



Learning to Rank

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These slides have been adapted from Shivani Agarwal's tutorial on "Ranking Methods in Machine Learning"
<https://www.siam.org/meetings/sdm10/tutorial1.pdf>

Ranking SVM

- Assign a rank to an input example
- Apple grading
 - U.S. Extra Fancy
 - U.S. Fancy
 - U.S. No. 1
 - U.S. No. 1 Hail
 - U.S. Utility



If i is 'US Extra fancy' and j is any other category then we want the score of i to be higher than that of j , i.e.,:

$$f(x_i) \geq f(x_j) + 1 - \xi_{ij}$$

These are the constraints in a ranking SVM. The objective function minimizes the sum of slacks and maximizes the margin.

Ranking in Recommendation Systems

Quora

Ask or Search Quora

Ask Question

Read

Answer

Notifications ²

Fayyaz

Feeds

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Top Stories

- Data Science
- Linux
- Programming Languages
- Mathematics
- Technology
- Computer Science
- Computer Programming
- Science
- Python (programming language)
- Data Analysis
- Big Data
- Proteomics
- Structural Biology
- Deep Learning

Popular on Quora

How would the U.S. military react if a U.S. president were to declare himself a dictator?



Balaji Viswanathan, Have been studying US history for a decade.
5.7k Views • Balaji is a Most Viewed Writer in Presidents of the United States.

Power resides where men believe it resides. No more and no less.

-- Game of

Thrones ... (more)

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Comments 3+



Question asked • Academia • 57m

Can a paper get rejected after a major revision?

I submitted a paper in a high I.F. journal as first, and corresponding author. The reviewers gave me a major revisions. I revised the pap... (more)

2 Answers

Answer

Pass

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Popular on Quora

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Ranking in Recommendation Systems

amazon.com Hello, Shivani Agarwal. We have [recommendations](#) for you. (Not Shivani?) FREE 2-Day Shipping: See details

Shivani's Amazon.com | Today's Deals | Gifts & Wish Lists | Gift Cards Your Account | Help

Shop All Departments Search All Departments Cart Wish List

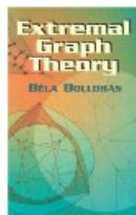
Your Amazon.com | Your Browsing History | Recommended For You | Rate These Items | Improve Your Recommendations | Your Profile | Your Communities | Learn More

Welcome to Your Amazon.com (If you're not Shivani Agarwal, click here.)

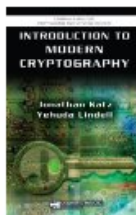
Today's Recommendations For You

Here's a daily sample of items recommended for you. Click here to [see all recommendations](#).

Page 1 of 44



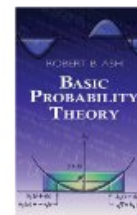
[Extremal Graph Theory](#)
(Paperback) by Béla Bollobás
\$20.42
[Fix this recommendation](#)



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★★★★★ (4) \$68.39
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★★★★★ (3) \$38.70
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★★★★★ (4) \$13.57
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- Ranking of Facebook posts

Ranking in Information Retrieval



The Google logo is centered on the page. It consists of the word "Google" in its signature multi-colored font (blue, red, yellow, blue, green, red) with a trademark symbol (TM) to the upper right. The logo is set against a white background with a faint, large watermark of the PIEAS Biomedical Informatics Research Lab seal in the background.

Google™

A search input field with a thin blue border. It contains the text "pieas" in a black, sans-serif font. The field is positioned below the Google logo and above the search buttons.

pieas

A rectangular button with a thin blue border and a light gray background. It contains the text "Google Search" in a black, sans-serif font.

Google Search

A rectangular button with a thin blue border and a light gray background. It contains the text "I'm Feeling Lucky" in a black, sans-serif font.

I'm Feeling Lucky

Ranking in Information Retrieval

Google search results for "pieas".

Search bar: pieas

Results: About 238,000 results (0.54 seconds)

PIEAS
www.pieas.edu.pk/ ▼
Official Website of Pakistan Institute of Engineering & Applied Sciences (PIEAS), Nilore, Islamabad, Pakistan.
[PhD Programmes - Achievements - Kaleidoscope](#)

Admission Schedule 2016 - PIEAS
www.pieas.edu.pk/red/schedule.cshhtml ▼
Feb 11, 2016 - Admission Schedule 2016. BS Admissions (2016-20) ...

Department of Nuclear Engineering - PIEAS
www.pieas.edu.pk/dne/ ▼
The vision of Department of Nuclear Engineering (DNE) is "to be a vibrant, ...

PIEAS University Islamabad Admission 2016 Last Date and ...
www.vstudents.org/education/pieas-university-admission/ ▼
Admissions are open in Pakistan institute of engineering & applied sciences (PIEAS) by its academic officials to brighten the future of enrolled candidates. This is ...

Pakistan Institute of Engineering and Applied Sciences ...
https://en.wikipedia.org/.../Pakistan_Institute_of_Engineering_and_Appli... ▼

Pakistan Institute of Engineering and Applied Sciences ★
Public university in Nilore, Islamabad, Pakistan
[Website](#) [Directions](#)

The Pakistan Institute of Engineering and Applied Sciences, is a public research university located in the Islamabad, Pakistan, near the remote town of Nilore. [Wikipedia](#)

