Support Vector Algorithms for Optimizing the Partial AUC

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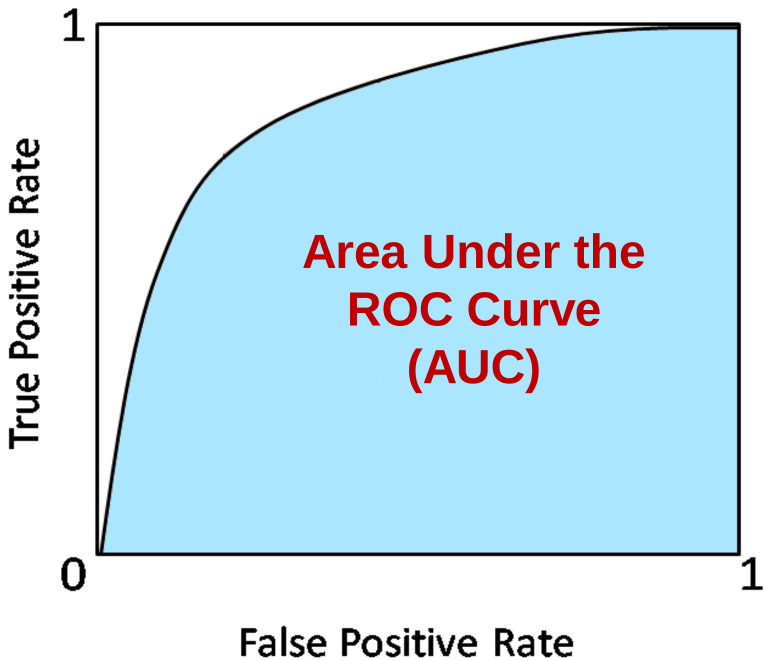
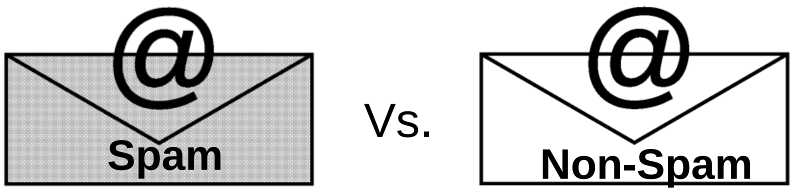
Based on work in ICML 2013 and KDD 2013

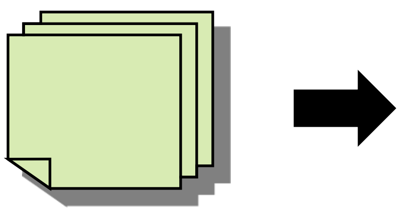
Receiver Operating Characteristic Curve



Binary Classification

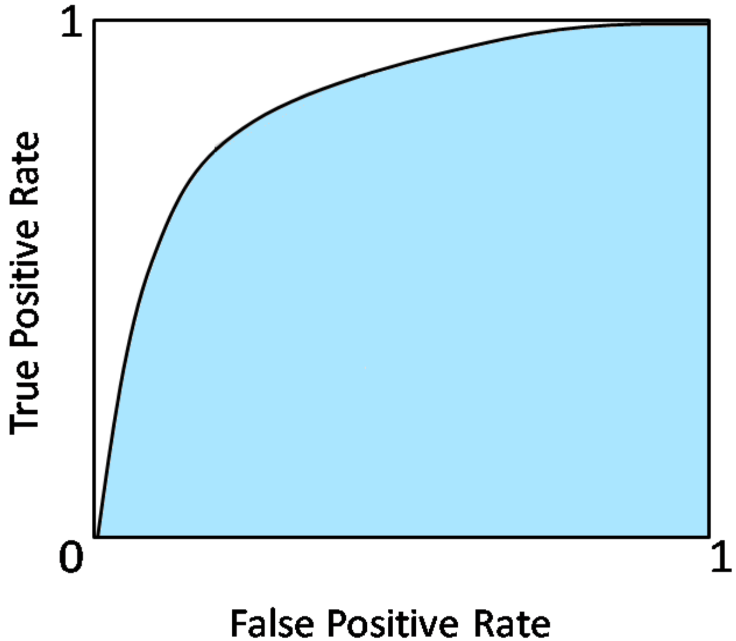


Bipartite Ranking

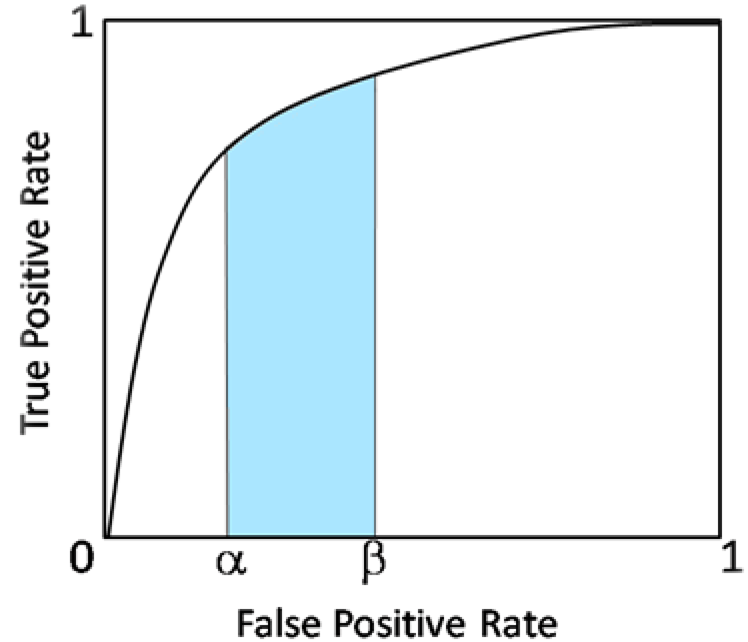


Ranking of documents

Partial AUC?



