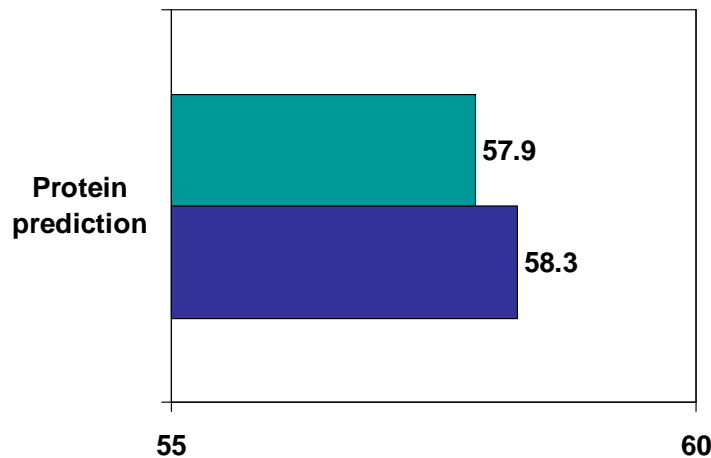
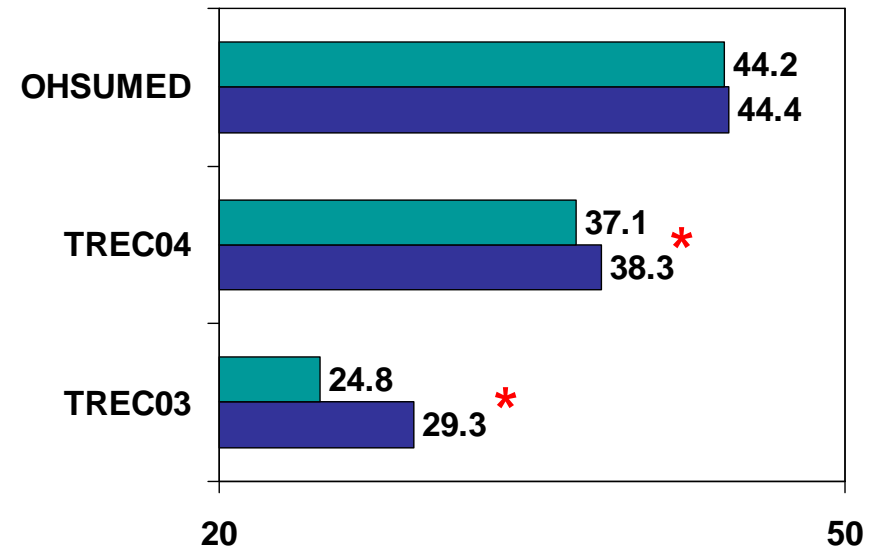
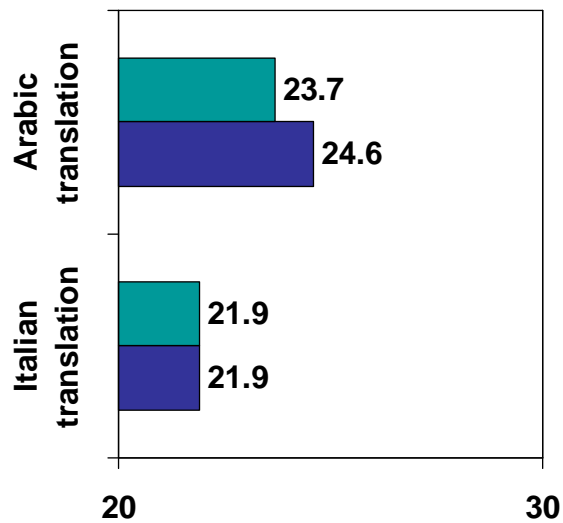
- Define density on pairs

$$p_{\text{train}}(x) \rightarrow p_{\text{train}}(s) \quad s = x_p^{(i)} - x_q^{(i)}$$

Importance Weighting Method



Evaluation (Importance Weighting)



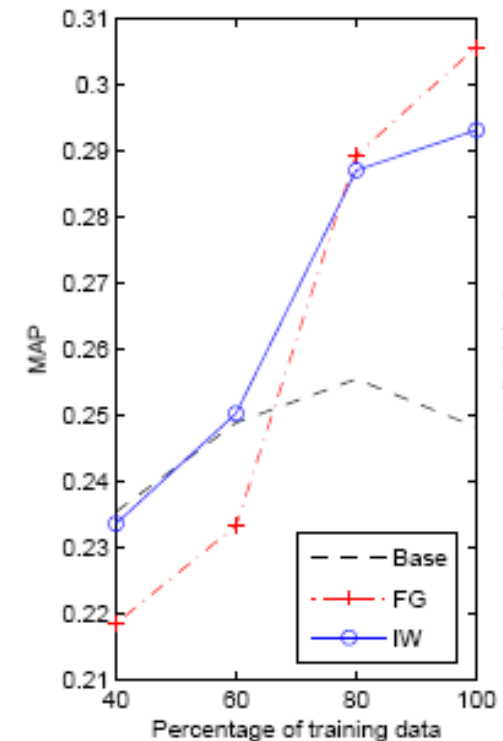
Importance Weighting is a stable method that improves or equals Baseline

Stability Analysis

How many lists are improved/degraded by the method?
Importance Weighting is most conservative
and rarely degrades in low data scenario

