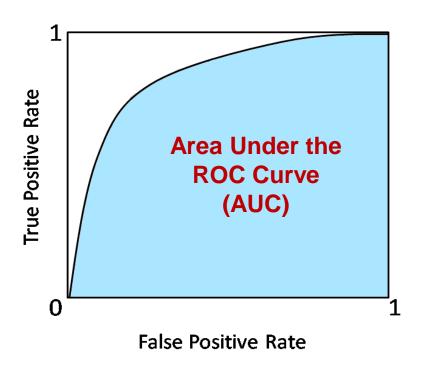
SVMpAUC-tight: A new algorithm for optimizing partial AUC based on a tight convex upper bound

Harikrishna Narasimhan and Shivani Agarwal

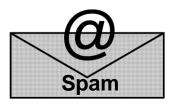


Department of Computer Science and Automation Indian Institute of Science, Bangalore



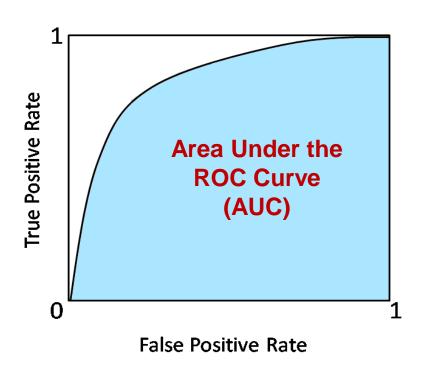


Binary Classification

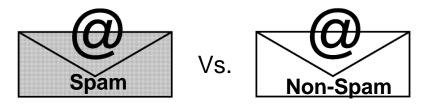


Vs.

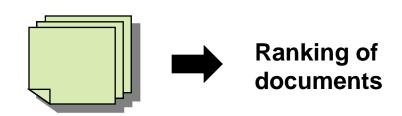




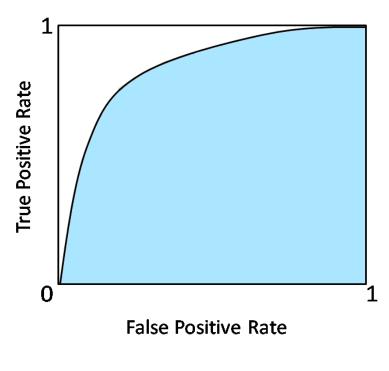
Binary Classification



Bipartite Ranking

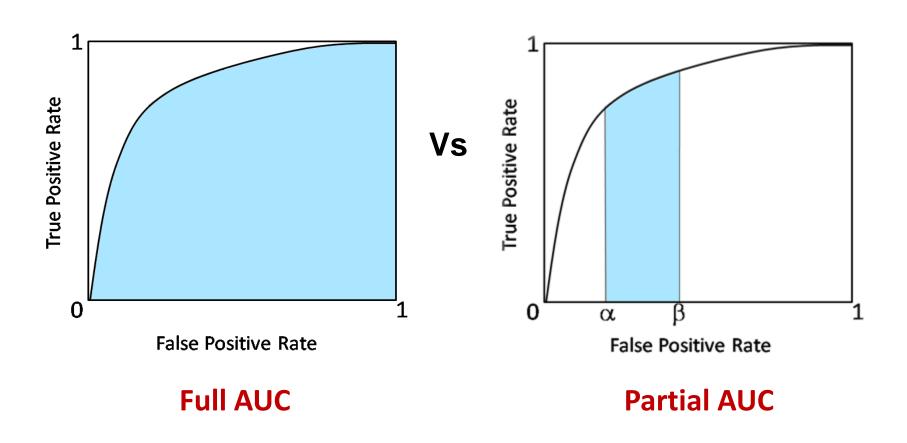


Partial AUC?



Full AUC

Partial AUC?



Ranking



learning to rank

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Applications - Feature vectors - Evaluation measures - Approaches

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Metric Learning to Rank. Brian McFee bmcfee@cs.ucsd.edu. Department of Computer Science and Engineering, University of California, San Diego, CA 92093 ...

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Metric Learning to Rank. Brian McFee bmcfee@cs.ucsd.edu. Department of Computer Science and Engineering, University of California, San Diego, CA 92093 ...