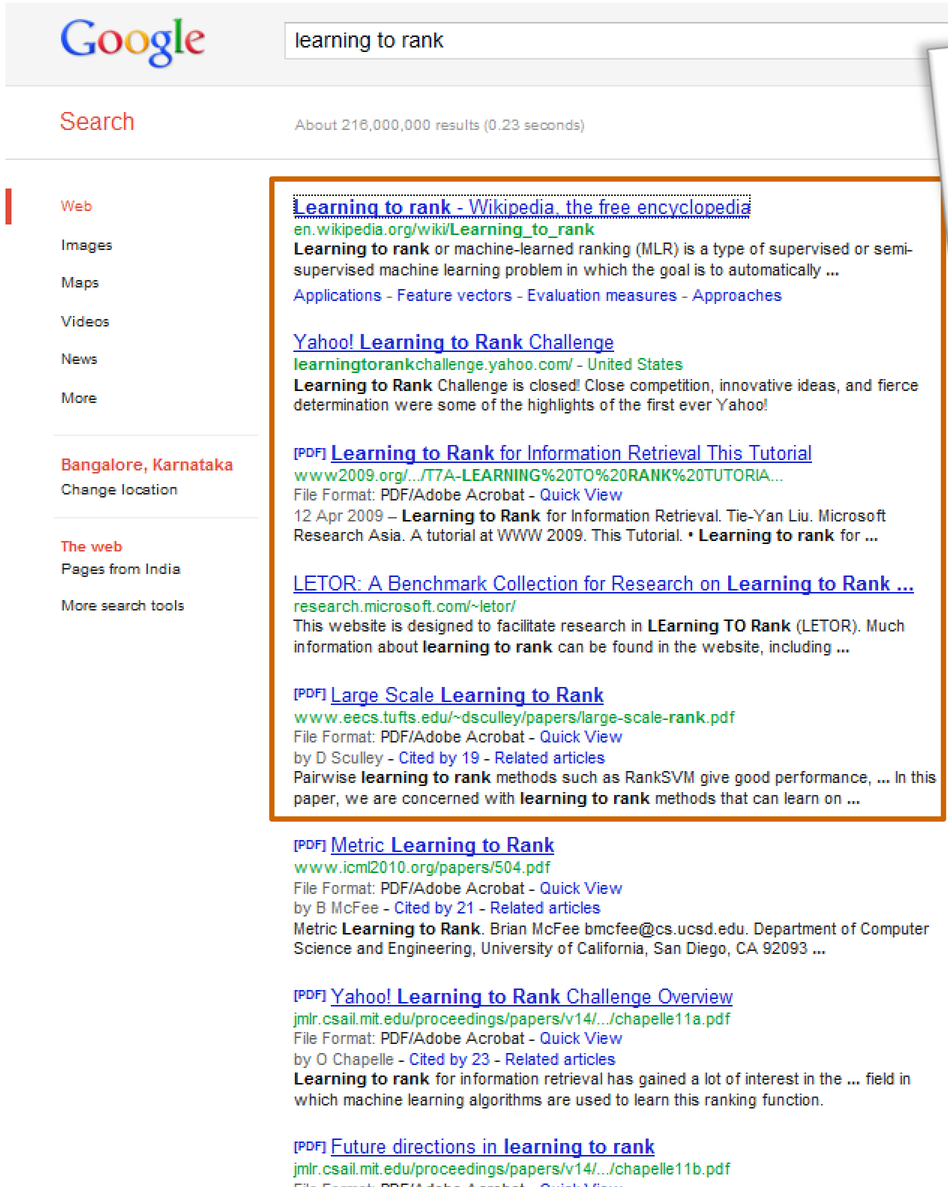
Vs



Full AUC

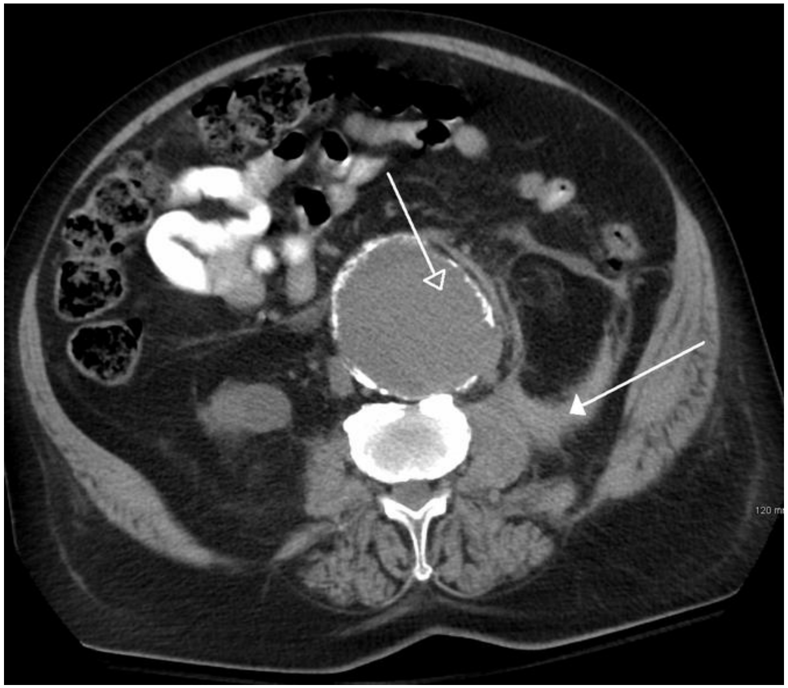
Partial AUC

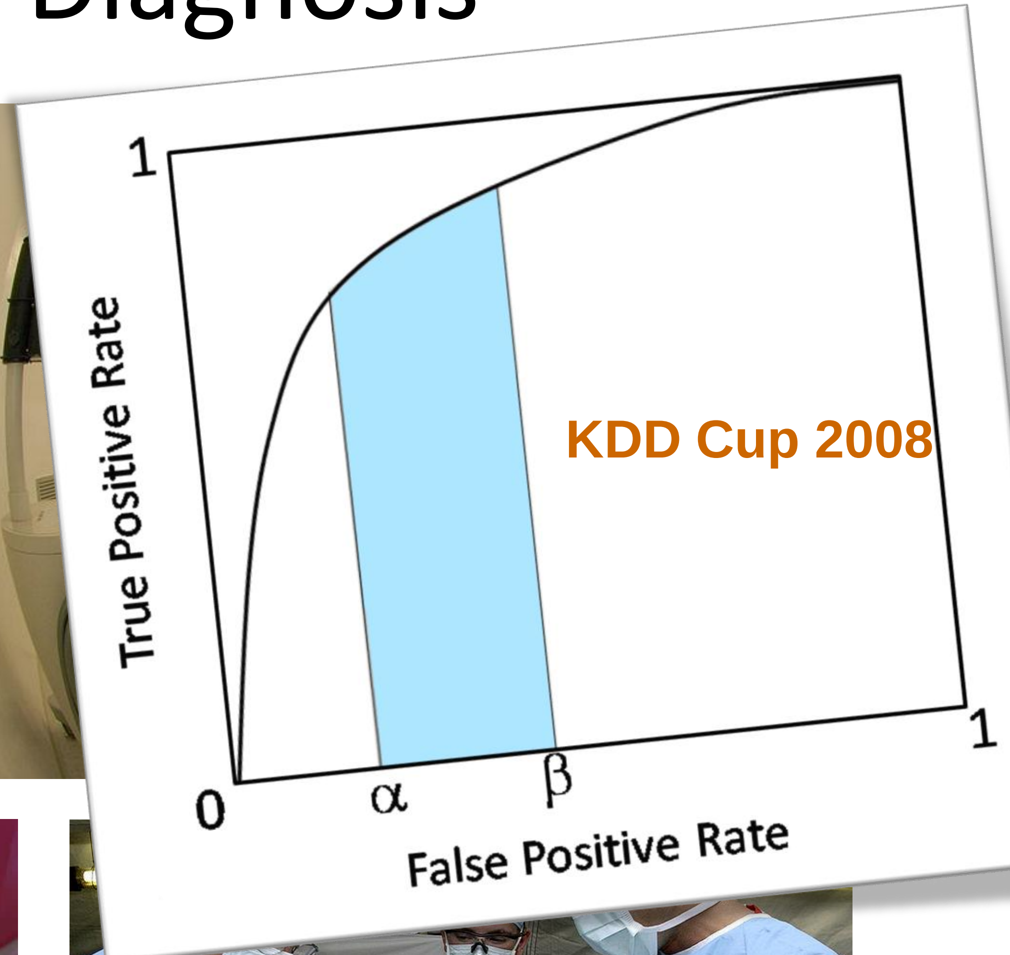
Ranking

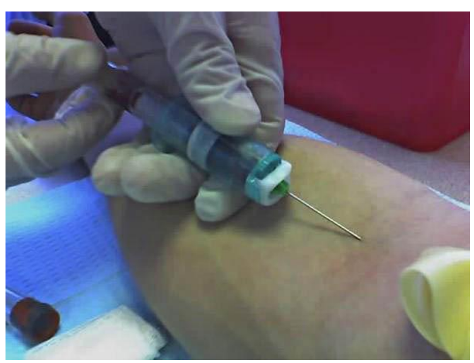


http://www.google.com/

Medical Diagnosis



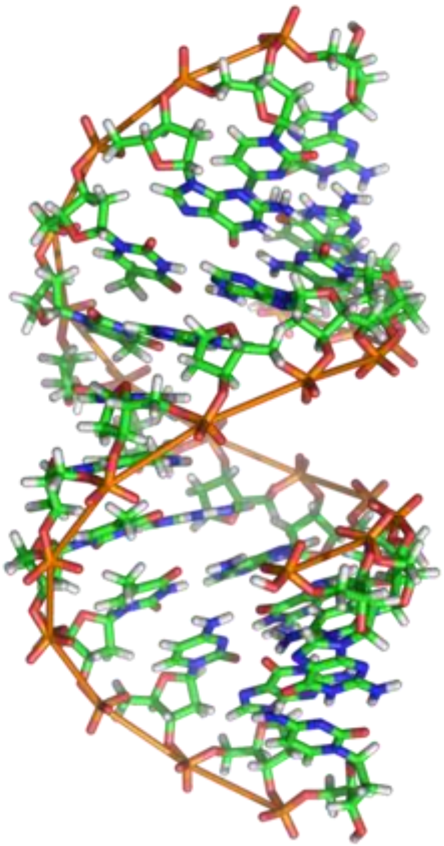


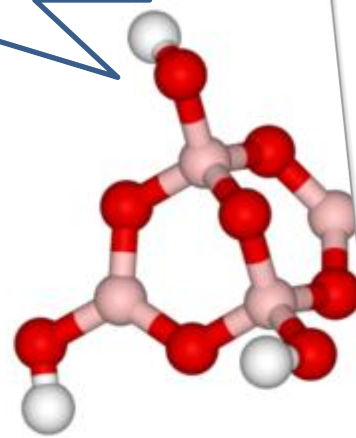


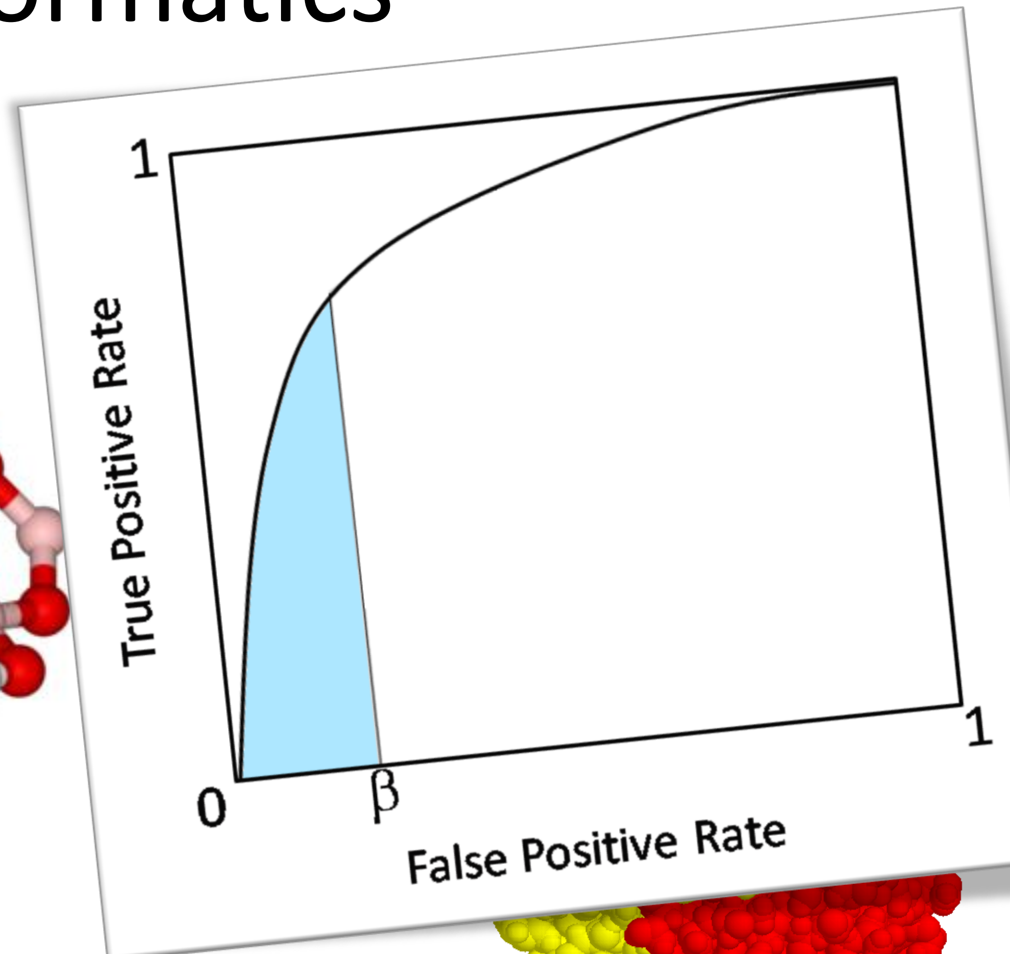
http://en.wikipedia.org/

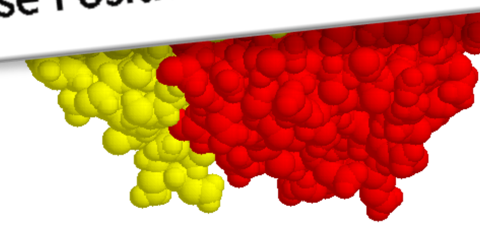
Bioinformatics

- Drug Discovery
- Gene Prioritization
- Protein Interaction Prediction
- ……









http://en.wikipedia.org/wiki
http://commons.wikimedia.org/
http://www.google.com/imghp

Partial Area Under the ROC Curve is critical to many applications

Partial AUC Optimization

- Asymmetric SVM:
  - Wu, S.-H., Lin, K.-P., Chen, C.-M., and Chen, M.-S. Asymmetric support vector machines: low false-positive learning under the user tolerance. In KDD, 2008.
- Boosting style algorithm:
  - Komori, O. and Eguchi, S. A boosting method for maximizing the partial area under the ROC curve. *BMC Bioinformatics*, 11:314, 2010.
  - Takenouchi, T., Komori, O., and Eguchi, S. An extension of the receiver operating characteristic curve and AUC-optimal classification. Neural Computation, 24, (10):2789–2824, 2012.
- Several heuristic approaches:
  - Pepe, M. S. and Thompson, M. L. Combining diagnostic test results to increase accuracy. *Biostatistics*, 1(2):123–140, 2000.
  - Ricamato, M. T. and Tortorella, F. Partial AUC maximization in a linear combination of dichotomizers. *Pattern Recognition*, 44(10-11):2669–2677, 2011.

Partial AUC Optimization

- Many of the existing approaches are either heuristic or solve special cases of the problem.
- **Our contribution**: New support vector methods for optimizing the general partial AUC measure.
- Based on Joachims' Structural SVM approach for optimizing full AUC, but leads to a trickier inner combinatorial optimization problem.
  - Joachims, T. A Support Vector Method for Multivariate Performance Measures. ICML, 2005.
  - Joachims, T. Training linear SVMs in linear time. KDD, 2006.
- Improvements over baselines on several real-world applications

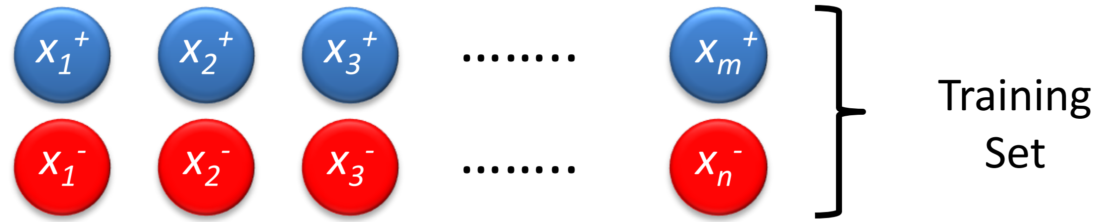
Outline

- Problem Setup
- **First cut:** Structural SVM Approach for Optimizing Partial AUC
- **Better Formulation:** Tighter Upper Bound on the Partial AUC Loss
- Experiments