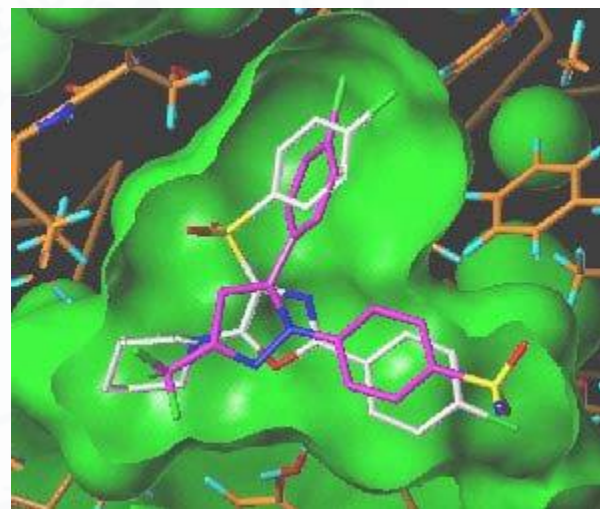
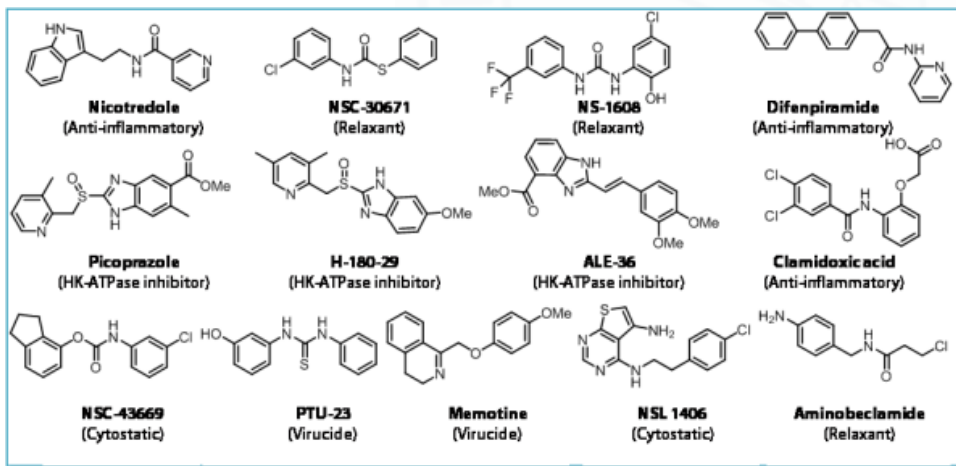
Address: Nilore



The image shows a Google search results page for the query "pieas". The search bar at the top contains the text "pieas". Below the search bar, there are tabs for "All", "Images", "News", "Videos", "More", and "Search tools". The "All" tab is selected. The search results show "About 238,000 results (0.54 seconds)". The first result is for "PIEAS" with the URL "www.pieas.edu.pk/" and a description: "Official Website of Pakistan Institute of Engineering & Applied Sciences (PIEAS), Nilore, Islamabad, Pakistan." Below this are links for "PhD Programmes - Achievements - Kaleidoscope", "Admission Schedule 2016 - PIEAS", "Department of Nuclear Engineering - PIEAS", "PIEAS University Islamabad Admission 2016 Last Date and ...", and "Pakistan Institute of Engineering and Applied Sciences ...". On the right side of the search results, there is a knowledge panel for "Pakistan Institute of Engineering and Applied Sciences" with a star rating, a "Website" button, and a "Directions" button. The panel also includes a description of the university and its address in Nilore. At the bottom of the page, there is a footer with the text "CIS 621: Machine Learning" and "PIEAS Biomedical Informatics Research Lab".

Ranking in Drug Discovery

- Given: A large number of molecules from a chemical library
- Output: Which one is the most promising?

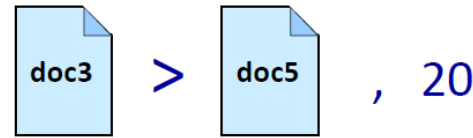
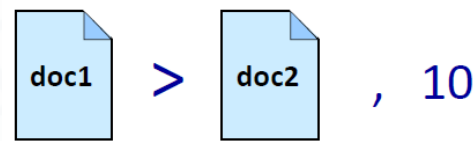


Ranking in Bioinformatics

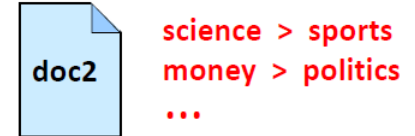
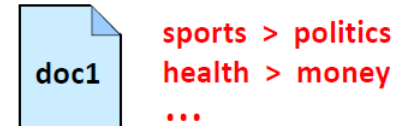
- Gene Discovery
 - Given: A set of genes and their activity in different conditions
 - Required output: What genes are important for a certain condition?