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Frue Positive Rate False Positive Rate

Medical Diagnosis



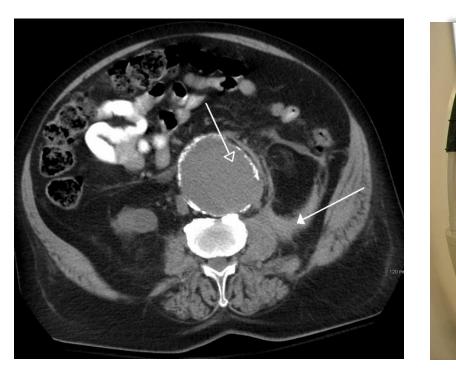


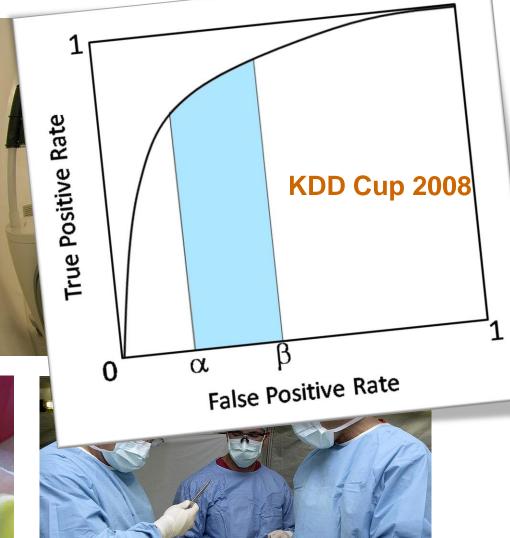






Medical Diagnosis



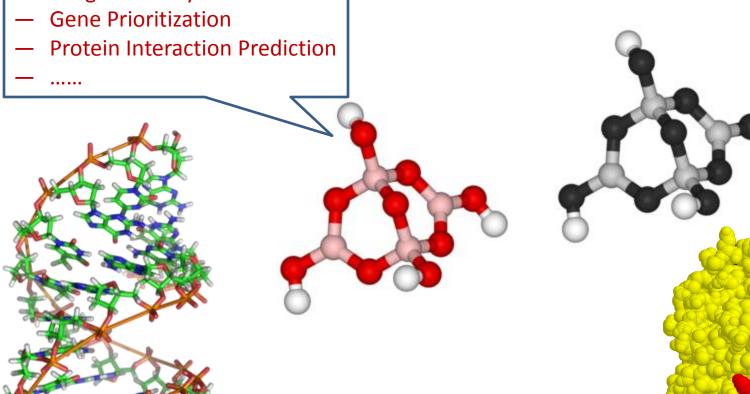






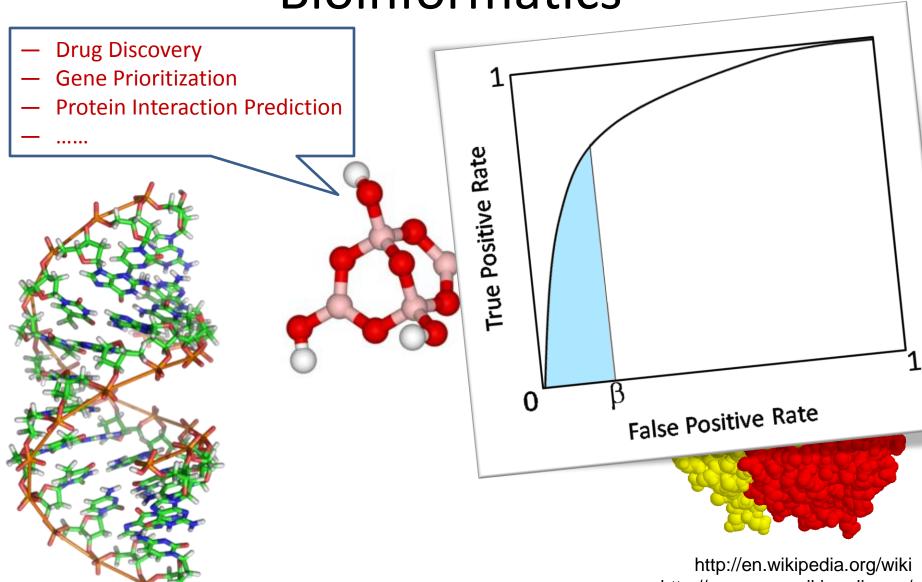
Bioinformatics





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Bioinformatics

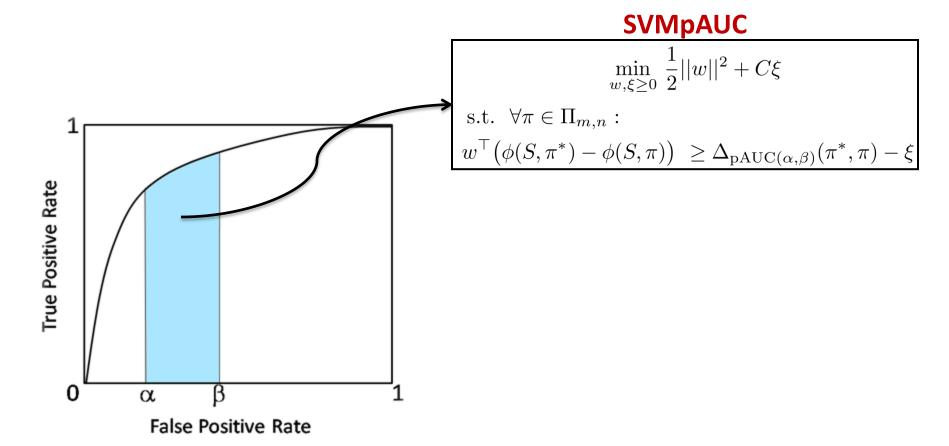


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Partial Area Under the ROC Curve is critical to many applications