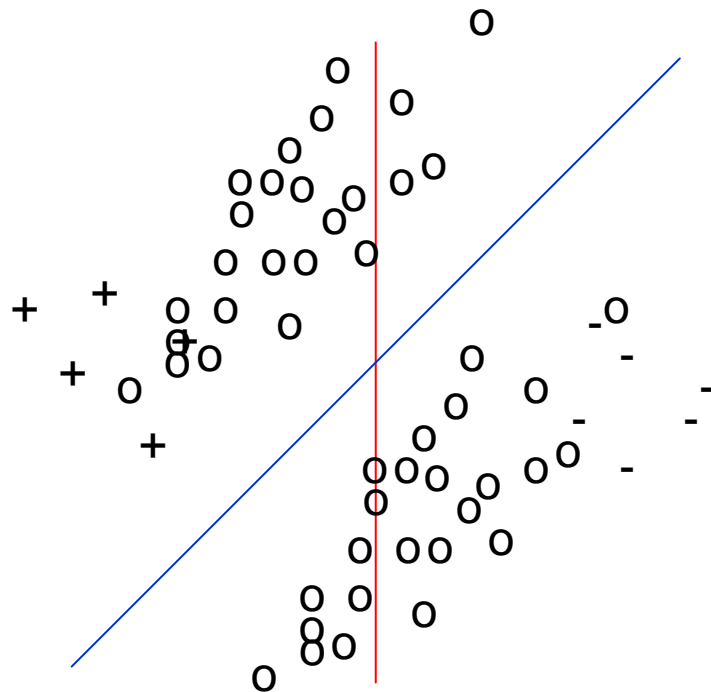
PROTEIN PREDICTION	% lists changed
Importance Weighting	32%
Feature Generation	45%
Pseudo Margin (next)	70%

TREC'03 Data Ablation



Low Density Separation Assumption in Classification

Classifier cuts through low density region,
revealed by clusters of data



Algorithms:

Transductive SVM [Joachim'99]

Boosting with Pseudo-Margin [Bennett'02]

$$\min \sum_{i \in \text{labeled}} \exp(-y_i F(x_i)) + \sum_{i \in \text{unlabeled}} \exp(-|F(x_i)|)$$

margin=
"distance"
to hyperplane

pseudo margin=
distance to hyperplane
assuming correct prediction

Low Density Separation in Ranking

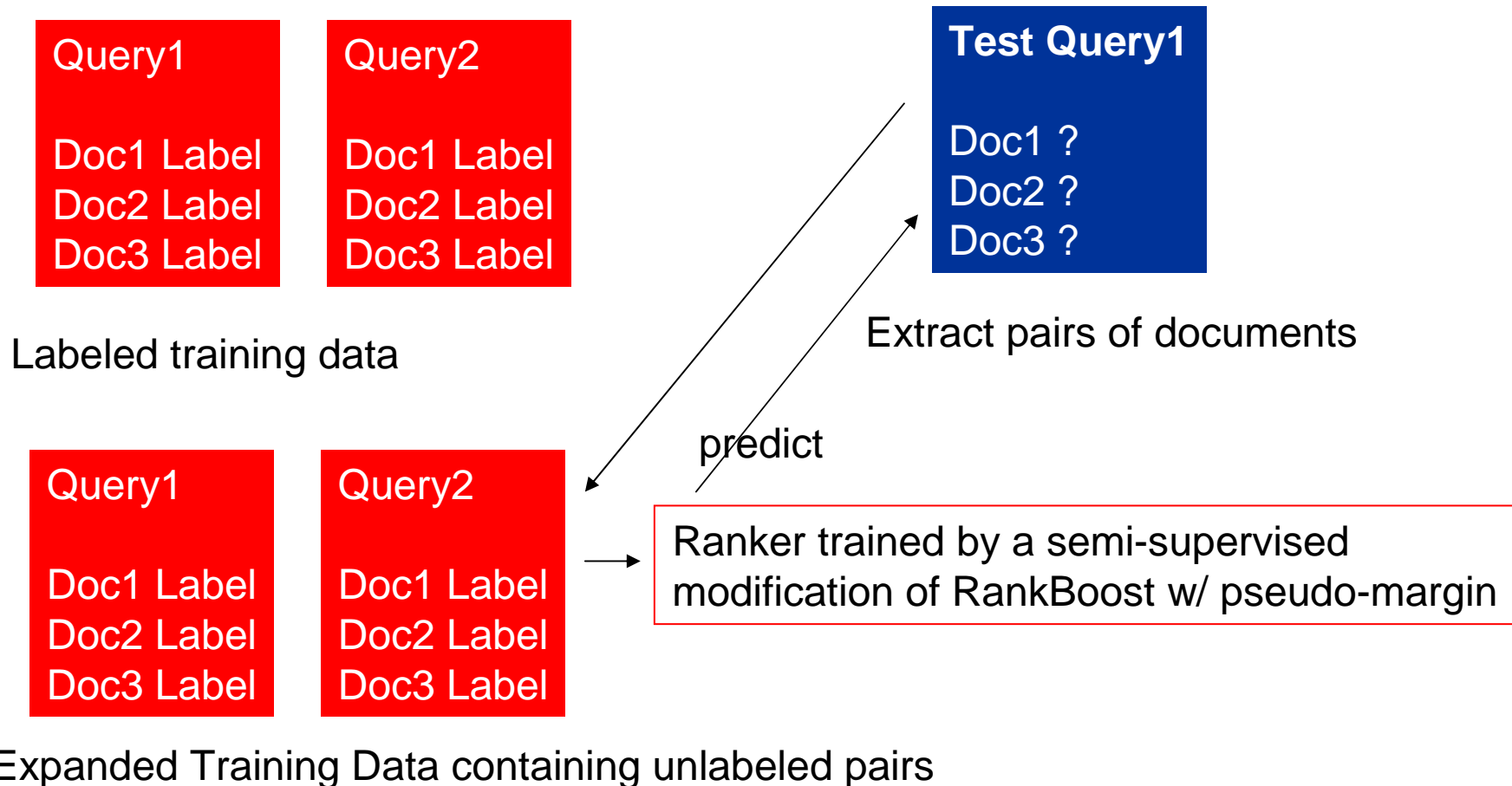
Test Query1

Doc1 ?
Doc2 ?
Doc3 ?