Types of Ranking Problems

- Instance Ranking



Instance Ranking



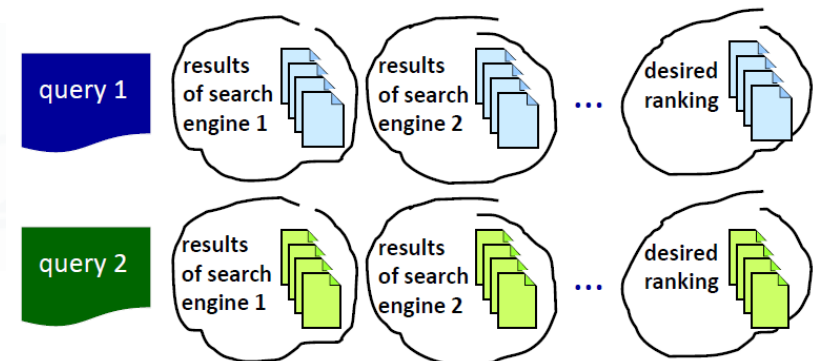
Label Ranking

- Label Ranking

- Subset Ranking



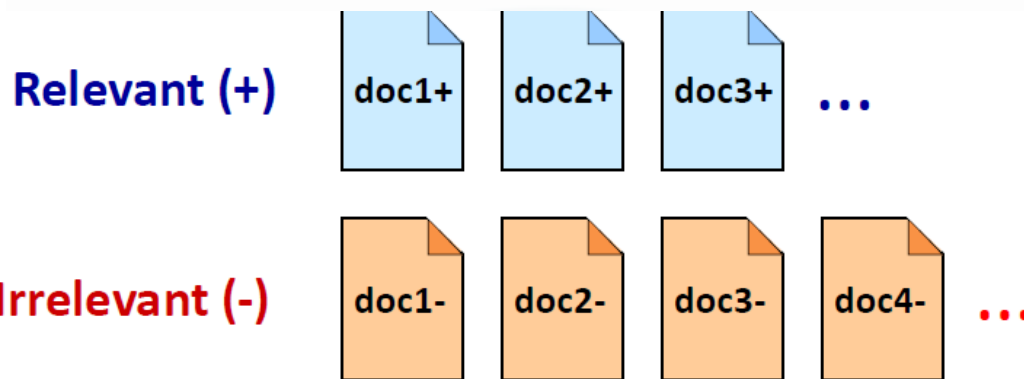
- Rank Aggregation



What we will cover

- Theory for Instance Ranking
 - Bipartite Ranking
 - K-partite Ranking
 - Ranking with Real-Valued Labels
 - General Instance Ranking
 - Properties of ranking methods
 - Ranking vs. Classification vs. Regression
 - AUC-ROC maximization
- Applications
 - Bioinformatics
 - Information Retrieval
- Further Reading and resources
 - Codes, etc.

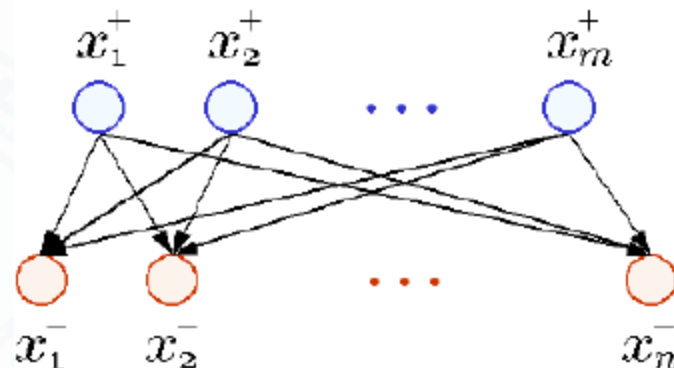
Bipartite Ranking



- Instance space: X
- Input: $S = \{S_+, S_-\}$
 - $S_+ = \{x_1^+, \dots, x_m^+\}$ (positive examples)
 - $S_- = \{x_1^-, \dots, x_n^-\}$ (negative examples)
- Output: Ranking function $f: X \rightarrow \mathbb{R}$
 - Isn't this the same as classification?
 - Or is it more closer to regression?

Bipartite Ranking Function

- In classification we require
 - $f(x) > 0$ for positive examples
 - $f(x) < 0$ for negative examples
- In regression
 - $f(x)$ should be as close as possible to the corresponding output
- The ranking function should be such that
 - $f(x) > f(x')$ if instance x should rank higher than x'
 - Any given positive instance should rank higher than any negative instance



Ranking Error

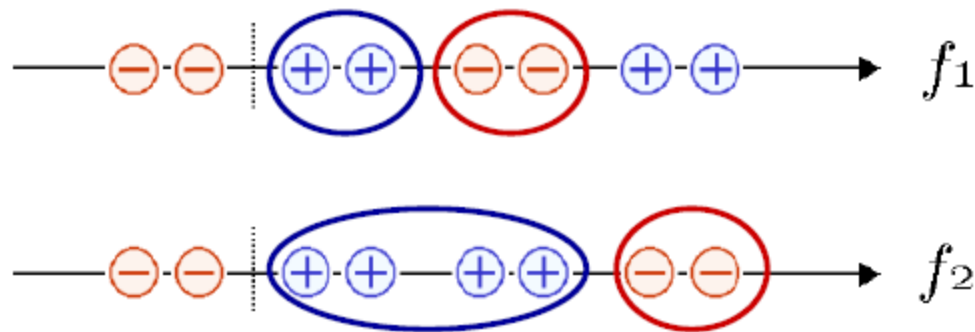
- If we have m positive instances and n negative instances, the number of possible 'pairings' becomes mn
 - Thus, the error for a given ranking function will be given by:

$$\widehat{\mathbf{er}}_S(f) = \frac{1}{mn} \sum_{i=1}^m \sum_{j=1}^n \mathbf{1}(f(x_i^+) < f(x_j^-))$$

Ranking Error

- What will be the classification and ranking errors of the following ranking functions?

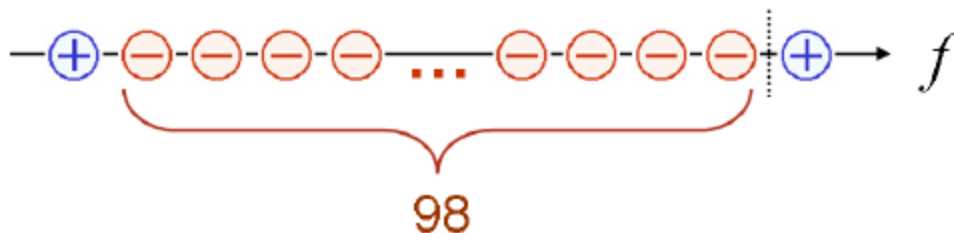
Example 1



Classification error = $\frac{1}{4}$
 Ranking error = $\frac{1}{4}$

Classification error = $\frac{1}{4}$
 Ranking error = $\frac{1}{2}$

Example 2



Classification error = $\frac{1}{100}$
 Ranking error = $\frac{1}{2}$

Ranking with Structured Risk Minimization

- SRM requires

$$f^* = \operatorname{argmin}_f \{ \underbrace{L(X, Y; f)}_{\text{Empirical Loss (or risk) term}} + \underbrace{\lambda g(\|f\|)}_{\text{Regularization Classifier Complexity (smoothing) term}} \}$$