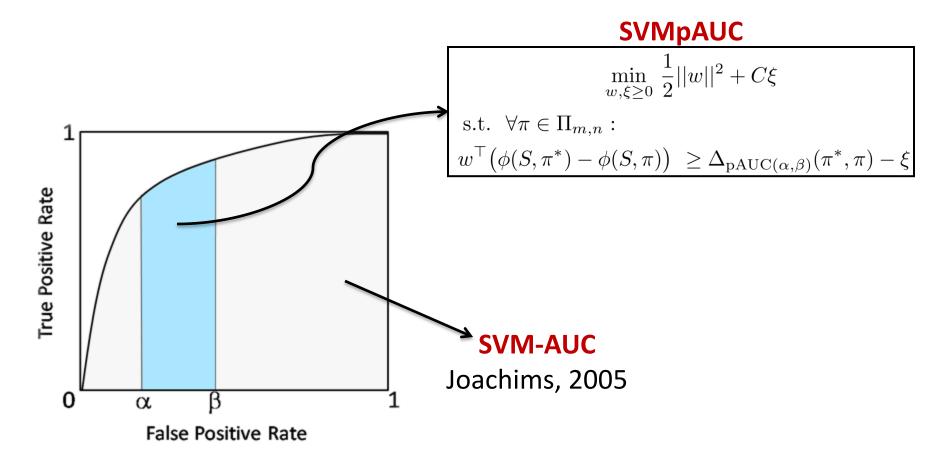
SVMpAUC (ICML 2013)

Narasimhan, H. and Agarwal, S. "A structural SVM based approach for optimizing partial AUC", ICML 2013.



SVMpAUC (ICML 2013)

Narasimhan, H. and Agarwal, S. "A structural SVM based approach for optimizing partial AUC", ICML 2013.



Improved Version of SVMpAUC

Tighter upper bound
Improved accuracy
Better runtime guarantee

Outline

- Overview of SVMpAUC
- Upper Bound Optimized by SVMpAUC
- Improved Formulation: SVMpAUC-tight
- Optimization Methods
- Experiments

Positive Instances









Training Set

$$X_1$$



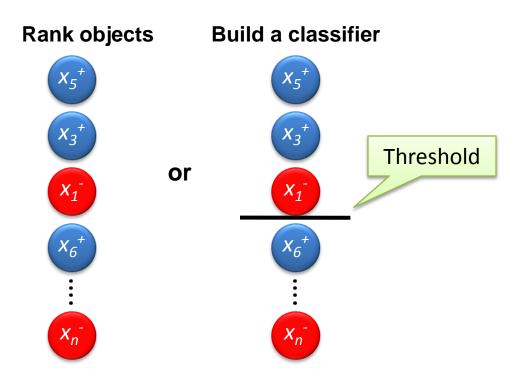




GOAL? Learn a scoring function $f:X o\mathbb{R}$

Positive Instances X_1^{\dagger} X_2^{\dagger} X_3^{\dagger} X_n^{\dagger} Training Set

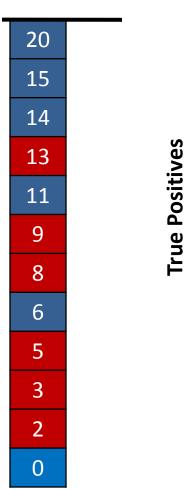
GOAL? Learn a scoring function $f:X\to\mathbb{R}$