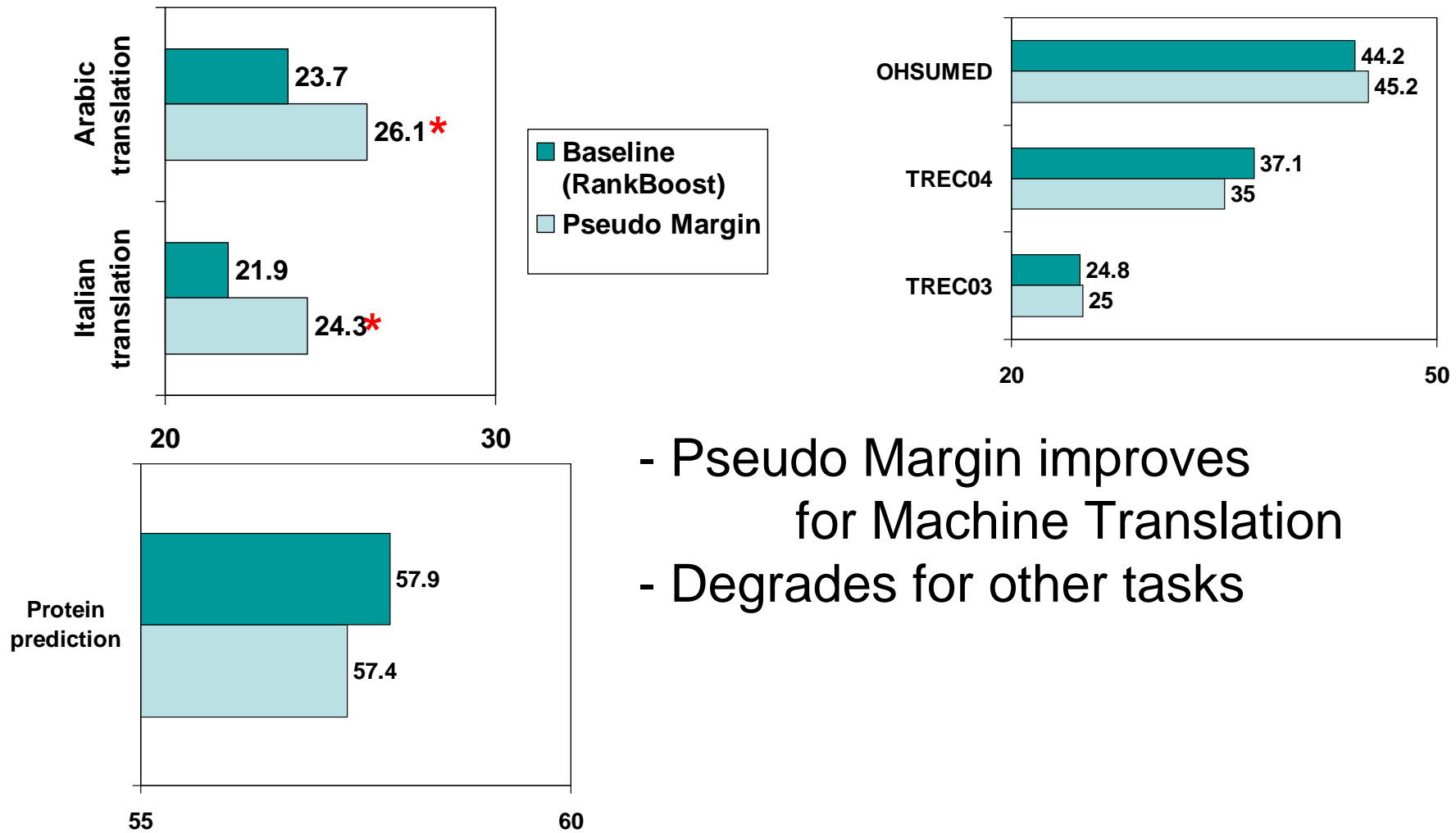
- 1 vs 2: $F(\text{Doc1}) \gg F(\text{Doc2})$ or $F(\text{Doc2}) \gg F(\text{Doc1})$
- 2 vs 3: $F(\text{Doc2}) \gg F(\text{Doc3})$ or $F(\text{Doc3}) \gg F(\text{Doc2})$
- 1 vs 3: $F(\text{Doc1}) \gg F(\text{Doc3})$ or $F(\text{Doc3}) \gg F(\text{Doc1})$
- Define Pseudo-Margin on unlabeled document pairs

$$\sum_{(i,j) \in \text{labeled}} \exp(-(F(x_i) - F(x_j))) + \sum_{(i,j) \in \text{unlabeled}} \exp(-|F(x_i) - F(x_j)|)$$

Pseudo Margin Method



Evaluation (Pseudo Margin)