Receiver Operating Characteristic Curve

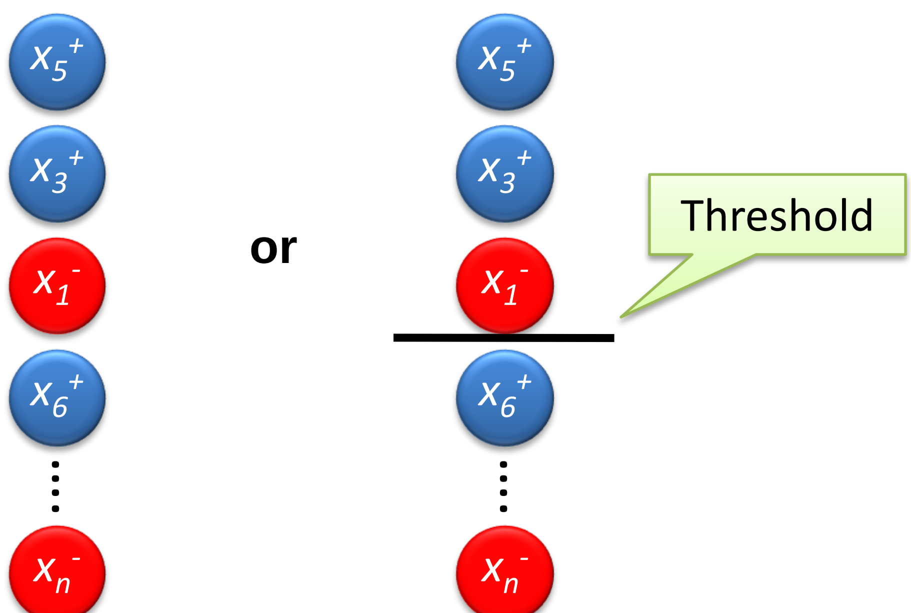
Positive Instances

Negative Instances

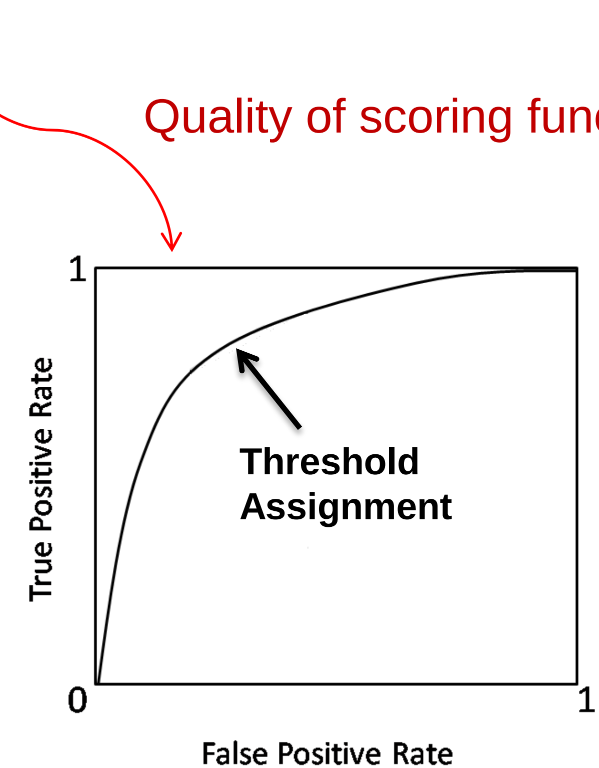


GOAL? Learn a scoring function $f : X \rightarrow \mathbb{R}$

Rank objects **Build a classifier**

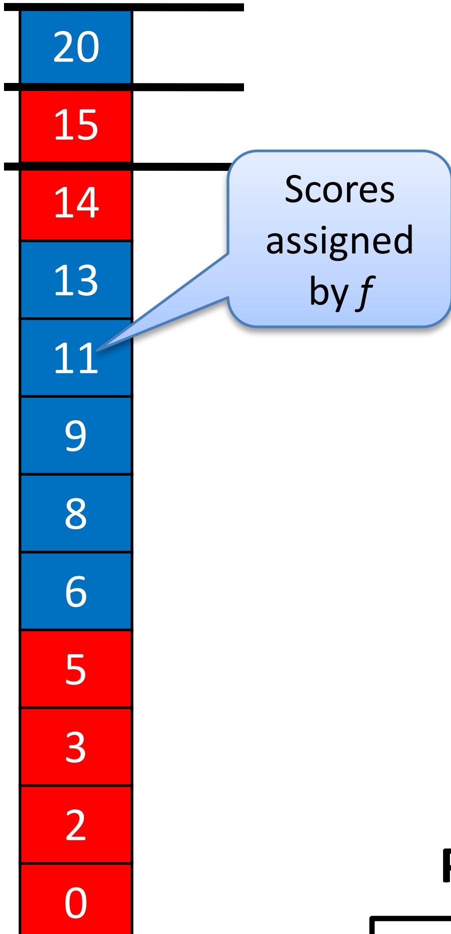


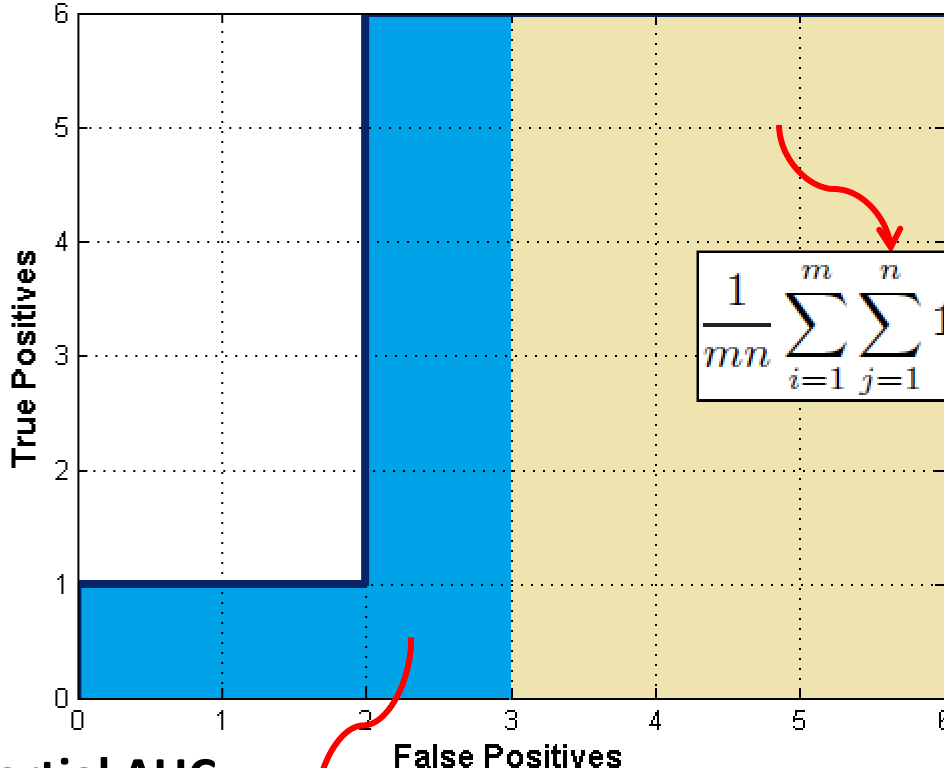
Quality of scoring function?



ROC Curve

Receiver Operating Characteristic Curve





Area Under the Curve (AUC)

$$\frac{1}{mn}\sum_{i=1}^{m}\sum_{j=1}^{n}\mathbf{1}\left(f(x_i^+) > f(x_j^-)\right)$$

Pair-wise accuracy

Partial AUC

$$\frac{1}{mn(\beta-\alpha)}\sum_{i=1}^{m}\sum_{j=j_\alpha+1}^{j_\beta}\mathbf{1}\left(f(x_i^+) > f(x_{(j)}^-)\right)$$

Partial AUC Optimization

Minimize: $\underbrace{1 - \widehat{\text{pAUC}}_f(\alpha, \beta)}$

Discrete and
Non-differentiable

$$\underbrace{\text{Convex Upper Bound on ``}1 - \widehat{\text{pAUC}}_f(\alpha, \beta)\text{''} + \text{Regularizer}}_{\text{Structural SVM Based Approach}}$$

- Extends Joachims' approach for full AUC optimization, but leads to a trickier combinatorial optimization step.
- Efficient solver with the same/lesser time complexity compared to that for full AUC.