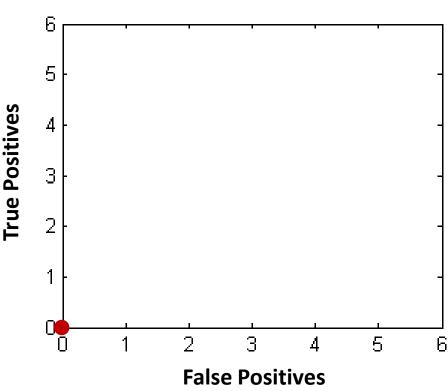


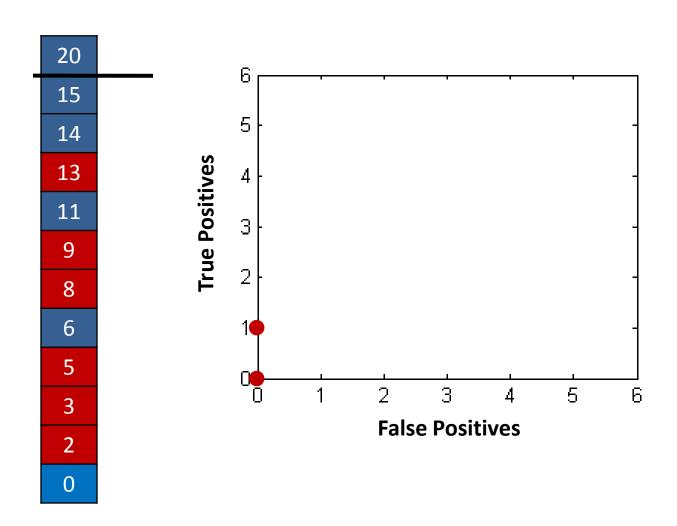
 X_3^+ **Positive Instances** X_1^+ X_m Training Set **Negative Instances** *X*₃ **GOAL?** Learn a scoring function $f:X\to\mathbb{R}$ **Build a classifier** Quality of scoring function? Rank objects X_5^{\dagger} X_5 X_3 **Threshold True Positive Rate** or X_1^{-} X_1^{-} **Threshold Assignment** X_6^+ X_6^+

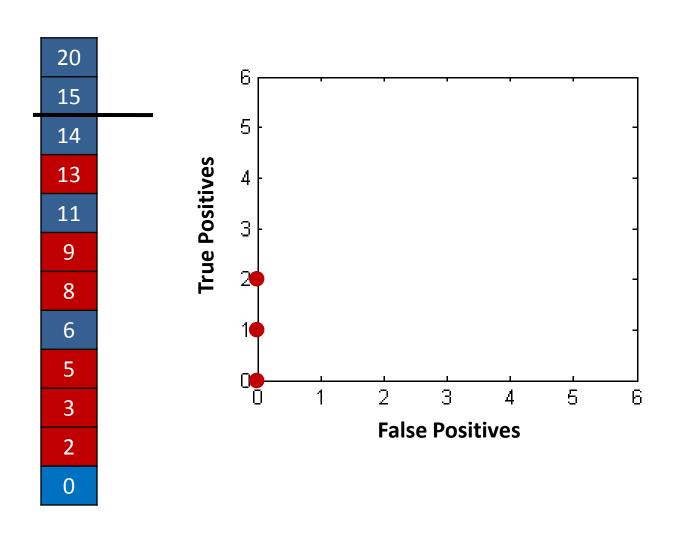
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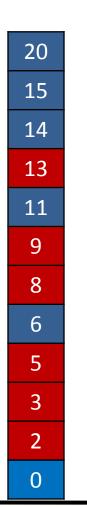
False Positive Rate