- Pseudo Margin improves for Machine Translation
- Degrades for other tasks

Analysis: Tied Ranks and Low Density Separation

Test Query1

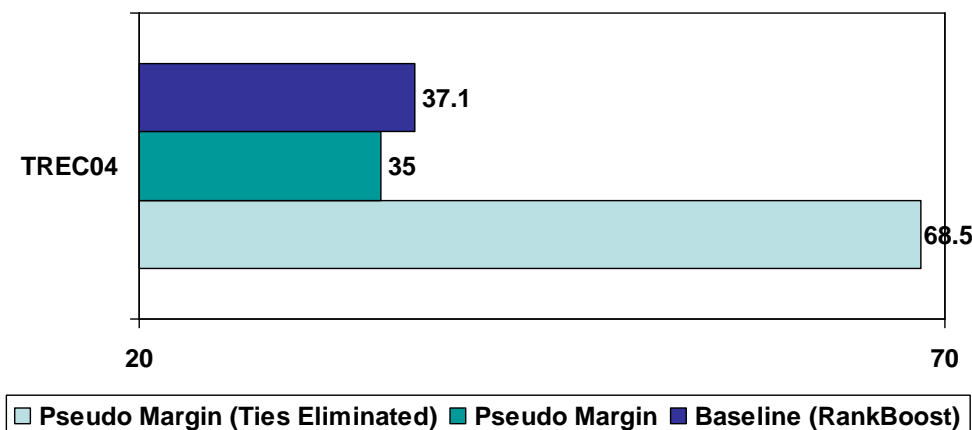
Doc1 ?

Doc2 ?

Doc3 ?

- 1 vs 2: $F(\text{Doc1}) \gg F(\text{Doc2})$ or $F(\text{Doc2}) \gg F(\text{Doc1})$
- Ignores the case $F(\text{Doc1}) = F(\text{Doc2})$

- But most documents are tied in Information Retrieval!
- If tied pairs are eliminated from semi-cheating experiment, Pseudo Margin improves drastically



Outline

1. Problem Setup
2. Investigating the Manifold Assumption
3. Local/Transductive Meta-Algorithm
 1. Change of Representation Assumption
 2. Covariate Shift Assumption
 3. Low Density Separation Assumption
4. Summary

Contribution 1

Investigated 4 assumptions on how unlabeled data helps ranking

- Ranker Propagation:
 - assumes ranker **vary smoothly over manifold** on lists
- Feature Generation method:
 - use on unlabeled test data to **learn better features**
- Importance Weighting method:
 - select training data to **match the test list's distribution**
- Pseudo Margin method:
 - assumes **rank differences are large** for unlabeled pairs

Contribution 2

Comparison on 3 applications, 6 datasets

	Information Retrieval	Machine Translation	Protein Prediction
Ranker Propagation	=	IMPROVE	BEST
Feature Generation	IMPROVE	DEGRADE	=
Importance Weighting	BEST	=	=
Pseudo Margin	=	BEST	=