X, Y is the training data
 f is the learning function

Structural Risk

The diagram illustrates the equation for f^* as the minimization of the sum of two terms. A bracket underneath the entire expression is labeled 'Structural Risk'. Two callout boxes point to the individual terms: a red box labeled 'Empirical Loss (or risk) term' points to the $L(X, Y; f)$ term, and a blue box labeled 'Regularization Classifier Complexity (smoothing) term' points to the $\lambda g(\|f\|)$ term.

- For ranking, we know the empirical error can be given by

$$\widehat{\mathbf{er}}_S(f) = \frac{1}{mn} \sum_{i=1}^m \sum_{j=1}^n \mathbf{1}(f(x_i^+) < f(x_j^-))$$

Ranking with SRM

- Find me a ranking function that minimizes the empirical error, possibly with some regularization, over some class of ranking functions
 - Examples: $f(x) = \langle w, x \rangle$
- Mathematically

$$\min_{f \in \mathcal{F}} \left[\frac{1}{mn} \sum_{i=1}^m \sum_{j=1}^n \ell(f, x_i^+, x_j^-) + \lambda N(f) \right]$$

$\ell(f, x_i^+, x_j^-)$: convex upper bound on $\mathbf{1}(f(x_i^+) < f(x_j^-))$

$N(f)$: regularizer

$\lambda > 0$: regularization parameter

$\mathcal{F}$: class of ranking functions

Ranking with SRM

- What should be loss function?
 - The ideal loss function would be:
 - Zero-one loss $\mathbf{1}(f(x_i^+) < f(x_j^-))$
 - Incurs a loss of 1 only if the ranking is not proper
 - Otherwise the loss is zero
 - Problems?
 - » Non-convex
 - » Discontinuous
 - Hinge-Loss

$$\ell_{\text{hinge}}(f, x_i^+, x_j^-) = \left(1 - \left(f(x_i^+) - f(x_j^-)\right)\right)_+ \quad [u_+ = \max(u, 0)]$$

Bipartite RankSVM Algorithm

- Primal

$$\min_w \lambda \|w\|^2 + \frac{1}{mn} \sum_{i=1}^m \sum_{j=1}^n l(x_i^+, x_j^-; w)$$

- Alternatively,

$$\min_{w, \xi > 0} \lambda \|w\|^2 + \frac{1}{mn} \sum_{i=1}^m \sum_{j=1}^n \xi_{ij}$$

Such that, for all $i = 1 \dots m$ and $j = 1 \dots n$

$$f(x_i) \geq f(x_j) + 1 - \xi_{ij}$$

Bipartite RankSVM Algorithm

Introducing Lagrange variables in the primal

$$\{\alpha_{ij} : 1 \leq i \leq m, 1 \leq j \leq n\}$$

we can get the dual optimization problem shown below

$$\min_{\alpha} \left[\frac{1}{2} \sum_{i=1}^m \sum_{j=1}^n \sum_{k=1}^m \sum_{l=1}^n \alpha_{ij} \alpha_{kl} \phi(x_i^+, x_j^-, x_k^+, x_l^-) - \sum_{i=1}^m \sum_{j=1}^n \alpha_{ij} \right]$$

$$\text{subject to } 0 \leq \alpha_{ij} \leq C \quad \forall i, j$$

where

$$\phi(x_i^+, x_j^-, x_k^+, x_l^-) = (K(x_i^+, x_k^+) - K(x_i^+, x_l^-) - K(x_j^-, x_k^+) + K(x_j^-, x_l^-))$$

$$C = \frac{1}{\lambda mn}$$

Can be solved using a standard QP Solver or other methods (Chapelle & Keerthi, 2010)

Other Algorithms

- RankBoost (Freund et al., 2003)
 - Combine outputs of multiple ‘weak’ ranking functions

$$\min_{f \in \mathcal{L}(\mathcal{F}_{\text{base}})} \left[\frac{1}{mn} \sum_{i=1}^m \sum_{j=1}^n \ell_{\text{exp}}(f, x_i^+, x_j^-) \right]$$

$$\ell_{\text{exp}}(f, x_i^+, x_j^-) = \exp \left(- \left(f(x_i^+) - f(x_j^-) \right) \right)$$

$$\mathcal{L}(\mathcal{F}_{\text{base}}) = \text{linear combinations of functions in some base class } \mathcal{F}_{\text{base}}$$

- RankNet (Burges et al, 2005): Neural network

$$\min_{f \in \mathcal{F}_{\text{neural}}} \left[\frac{1}{mn} \sum_{i=1}^m \sum_{j=1}^n \ell_{\text{logistic}}(f, x_i^+, x_j^-) \right]$$

$$\ell_{\text{logistic}}(f, x_i^+, x_j^-) = \log \left(1 + \exp \left(- \left(f(x_i^+) - f(x_j^-) \right) \right) \right)$$

$$\mathcal{F}_{\text{neural}} = \text{functions represented by some class of neural networks}$$

K-partite ranking

Input: Training sample $S = (S_1, S_2, \dots, S_k)$:

$S_k = (x_1^k, \dots, x_{n_k}^k) \in X^{n_k}$ (examples of rating k)