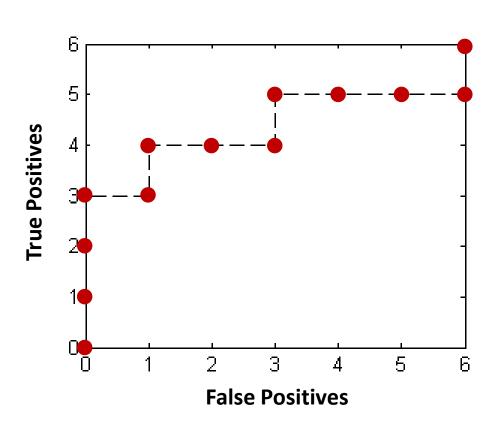




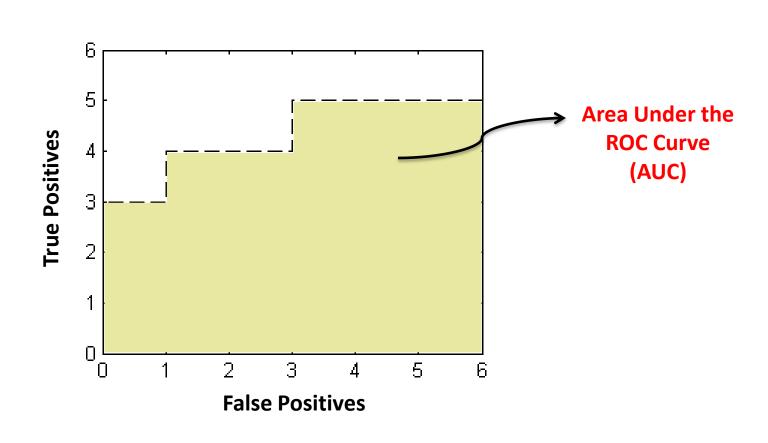


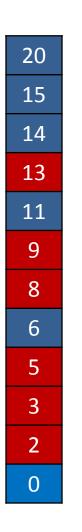


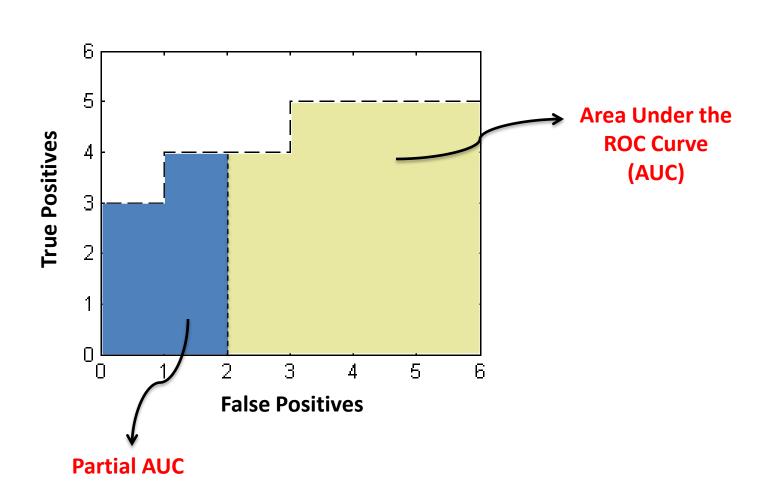


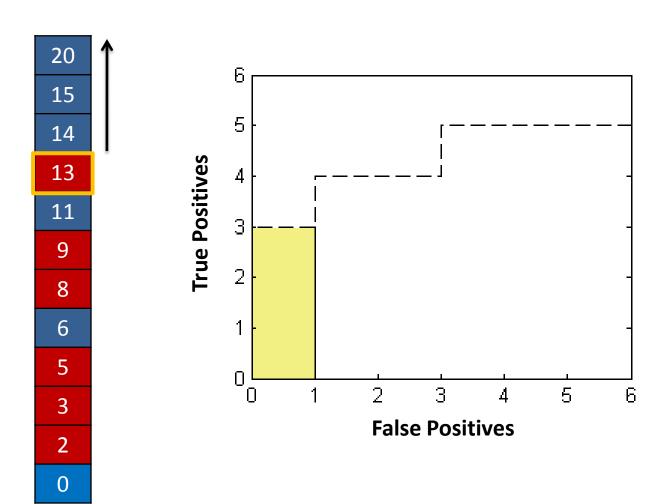


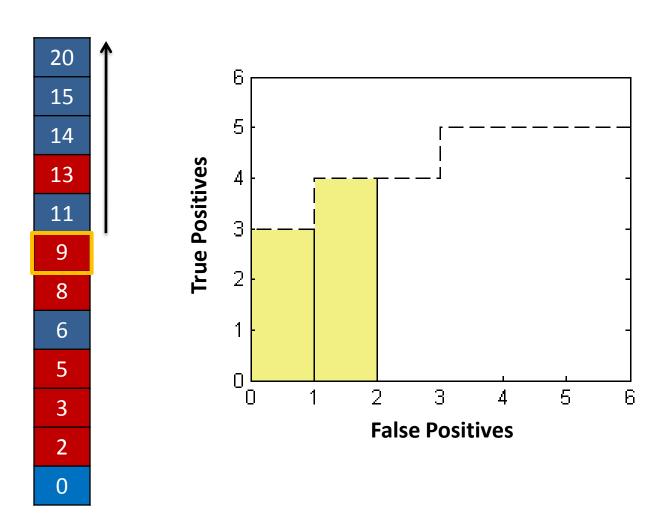




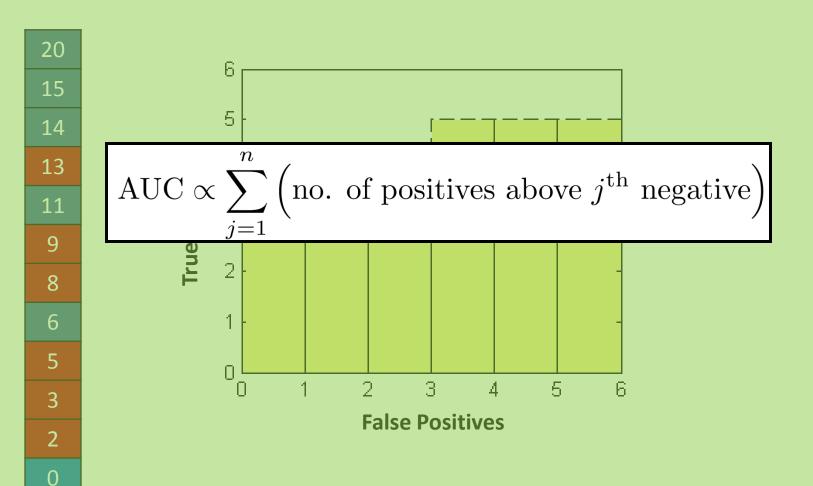




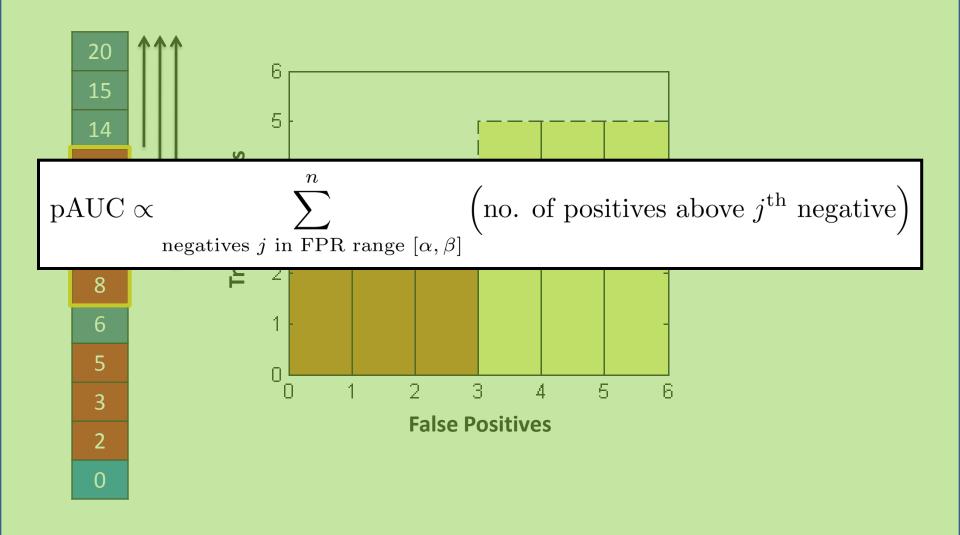