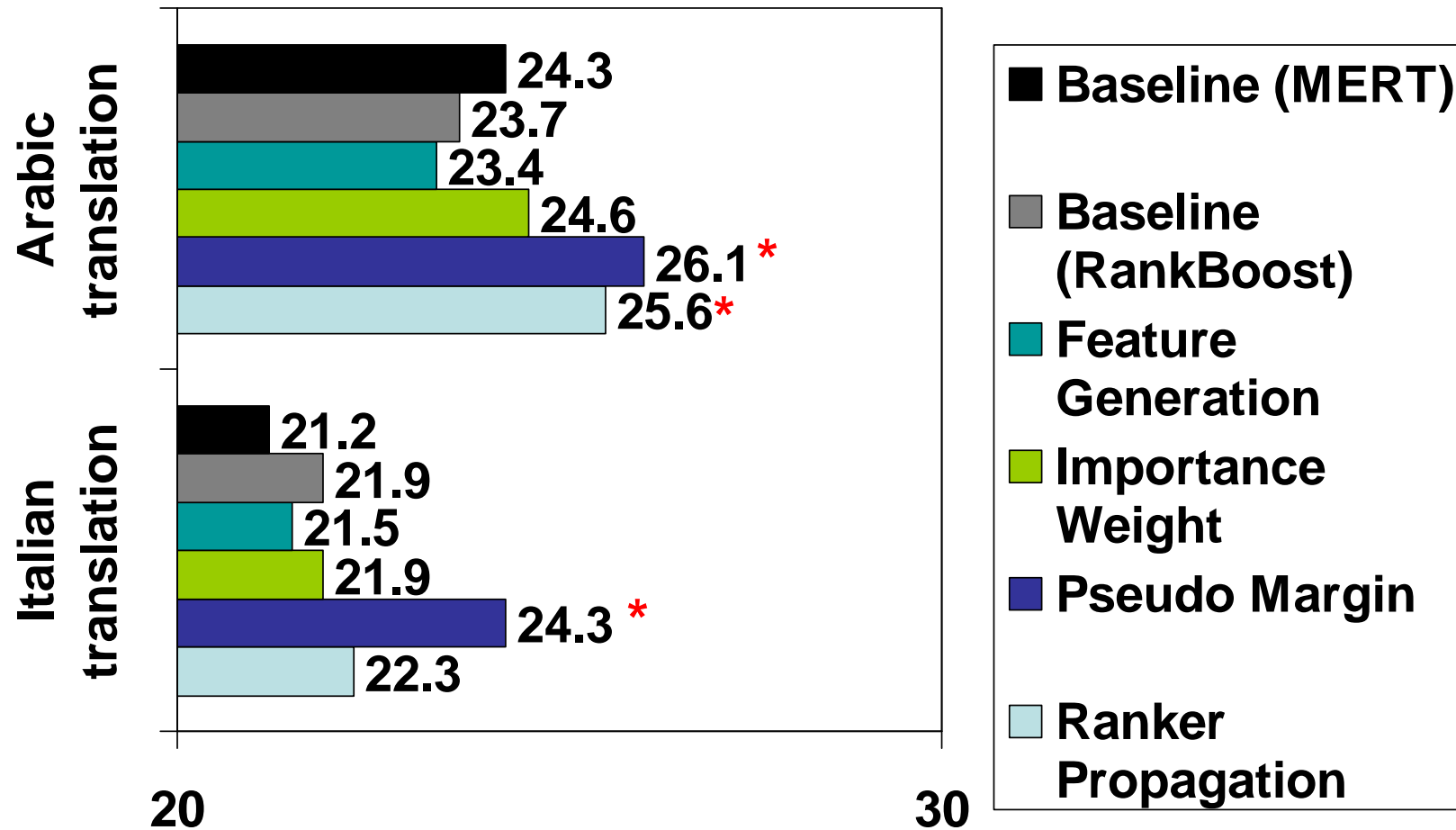
Future Directions

- Semi-supervised ranking works! Many future directions are worth exploring:
 - Ranker Propagation with Nonlinear Rankers
 - Different kinds of List Kernels
 - Speed up Local/Transductive Meta-Algorithm
 - Inductive semi-supervised ranking algorithms
 - Statistical learning theory for proposed methods

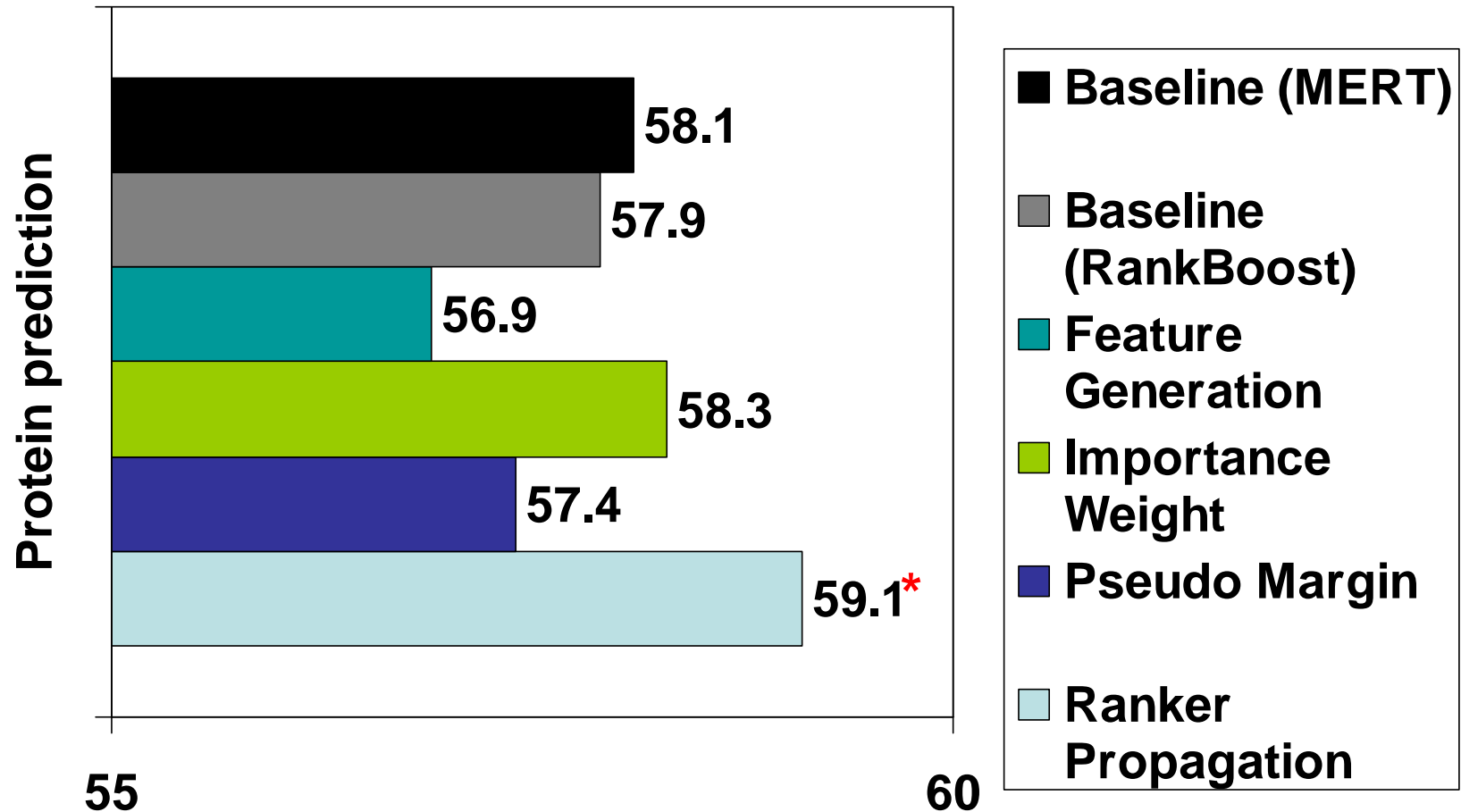
Thanks for your attention!