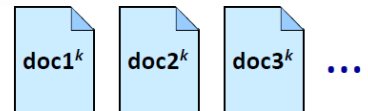
$\vdots$

$S_2 = (x_1^2, \dots, x_{n_2}^2) \in X^{n_2}$ (examples of rating 2)

$S_1 = (x_1^1, \dots, x_{n_1}^1) \in X^{n_1}$ (examples of rating 1)

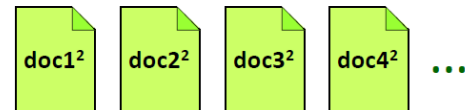
Output: Ranking function $f : X \rightarrow \mathbb{R}$

Rating k

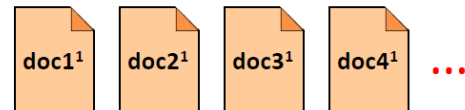


$\vdots$

Rating 2



Rating 1



Empirical error:

$$\widehat{\mathbf{er}}_S(f) = \left(\frac{1}{\sum_{1 \leq a < b \leq k} n_a n_b} \right) \sum_{1 \leq a < b \leq k} \sum_{i=1}^{n_b} \sum_{j=1}^{n_a} (b - a) \mathbf{1}(f(x_i^b) < f(x_j^a))$$

K-partite Ranking with SRM

Minimize a convex upper bound on the empirical ranking error, possibly with some regularization, over some class of ranking functions:

$$\min_{f \in \mathcal{F}} \left[\left(\frac{1}{\sum_{1 \leq a < b \leq k} n_a n_b} \right) \sum_{1 \leq a < b \leq k} \sum_{i=1}^{n_b} \sum_{j=1}^{n_a} \ell(f, x_i^b, x_j^a, (b-a)) + \lambda N(f) \right]$$

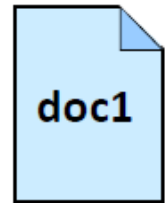
where

- $\ell(f, x_i^b, x_j^a, (b-a))$: convex upper bound on $(b-a) \mathbf{1}(f(x_i^b) < f(x_j^a))$
- $N(f)$: regularizer
- $\lambda > 0$: regularization parameter
- $\mathcal{F}$: class of ranking functions

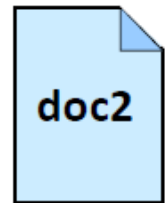
Ranking with Real-Valued Labels

- ▶ Instance space X
- ▶ Real-valued labels $Y = \mathbb{R}$
- ▶ **Input:** Training sample $S = ((x_1, y_1), \dots, (x_m, y_m)) \in (X \times \mathbb{R})^m$
- ▶ **Output:** Ranking function $f : X \rightarrow \mathbb{R}$
- ▶ Empirical error:

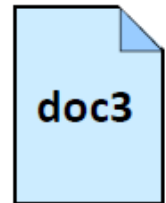
$$\widehat{\mathbf{er}}_S(f) = \frac{1}{\binom{m}{2}} \sum_{1 \leq i < j \leq m} |y_i - y_j| \mathbf{1} \left((y_i - y_j)(f(x_i) - f(x_j)) < 0 \right)$$



y_1



y_2



y_3

...

Real-Valued Ranking with SRM

Minimize a convex upper bound on the empirical ranking error, possibly with some regularization, over some class of ranking functions:

$$\min_{f \in \mathcal{F}} \left[\frac{1}{\binom{m}{2}} \sum_{1 \leq i < j \leq m} \ell(f, (x_i, y_i), (x_j, y_j)) + \lambda N(f) \right]$$

where

- $\ell(f, (x_i, y_i), (x_j, y_j))$: convex upper bound on
 $|y_i - y_j| \mathbf{1} \left((y_i - y_j)(f(x_i) - f(x_j)) < 0 \right)$
- $N(f)$: regularizer
- $\lambda > 0$: regularization parameter
- $\mathcal{F}$: class of ranking functions

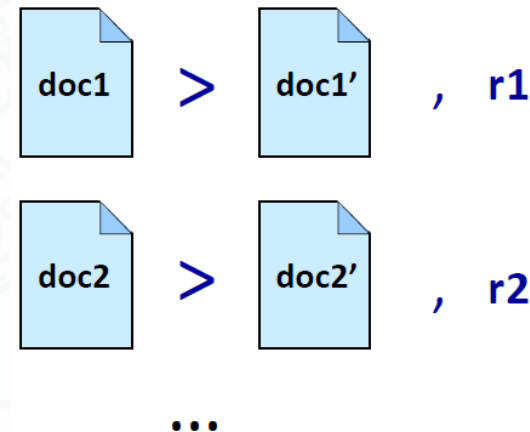
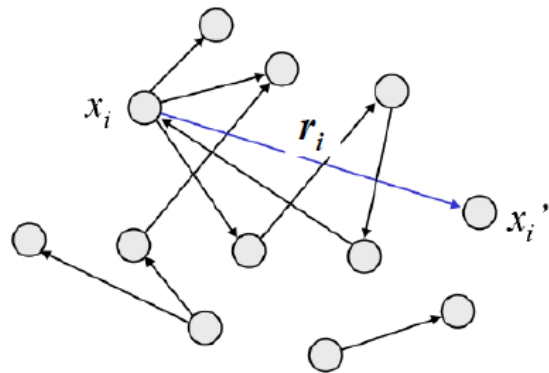
Generalized Instance Ranking

- Each example is paired with another example and the difference between their ranks is given during training

► Instance space X

► **Input:** Training sample $S = ((x_1, x'_1, r_1), \dots, (x_m, x'_m, r_m)) \in (X^2 \times \mathbb{R}_+)^m$