Outline

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Structural SVM Based Approach

Ordering of $\{x_1, x_2, \ldots, x_s\}$

$$\pi: \quad \begin{array}{c|c} & n \\ \hline m & \begin{array}{|c|c|c|c|c|} \hline 0 & 0 & 0 & 0 & 0 \\ \hline 1 & 1 & 0 & 0 & 0 \\ \hline 1 & 1 & 0 & 0 & 1 \\ \hline 1 & 1 & 0 & 0 & 1 \\ \hline \end{array} \end{array}$$

compared with

$$\pi^*: \quad \begin{array}{|c|c|c|c|c|} \hline 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 \\ \hline \end{array}$$

IDEAL

Upper Bound on (1 – pAUC)

Regularizer

$$\min_{w,\xi \geq 0} \boxed{\frac{1}{2}||w||^2} + C\boxed{\xi}$$

s.t.

$$\boxed{\forall \pi \in \Pi_{m,n}} : \quad w^\top \left(\phi(S,\pi^*) - \phi(S,\pi)\right) \geq \Delta_{\mathrm{pAUC}(\alpha,\beta)}(\pi^*,\pi) - \xi$$

pAUC Loss

Exponential Number of Output Matrices!!

Cutting-plane Solver

Converges in constant number of iterations

$$\min_{w,\xi\geq 0} \frac{1}{2}||w||^2 + C\xi$$

s.t. $\forall \pi \in \mathcal{C}$:

$$\boxed{w^\top \left(\phi(S,\pi^*) - \phi(S,\pi)\right) \geq \Delta_{\mathrm{pAUC}(\alpha,\beta)}(\pi^*,\pi) - \xi}$$

Repeat:

1. Solve OP for a subset of constraints.
2. Add the most violated constraint.

Break down!

$$\underset{\pi}{\mathrm{argmax}} \ \Delta_{\mathrm{pAUC}(\alpha,\beta)}(\pi^*,\pi) + w^\top \left(\phi(S,\pi^*) - \phi(S,\pi)\right)$$

Full AUC

0	1	0	1	0
1	1	0	0	0
1	1	0	0	1
1	1	0	0	1

Partial AUC

0	1	0	1	0
1	1	0	0	0
1	1	0	0	1
1	1	0	0	1

?

Trickier Optimization Problem

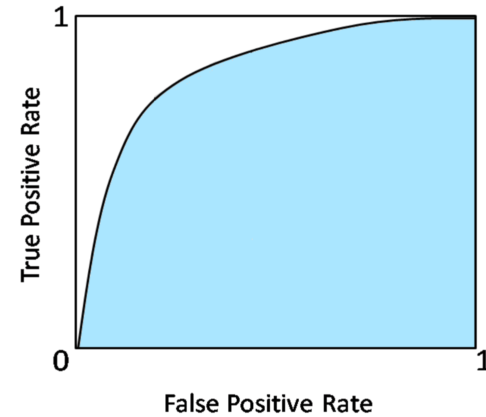
Full AUC

All Pairs

$$\frac{1}{mn}\sum_{i=1}^{m}\sum_{j=1}^{n}\mathbb{1}\left(f(x_i^+) > f(x_j^-)\right)$$

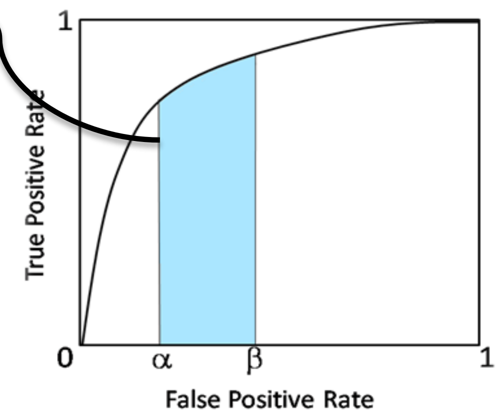
0	1	0	1	0
1	1	0	0	0
1	1	0	0	1
1	1	0	0	1

➡ $\sum$ ➡ **AUC**



Partial AUC

$$\frac{1}{mn(\beta-\alpha)}\sum_{i=1}^{m}\sum_{j=j_\alpha+1}^{j_\beta}\mathbb{1}\left(f(x_i^+) > f(x_{(j)}^-)\right)$$



Subset of negative instances in the FPR range [α, β] – **changes with ordering**

Trickier Optimization Problem

Full AUC

All Pairs

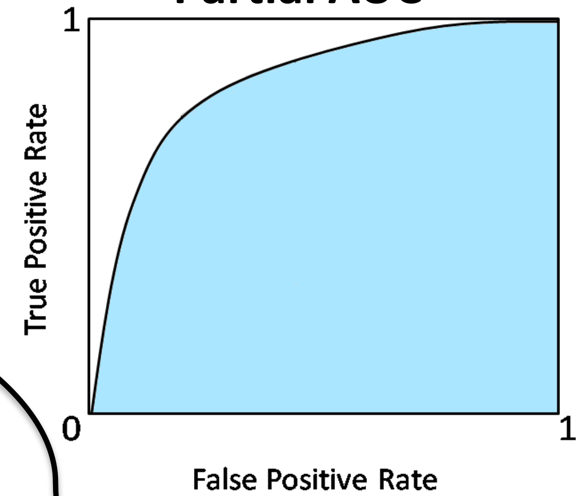
$$\frac{1}{mn}\sum_{i=1}^{m}\sum_{j=1}^{n}\mathbb{1}\left(f(x_i^+) > f(x_j^-)\right)$$

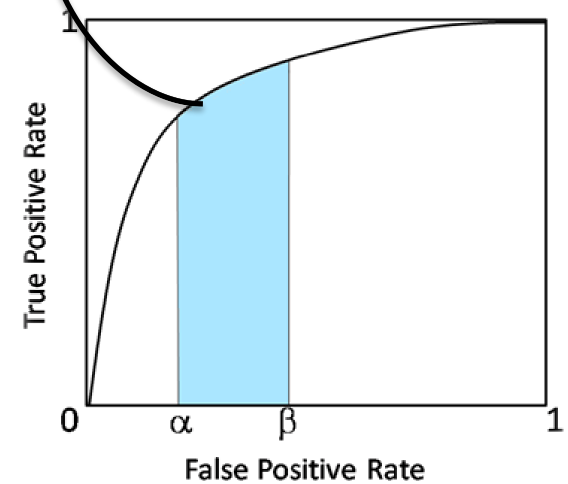
Partial AUC

$$\frac{1}{mn(\beta-\alpha)}\sum_{i=1}^{m}\sum_{j=j_\alpha+1}^{j_\beta}\mathbb{1}\left(f(x_i^+) > f(x_{(j)}^-)\right)$$