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 - NSF Graduate Fellowship (2005-2008)
 - RA support from my advisor's NSF Grant IIS-0326276 (2004-2005) and NSF Grant IIS-0812435 (2008-2009)
- Related publications:
 - Duh & Kirchhoff, *Learning to Rank with Partially-Labeled Data*, ACM SIGIR Conference, 2008
 - Duh & Kirchhoff, *Semi-supervised Ranking for Document Retrieval*, under journal review

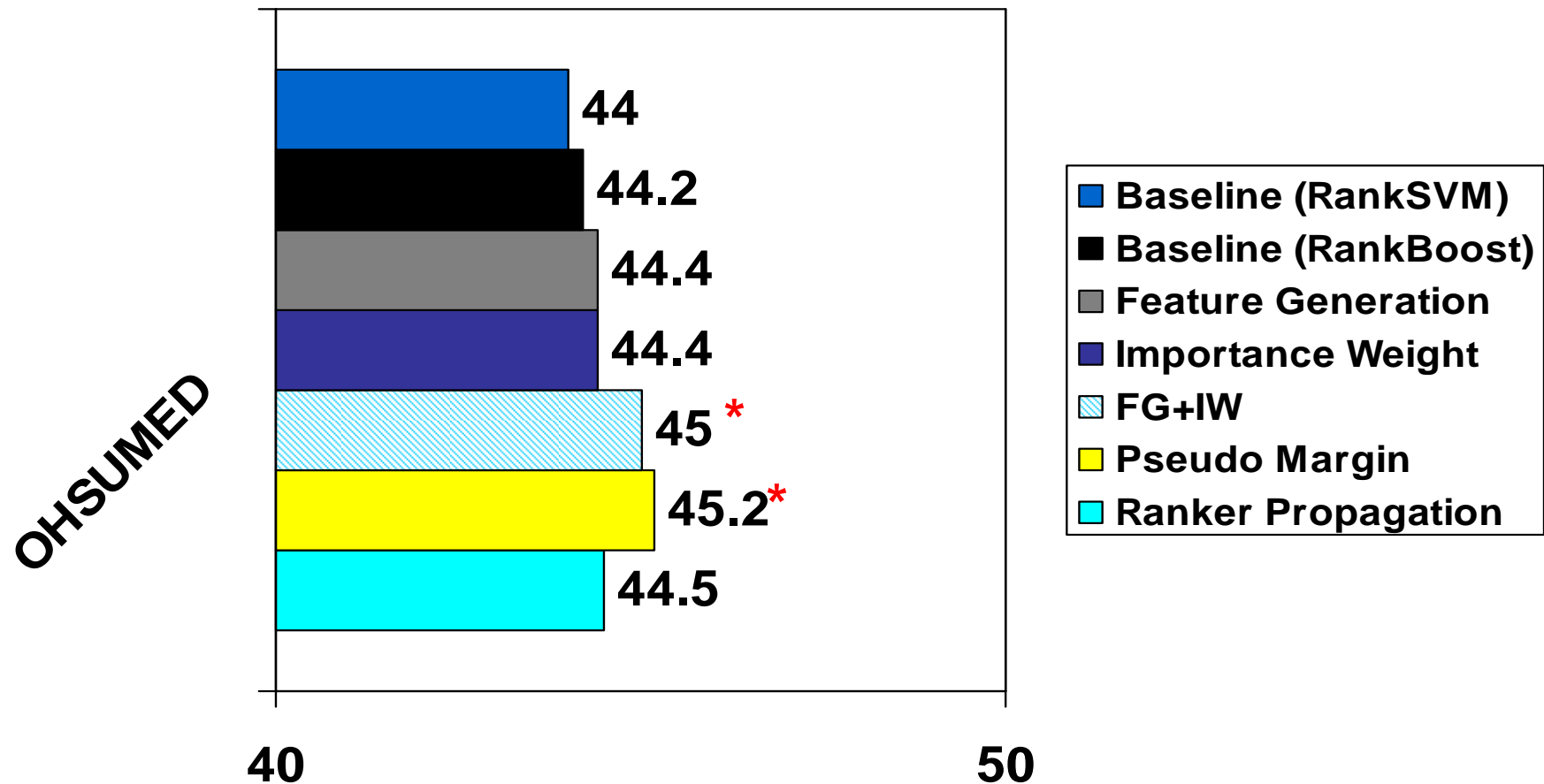
Machine Translation: Overall Results



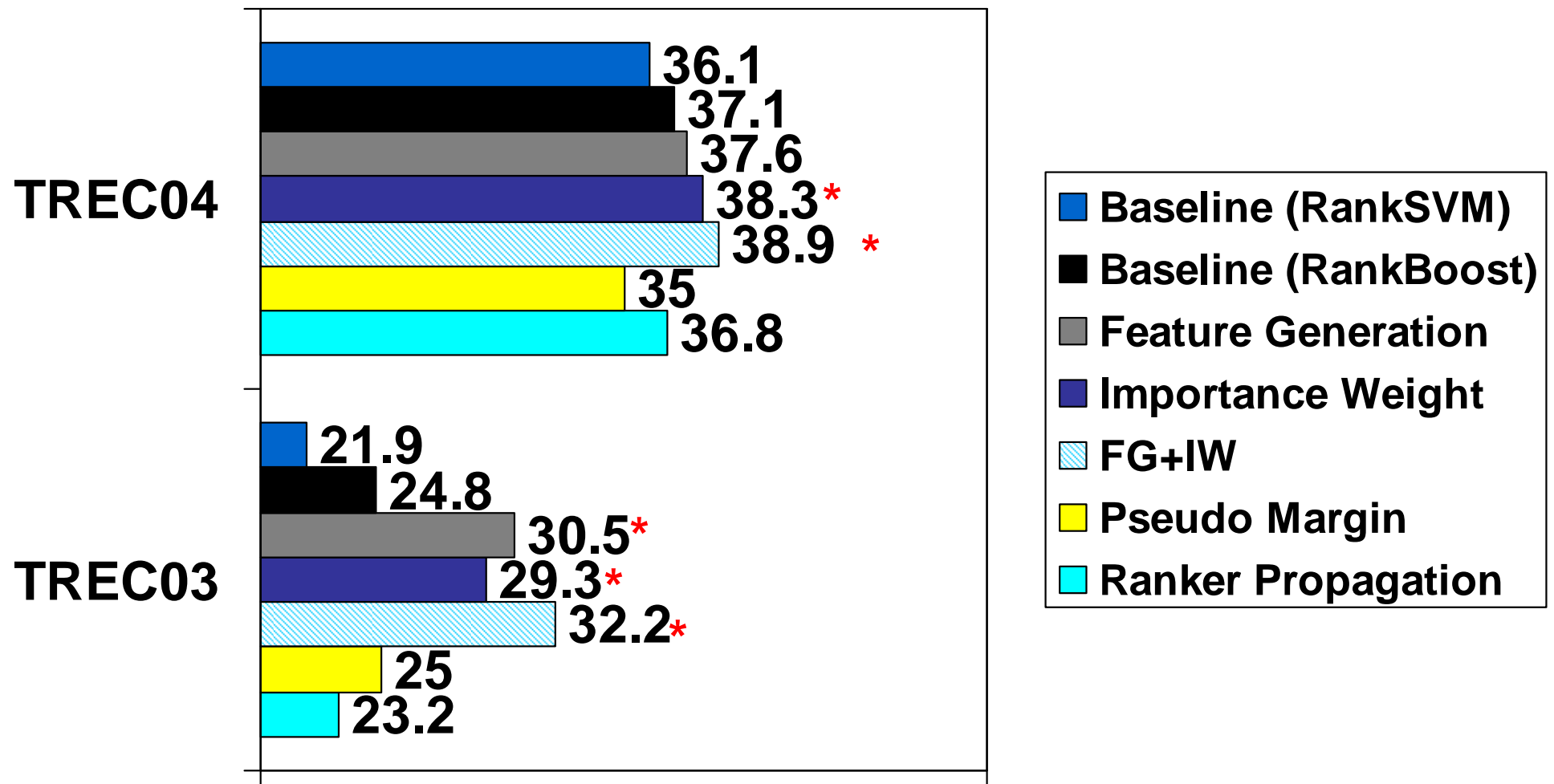
Protein Prediction: Overall Results



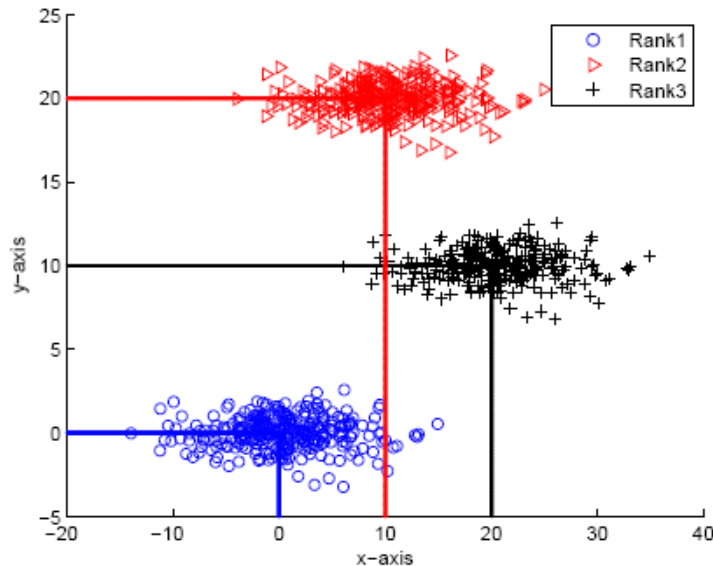
OHSUMED: Overall Results



TREC: Overall Results



Supervised Feature Extraction for Ranking



Linear Discriminant Analysis (LDA)

$$\arg \max_{\alpha} \frac{\alpha^T B \alpha}{\alpha^T W \alpha}$$

B: between-class scatter

W: within-class scatter

RankLDA $\arg \max_{\alpha} \frac{\alpha^T \tilde{B} \alpha}{\alpha^T W \alpha}$