► **Output:** Ranking function $f : X \rightarrow \mathbb{R}$



► Empirical error: $\widehat{\text{er}}_S(f) = \frac{1}{m} \sum_{i=1}^m r_i \mathbf{1}(f(x_i) < f(x'_i))$

Generalized Instance Ranking with SRM

Minimize a convex upper bound on the empirical ranking error, possibly with some regularization, over some class of ranking functions:

$$\min_{f \in \mathcal{F}} \left[\frac{1}{m} \sum_{i=1}^m \ell(f, x_i, x'_i, r_i) + \lambda N(f) \right]$$

where

- $\ell(f, x_i, x'_i, r_i)$: convex upper bound on $r_i \mathbf{1}(f(x_i) < f(x'_i))$
- $N(f)$: regularizer
- $\lambda > 0$: regularization parameter
- $\mathcal{F}$: class of ranking functions

General RankSVM

$$\min_{f \in \mathcal{F}_K} \left[\frac{1}{m} \sum_{i=1}^m \ell_{\text{hinge}}(f, x_i, x'_i, r_i) + \frac{\lambda}{2} \|f\|_K^2 \right]$$

$$\ell_{\text{hinge}}(f, x_i, x'_i, r_i) = \left(r_i - (f(x_i) - f(x'_i)) \right)_+ \quad [u_+ = \max(u, 0)]$$

$\mathcal{F}_K$ = reproducing kernel Hilbert space (RKHS)
with kernel function K

$$N(f) = \frac{\|f\|_K^2}{2}$$

[Herbrich et al, 2000; Joachims, 2002]

SVMRank Tools



SVM^{rank}



Support Vector Machine for Ranking

Author: [Thorsten Joachims <thorsten@joachims.org>](mailto:thorsten@joachims.org)
[Cornell University](#)
[Department of Computer Science](#)

Version: 1.00
Date: 21.03.2009

Overview

SVM^{rank} is an instance of *SVM^{struct}* for efficiently training Ranking SVMs as defined in [Joachims, 2002c]. *SVM^{rank}* solves the same optimization problem as *SVM^{light}* with the '-z p' option, but it is much faster. On the LETOR 3.0 dataset it takes about a second to train on any of the folds and datasets. The algorithm for solving the quadratic program is a straightforward extension of the ROC-area optimization algorithm described in [Joachims, 2006] for multiple rankings using the one-slack formulation of *SVM^{struct}*. However, since I did not want to spend more than an afternoon on coding *SVM^{rank}*, I only implemented a simple separation oracle that is quadratic in the number of items in each ranking (not the $O[k \cdot \log k]$ separation oracle described in [Joachims, 2006]). While this makes the implementation not very suitable for the special case of ordinal regression [Herbrich et al, 1999], it means that it is nevertheless fast for small rankings (i.e. $k < 1000$) and scales linearly in the number of rankings (i.e. queries).

Source Code

The program is free for scientific use. Please contact me, if you are planning to use the software for commercial purposes. The software must not be further distributed without prior permission of the author. If you use *SVM^{rank}* in your scientific work, please cite as

- T. Joachims, *Training Linear SVMs in Linear Time*, Proceedings of the ACM Conference on Knowledge Discovery and Data Mining (KDD), 2006. [\[Postscript \(gz\)\]](#) [\[PDF\]](#)

The implementation was developed on Linux with gcc, but compiles also on Solaris, Cygwin, Windows (using MinGW) and Mac (after small modifications, see [FAQ](#)). The source code is available at the following location:

http://download.joachims.org/svm_rank/current/svm_rank.tar.gz

https://www.cs.cornell.edu/people/tj/svm_light/svm_rank.html

<https://sourceforge.net/p/lemur/wiki/RankLib/> (Java)

<http://fa.bianp.net/blog/2012/learning-to-rank-with-scikit-learn-the-pairwise-transform/>

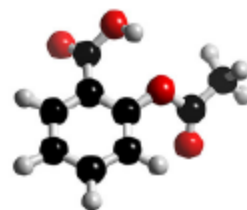
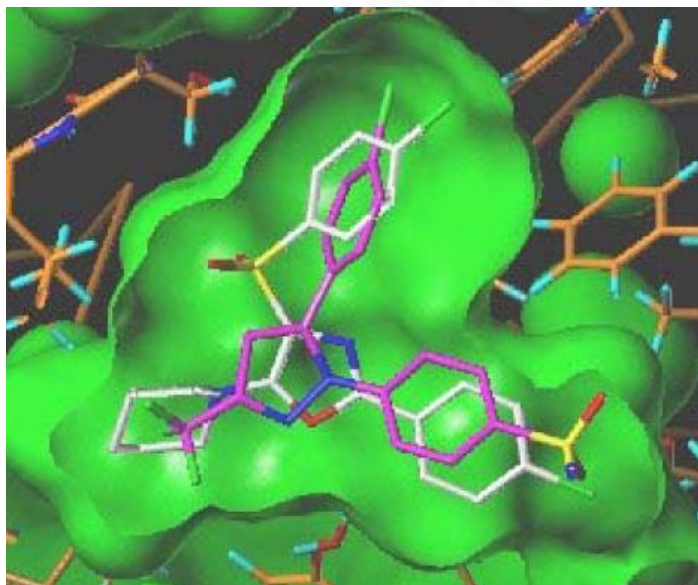
<http://faculty.pieas.edu.pk/fayyaz/studpro.html#pylemmings-a-software-suite-for-multiple-instance-learning>

Properties

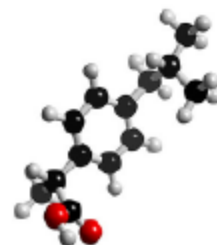
- Ranking SVM maximizes the AUC score
 - Because it ensures that positive examples rank higher than negative examples
 - Ulf Brefeld, Tobias Scheffer. n.d. “AUC Maximizing Support Vector Learning.”
- Similar methods for maximizing Average Precision
 - Yue, Yisong, Thomas Finley, Filip Radlinski, and Thorsten Joachims. 2007. “A Support Vector Method for Optimizing Average Precision.” In *Proceedings of the 30th Annual International ACM SIGIR Conference on Research and Development in Information Retrieval*, 271–78. SIGIR '07. New York, NY, USA: ACM. doi:10.1145/1277741.1277790.