Subset of negative instances in the FPR range [α, β] – **changes with ordering**

Partial AUC





Can be implemented in **O((m+n) log (m+n))** time complexity

Inputs: $S = (S_+, S_-)$, α, β, w

For $i = 1, \ldots, m$ **do**

Optimize over $r_i \in \{0, \ldots, j_\alpha - 1\}$:

$$\pi^{(1)}_{i,(j)_w} = \begin{cases} \mathbf{1}(w^\top x^{\pm}_{i,(j)_w} \leq 0)\,, & j \in \{1, \ldots, j_\alpha - 1\} \\ 0\,, & j \in \{j_\alpha, \ldots, n\} \end{cases}$$

Optimize over $r_i \in \{j_\alpha\}$:

$$\pi^{(2)}_{i,(j)_w} = \begin{cases} 1\,, & j \in \{1, \ldots, j_\alpha\} \\ 0\,, & j \in \{j_\alpha + 1, \ldots, n\} \end{cases}$$

Optimize over $r_i \in \{j_\alpha + 1, \ldots, n\}$:

$$\pi^{(3)}_{i,(j)_w} = \begin{cases} 1\,, & j \in \{1, \ldots, j_\alpha + 1\} \\ \mathbf{1}(w^\top x^{\pm}_{i,(j)_w} \leq 1)\,, & j \in \{j_\alpha + 2, \ldots, j_\beta\} \\ \mathbf{1}(w^\top x^{\pm}_{i,(j)_w} \leq n\beta - j_\beta)\,, & j = j_\beta + 1 \\ \mathbf{1}(w^\top x^{\pm}_{i,(j)_w} \leq 0)\,, & j \in \{j_\beta + 2, \ldots, n\} \end{cases}$$

$$\bar{k} = \underset{k \in \{1,2,3\}}{\text{argmax}} \left\{ \begin{array}{l} \text{term inside sum over } i \text{ in} \\ \text{Eq. (4) evaluated at } \pi^{(k)}_i \end{array} \right\}$$

$\bar{\pi}_i = \pi^{(\bar{k})}_i$

End For

Output: $\bar{\pi}$

Partial AUC

0	1	0	1	0
1	1	0	0	0
1	1	0	0	1
1	1	0	0	1

Optimize rows independently

0	1	0	1	0
1	1	0	0	0
1	1	0	0	1
1	1	0	0	1

H. Narasimhan and S. Agarwal. *A Structural SVM Based Approach for Optimizing Partial AUC*. ICML, 2013.

Outline

- Problem Setup
- **First cut:** Structural SVM Approach for Optimizing Partial AUC
- **Better Formulation:** Tighter Upper Bound on the Partial AUC Loss
- Experiments

Better Formulation

- Tighter upper bound on partial AUC loss
- Lesser time for finding most-violated constraint!
- Better guarantee on number of cutting-plane iterations!

$$\max_{z \in \mathcal{Z}_\beta} \sum_{x_j^- \in z} \sum_{i=1}^{m} \mathbf{1}\big(f(x_i^+) < f(x_j^-)\big)$$

Max over subsets of negative instances

Truncated form of earlier objective

H. Narasimhan and S. Agarwal. *SVM_pAUC^tight: A New Support Vector Method for Optimizing Partial AUC Based on a Tight Convex Upper Bound*. KDD, 2013. *To appear*.

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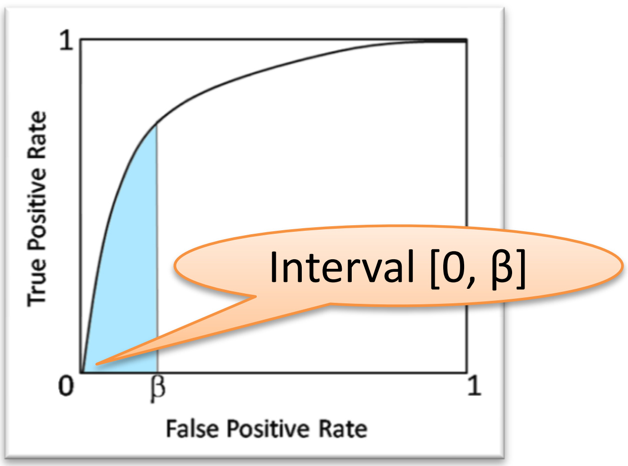
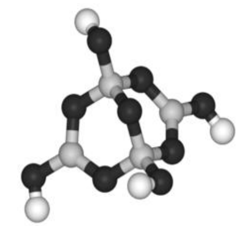
SVMpAUC^{struct} vs. Baseline Methods



Drug Discovery

50 active compounds / 2092 inactive compounds

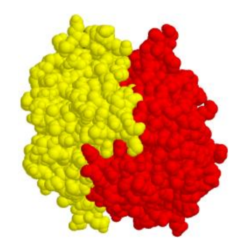
	pAUC(0, 0.1)
SVM$_{pAUC}$[0,0.1]	**65.25**
SVM$_{AUC}$	62.64 *
ASVM[0,0.1]	63.80
pAUCBoost[0,0.1]	43.89 *
Greedy-Heuristic[0,0.1]	8.33 *



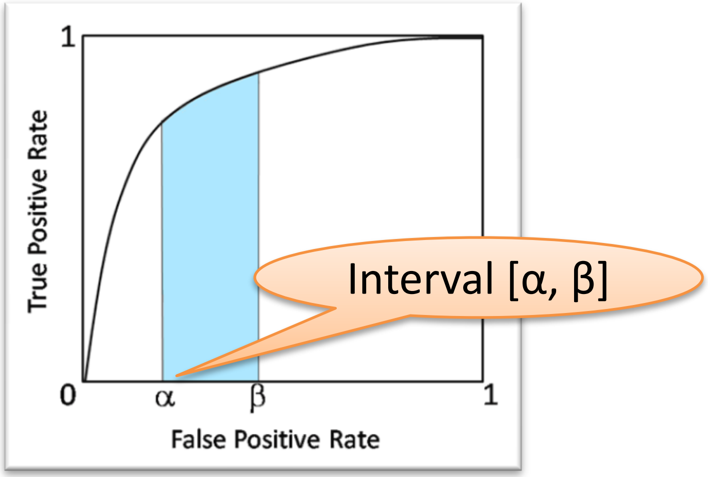
Protein-Protein Interaction Prediction

~3x10^3 interacting pairs / ~2x10^5 non-interacting pairs

	pAUC(0, 0.1)
SVM$_{pAUC}$[0,0.1]	**51.79**
SVM$_{AUC}$	39.72 *
ASVM[0,0.1]	44.51 *
pAUCBoost[0,0.1]	48.65 *
Greedy-Heuristic[0,0.1]	47.33 *