s.t. $\alpha^T B_{13} \alpha > \alpha^T B_{12} \alpha$

$$\alpha^T B_{13} \alpha > \alpha^T B_{23} \alpha$$

OHSUMED

Baseline: 44.2

Feature Generation: 44.4

w/ RankLDA: 44.8

KLIEP Optimization

$$\begin{aligned}KL(p_{test}(x) // w(x) * p_{train}(x)) &= \int p_{test}(x) \log \frac{p_{test}(x)}{w(x) * p_{train}(x)} dx \\ &= \int p_{test}(x) \log \frac{p_{test}(x)}{p_{train}(x)} dx - \int p_{test}(x) \log w(x) dx \\ \mathcal{O}_{KLIEP} &= \int p_{test}(x) \log w(x) dx \\ &\approx \frac{1}{U_{pair}} \sum_{u=1}^{U_{pair}} \log w(x_u) \\ &= \frac{1}{U_{pair}} \sum_{u=1}^{U_{pair}} \log \sum_{b=1}^B \beta_b \psi_b(x_u)\end{aligned}$$

constraints that $\beta \geq 0$

$$1 = \int w(x) p_{train}(x) dx \approx \frac{1}{L_{pair}} \sum_{x=1}^{L_{pair}} \sum_b^B \beta_b \psi(x_l)$$

List Kernel Proof: Symmetricity

Proposition 8.3.1. *The function $K(x,y)$ in Algorithm 10 is symmetric, i.e. $K(x,y) = K(y,x)$.*

Proof.