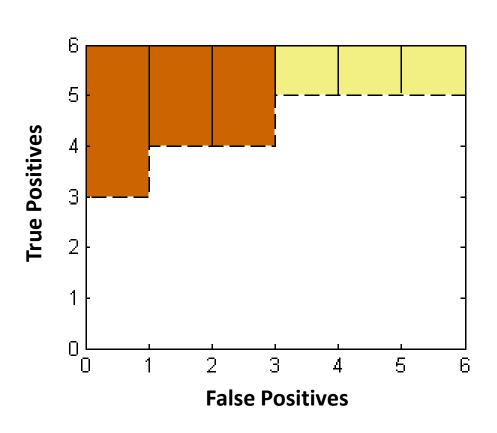






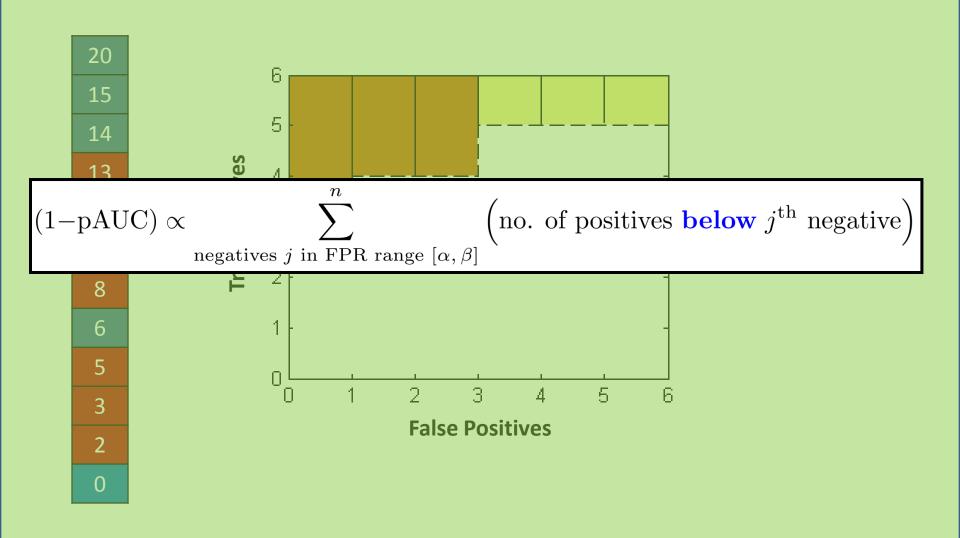






$$\beta = 0.5$$

Top 3 negatives!

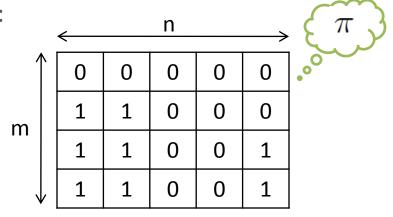


(1 - pAUC) for f

Convex Upper Bound (1 - pAUC) for f

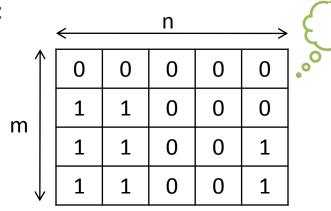
Convex Upper Bound
$$(1 - pAUC) for f + Regularizer$$

Ordering of training examples:



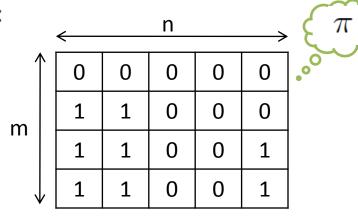
Narasimhan and Agarwal, 2013

Ordering of training examples:



Scoring function f

Ordering of training examples:

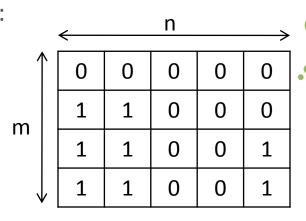


Scoring function f

$$\begin{array}{c} (1-\mathrm{pAUC}) \\ \text{for } \pi \end{array} + \begin{array}{c} \operatorname{term\ capturing} \\ \text{agreement\ between} \ \pi \ \text{and} \ f \\ \text{on\ all\ pairs} \end{array}$$

SVMpAUC: Structural SVM Approach
Narasimhan and Agarwal, 2013

Ordering of training examples:



Scoring function f

$$\max_{\substack{\text{ordering matrices } \pi \\ \text{of size } m \times n}} \left((1 - \text{pAUC}) + \underset{\text{on all pairs}}{\text{term capturing}} + \underset{\text{on all pairs}}{\text{term capturing}} \right)$$

SVMpAUC: Structural SVM Approach
Narasimhan and Agarwal, 2013

Convex Upper Bound

$$(1-pAUC)$$
 for f + Regularizer



$$\max_{\substack{\text{ordering matrices } \pi \\ \text{of size } m \times n}} \left((1 - \text{pAUC}) \atop \text{for } \pi \right) + \text{agreement between } \pi \text{ and } f \atop \text{on all pairs} \right)$$

$$\max_{\substack{\text{ordering matrices } \pi \\ \text{of size } m \times n}} \left((1 - \text{pAUC}) + \underset{\text{on all pairs}}{\text{term capturing}} + \underset{\text{on all pairs}}{\text{term capturing}} \right)$$

How does this upper bound look?

Convex Upper Bound
$$(1 - pAUC) for f + Regularizer$$

$$\max_{\substack{\text{ordering matrices } \pi \\ \text{of size } m \times n}} \left((1 - \text{pAUC}) + \text{agreement between } \pi \text{ and } f \right)$$

Can we obtain a tighter upper bound?

Outline

- Overview of SVMpAUC
- Upper Bound Optimized by SVMpAUC
- Improved Formulation: SVMpAUC-tight
- Optimization Methods
- Experiments

1 - pAUC

```
\sum_{\substack{\text{negatives } j \text{ in} \\ \text{FPR range } [\alpha, \beta]}}^{n} \left(\text{no. of positives below } j^{\text{th}} \text{ negative}\right)
```

1 - pAUC

1 - pAUC

1 - pAUC

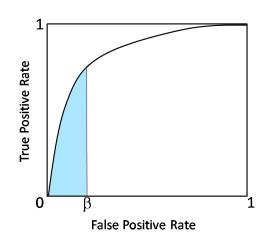
$$\underset{\text{negatives } j \text{ in } i=1}{\overset{m}{\sum}} \sum_{i=1}^{m} \mathbf{1} \left(f(x_i^+) - f(x_j^-) \le 0 \right)$$

$$\underset{\text{FPR range } [\alpha, \beta]}{\overset{m}{\sum}} \sum_{i=1}^{m} \mathbf{1} \left(f(x_i^+) - f(x_j^-) \le 0 \right)$$

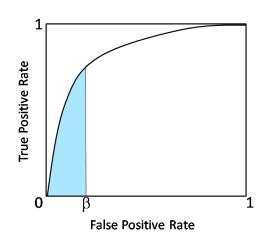
$$\leq \sum_{\text{negatives } j \text{ in }}^{n} \sum_{i=1}^{m} \frac{\text{hinge-loss}(f(x_i^+) - f(x_j^-))}{\text{hinge-loss}(f(x_i^+) - f(x_j^-))}$$

FPR range $[\alpha, \beta]$ pair-wise hinge loss!

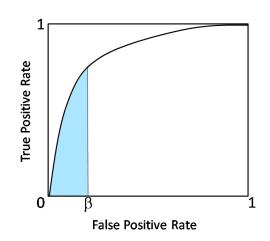
$$\max_{\substack{\text{ordering matrices } \pi \\ \text{of size } m \times n}} \left((1 - \text{pAUC}) + \text{agreement between } \pi \text{ and } f \right)$$



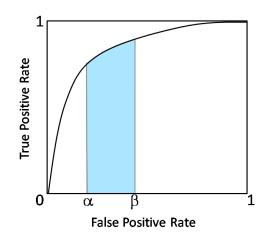
$$\max_{\substack{\text{ordering matrices } \pi \\ \text{of size } m \times n}} \left((1 - \text{pAUC}) \atop \text{for } \pi \right) + \text{agreement between } \pi \text{ and } f \atop \text{on all pairs} \right)$$