SVMpAUC^{struct} vs. Baseline Methods



KDD Cup 2008

Breast Cancer Detection

~600 malignant ROIs / ~10^5 benign ROIs

	pAUC$(0.2s, 0.3s)$
SVM$_{\text{pAUC}}[0.2s, 0.3s]$	51.44
SVM$_{\text{AUC}}$	50.50
pAUCBoost$[0.2s, 0.3s]$	48.06 *
Greedy-Heuristic$[0.2s, 0.3s]$	46.99 *

SVMpAUC^{tight} vs. SVMpAUC^{struct}

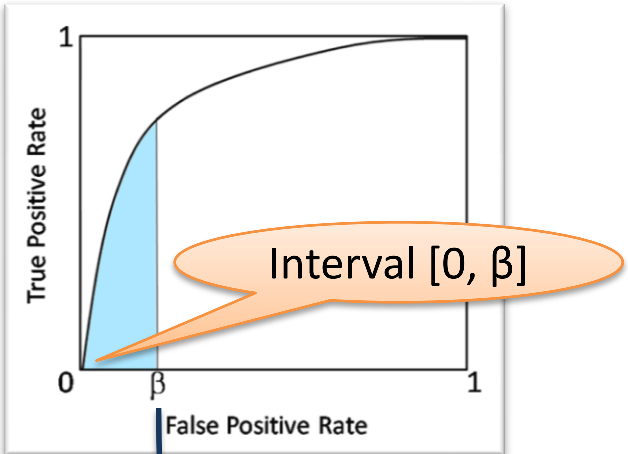
Partial AUC in [0, β]

	$\mathrm{SVM}_{\mathrm{pAUC}}^{\mathrm{tight}}[0, 0.1]$	$\mathrm{SVM}_{\mathrm{pAUC}}^{\mathrm{struct}}[0, 0.1]$	$\mathrm{SVM}_{\mathrm{AUC}}$
PPI	**52.95**	51.96 *	39.72 *
Cheminformatics	**65.30**	65.28	62.78
KDD Cup 2001	69.91	**70.12**	62.23 *
Leukemia	**30.44**	24.64 *	28.83
Ovarian Cancer	91.84	91.84	**92.17**

Partial AUC in [α, β]

	$\mathrm{SVM}_{\mathrm{pAUC}}^{\mathrm{tight}}[0.2s, 0.3s]$	$\mathrm{SVM}_{\mathrm{pAUC}}^{\mathrm{struct}}[0.2s, 0.3s]$	$\mathrm{SVM}_{\mathrm{AUC}}$
KDD Cup 2008	**53.43**	51.89	50.66

Run-time Analysis



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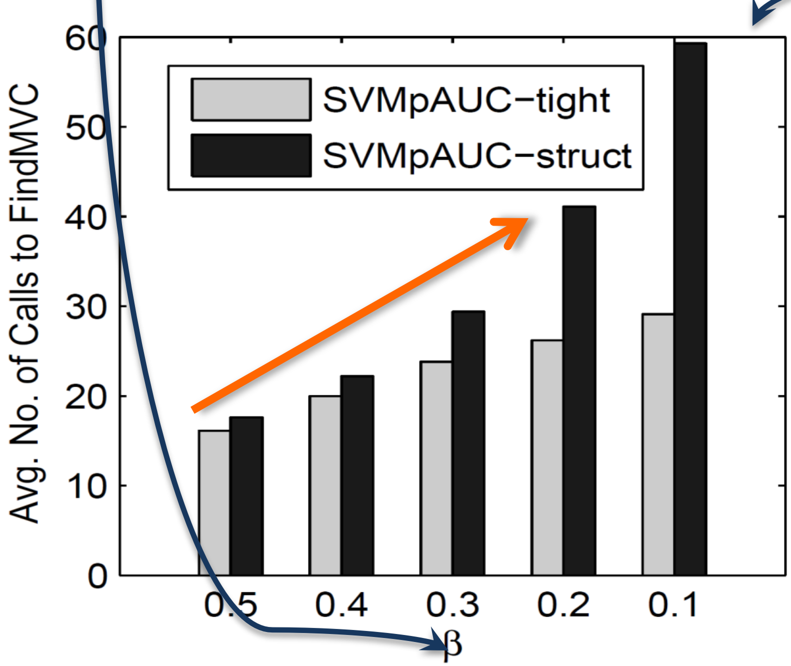

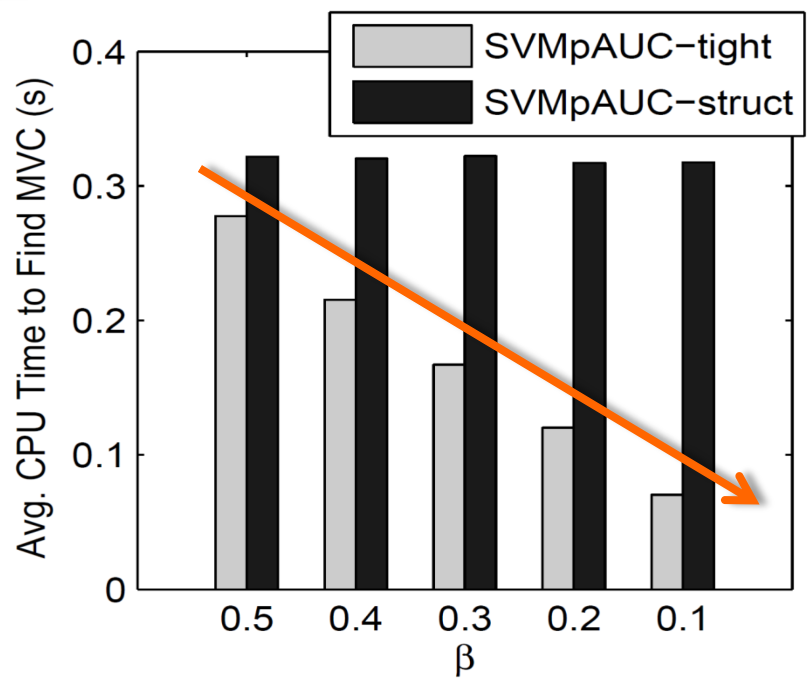

Conclusions

- A new structural SVM based approach for optimizing partial AUC
- Efficient algorithm for solving the inner combinatorial optimization step
- Improved algorithm that optimizes a tighter upper bound on the partial AUC loss
- Experimental results confirm the effectiveness of our methods

Questions?