$$\begin{aligned} K(x,y) &= \frac{\sum_{m=1}^M \lambda_x^m \lambda_y^{a(m)} \cdot | \langle u_x^m, u_y^{a(m)} \rangle |}{(\|\lambda_x\| \cdot \|\lambda_y\|)} \\ &= \frac{\sum_{m=1}^M \lambda_y^{a(m)} \lambda_x^m \cdot | \langle u_y^{a(m)}, u_x^m \rangle |}{(\|\lambda_y\| \cdot \|\lambda_x\|)} \\ &= \frac{\sum_{m=1}^M \lambda_y^m \lambda_x^{a^{-1}(m)} \cdot | \langle u_y^m, u_x^{a^{-1}(m)} \rangle |}{(\|\lambda_y\| \cdot \|\lambda_x\|)} \\ &= K(y,x) \end{aligned}$$

List Kernel Proof: Cauchy-Schwartz Inequality

Proposition 8.3.2. *The function $K(x,y)$ in Algorithm 10 satisfies the Cauchy-Schwartz Inequality, i.e. $K(x,y)^2 \leq K(x,x)K(y,y)$.*

Proof. First, we show that $K(x,x) = 1$:

$$\begin{aligned}
 K(x,x) &= \frac{\sum_{m=1}^M \lambda_x^m \lambda_x^{a(m)} \cdot | \langle u_x^m, u_x^{a(m)} \rangle |}{(\|\lambda_x\| \cdot \|\lambda_x\|)} \\
 &= \frac{\sum_{m=1}^M \lambda_x^m \lambda_x^m \cdot | \langle u_x^m, u_x^m \rangle |}{(\|\lambda_x\| \cdot \|\lambda_x\|)} \\
 &= \frac{\sum_{m=1}^M \lambda_x^m \lambda_x^m}{(\|\lambda_x\| \cdot \|\lambda_x\|)} \\
 &= \frac{\|\lambda\|^2}{(\|\lambda_x\| \cdot \|\lambda_x\|)} = 1
 \end{aligned}$$

The second step follows from the fact that maximum bipartite matching would achieve $a(m) = m \forall m$ since $\langle u_x^m, u_x^m \rangle = 1$ and $\langle u_x^m, u_x^{m'} \rangle = 0$ for any $m \neq m'$. The third step is a result of $\langle u_x^m, u_x^m \rangle = 1$.

Next we show that $K(x,y)^2$ is bounded by 1. Note that $\langle u_x^m, u_y^{a(m)} \rangle \leq 1$, so that $K(x,y) \leq \frac{\sum_{m=1}^M \lambda_x^m \lambda_y^{a(m)}}{(\|\lambda_x\| \cdot \|\lambda_y\|)} \leq 1$ where the last inequality follows from applying Cauchy-Schwartz to the vectors of

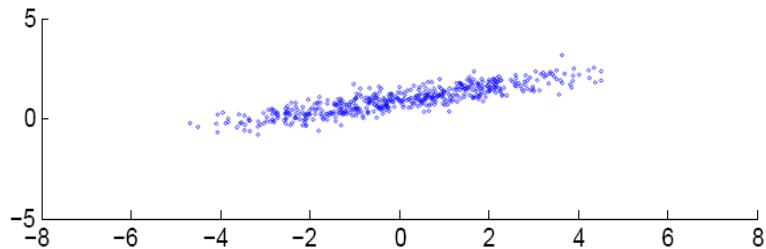
List Kernel Proof: Mercer's Theorem

Theorem 8.3.3 (Mercer's Theorem, c.f. [123]). *Every positive (semi) definite, symmetric function is a kernel: i.e., there exists a feature mapping ϕ such that it is possible to write: $K(x,y) = \langle \phi(x), \phi(y) \rangle$.*

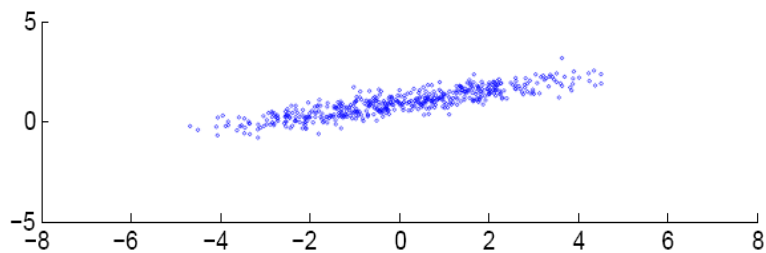
Proposition 8.3.4. *The function $K(x,y)$ in Algorithm 10 satisfies the Mercer Theorem.*

Proof. We have already proved that $K(x,y)$ is symmetric. To see that it is positive semi-definite, we just need to observe that $K(x,y) \geq 0$ for any x,y . We prove this by contradiction: Suppose $K(x,y) < 0$ for some x,y . This implies that $\sum_{m=1}^M \lambda_x^m \lambda_y^{a(m)} \cdot | \langle u_x^m, u_y^{a(m)} \rangle |$ is negative. However, by construction, we will only obtain non-negative eigenvalues λ_x from PCA. Further, the absolute value operation $| \langle u_x^m, u_y^{a(m)} \rangle |$ ensures non-negativity. Thus, the statement that $K(x,y) < 0$ for some x,y is false. \square

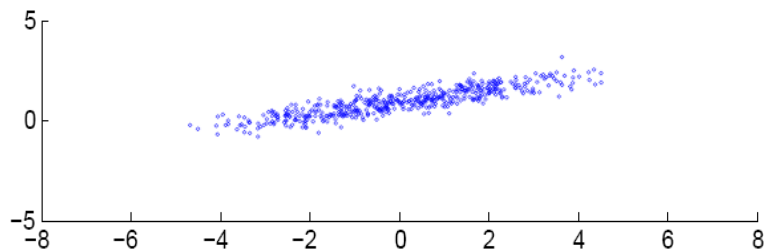
Invariance Properties for Lists



Shift-invariance



Scale-invariance



Rotation-invariance