Applications

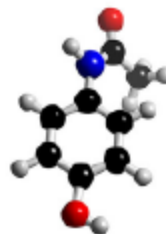
- Drug Discovery
 - Input



$$\text{pIC}_{50} = 5.6718$$



$$\text{pIC}_{50} = 8.2991$$



$$\text{pIC}_{50} = 4.1317$$

...

Agarwal et al., 2010

- Dataset (from Sutherland et al., 2004)

Data Set	No. of Compounds	No. of Chemical (2.5D) Descriptors	pIC ₅₀ Values
DHFR inhibitors	361	70	3.3 – 9.8
COX2 inhibitors	292	74	4.0 – 9.0

2.5D chemical descriptors
Gaussian kernel

Training size	Ranking error	
	SVR	RankSVM
24	0.4755	0.4601
48	0.3430	0.3509
72	0.2840	0.2726
96	0.2483	0.2351
120	0.2171	0.2121
144	0.2023	0.2032
168	0.2019	0.1817
192	0.1808	0.1749
216	0.1816	0.1722
237	0.1714	0.1681

FP2 molecular fingerprints
Tanimoto kernel

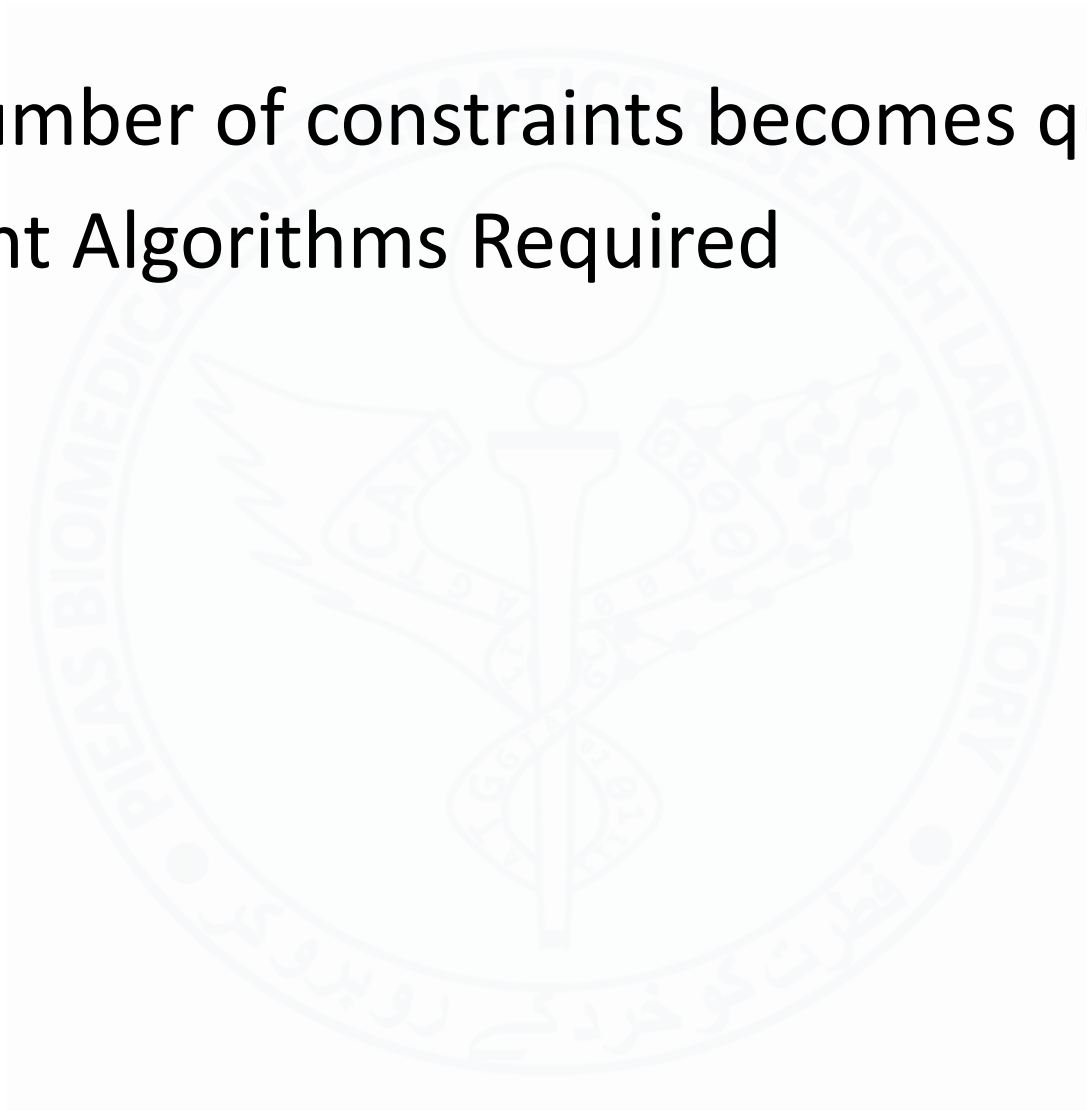
Training size	Ranking error	
	SVR	RankSVM
24	0.3793	0.3546
48	0.2905	0.2896
72	0.2517	0.2421
96	0.2343	0.2201
120	0.2147	0.2052
144	0.2166	0.1988
168	0.2096	0.1966
192	0.2056	0.1962
216	0.1907	0.1787
237	0.1924	0.1798

Potential Application Areas

- Student Grades Prediction
- Binding Affinity Prediction
- Amyloidogenicity Prediction
- Document Ranking
- Remote Homology Detection
 - Liu, Bin, Junjie Chen, and Xiaolong Wang. 2015. “Application of Learning to Rank to Protein Remote Homology Detection.” *Bioinformatics* 31 (21): 3492–98.
doi:10.1093/bioinformatics/btv413.

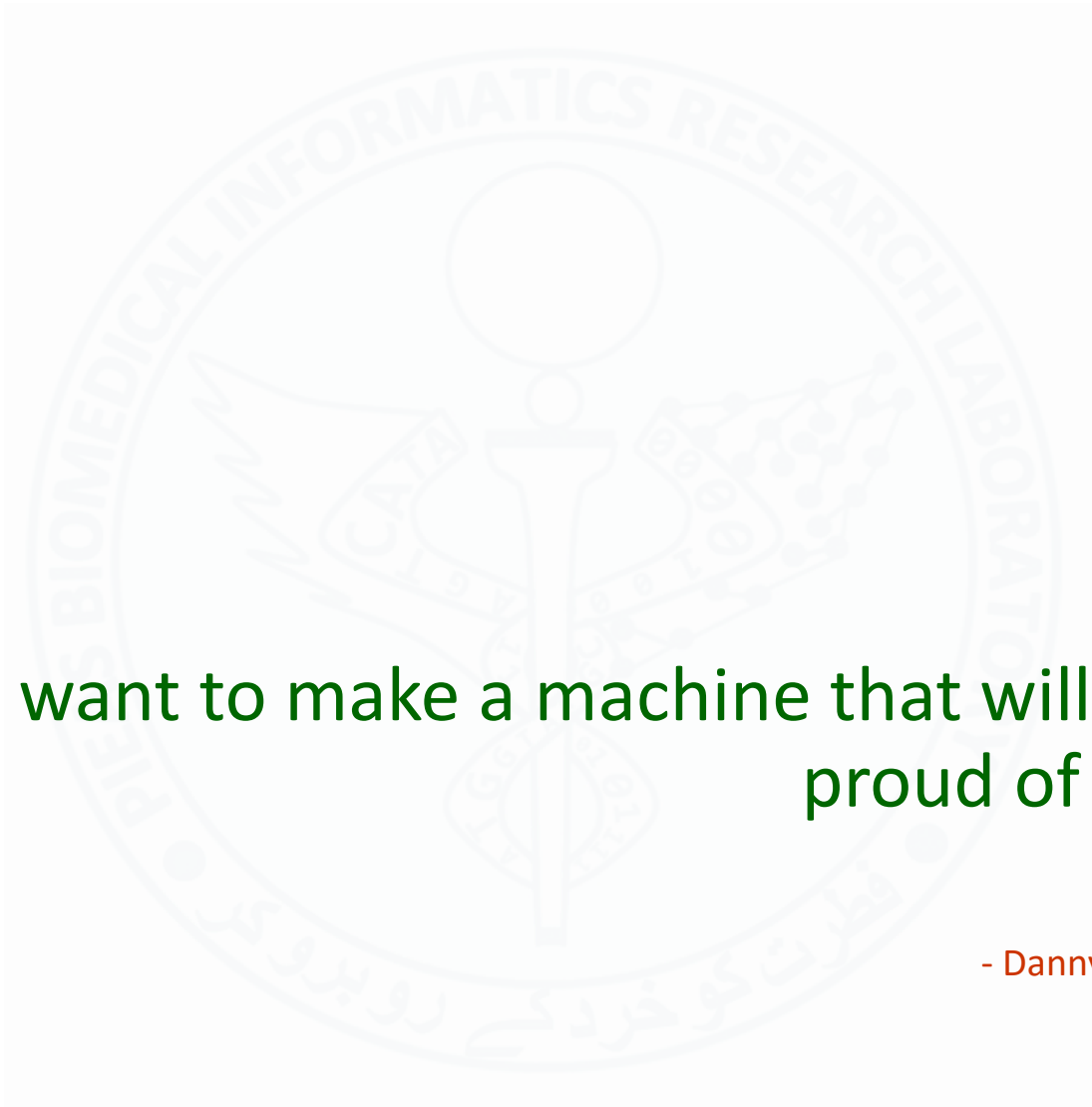
Issues

- The number of constraints becomes quadratic
- Efficient Algorithms Required



Required Reading

- Yu, Hwanjo, and Sungchul Kim. 2012. “SVM Tutorial — Classification, Regression and Ranking.” In *Handbook of Natural Computing*, edited by Grzegorz Rozenberg, Thomas Bäck, and Joost N. Kok, 479–506. Springer Berlin Heidelberg.
http://link.springer.com/referenceworkentry/10.1007/978-3-540-92910-9_15.
- Yue, Yisong, Thomas Finley, Filip Radlinski, and Thorsten Joachims. 2007. “A Support Vector Method for Optimizing Average Precision.” In *Proceedings of the 30th Annual International ACM SIGIR Conference on Research and Development in Information Retrieval*, 271–78. SIGIR '07. New York, NY, USA: ACM. doi:10.1145/1277741.1277790.



We want to make a machine that will be
proud of us.

- Danny Hillis