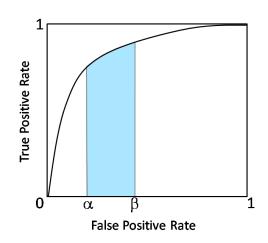
Subset of pairs of positive-negative examples $\max_{\substack{\text{ordering matrices } \pi \\ \text{of size } m \times n}} \left(\frac{(1 - \text{pAUC})}{\text{for } \pi} + \text{agreement between } \frac{\pi}{\pi} \text{ and } f \right)$



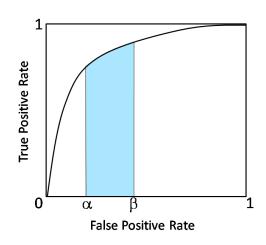
Subset of pairs of positive-negative examples $\max_{\substack{\text{ordering matrices } \pi \\ \text{of size } m \times n}} \left(\frac{(1-\text{pAUC})}{\text{for } \pi} + \text{agreement between } \frac{1}{\pi} \text{ and } f \right)$



$$\frac{\max}{\text{ordering matrices } \pi} \left((1 - \text{pAUC}) + \frac{\text{term capturing}}{\text{agreement between } \pi \text{ and } f} \right) \\
\text{for } \pi + \frac{\text{on all pairs}}{\text{on all pairs}}$$



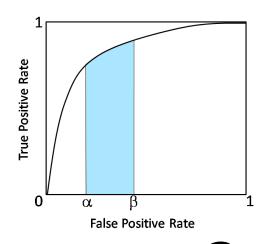
$$\max_{\substack{\text{ordering matrices } \pi \\ \text{of size } m \times n}} \left((1 - \text{pAUC}) + \underset{\text{on all pairs}}{\text{term capturing}} + \underset{\text{on all pairs}}{\text{term capturing}} \right)$$



approx. pair-wise hinge loss + extra term

$$\max_{\substack{\text{ordering matrices } \pi \\ \text{of size } m \times n}} \left((1 - \text{pAUC}) + \underset{\text{on all pairs}}{\text{term capturing}} + \underset{\text{on all pairs}}{\text{term capturing}} \right)$$

 \leq



approx. pair-wise hinge loss + extra term

$$\max_{\substack{\text{ordering matrices } \pi \\ \text{of size } m \times n}} \left((1 - \text{pAUC}) \atop \text{for } \pi \right) + \text{agreement between } \pi \text{ and } f \atop \text{on all pairs} \right)$$

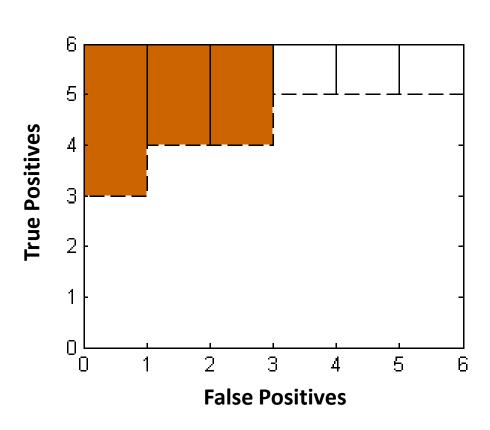
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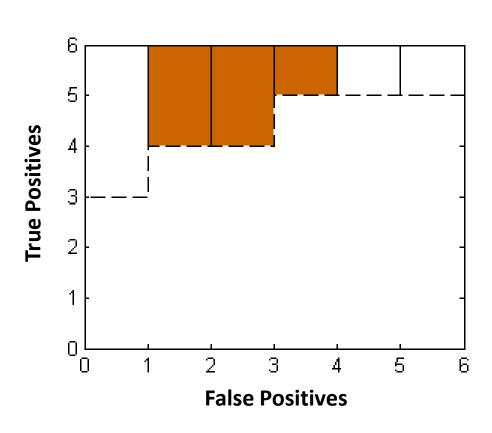
$$\alpha = 0$$
, $\beta = 0.5$





$$3 + 2 + 2 = 7$$

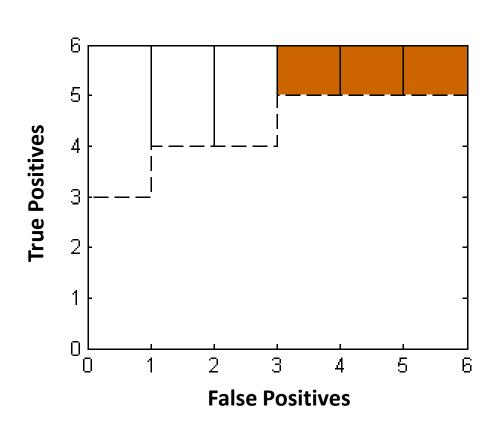
 $\alpha = 0$, $\beta = 0.5$



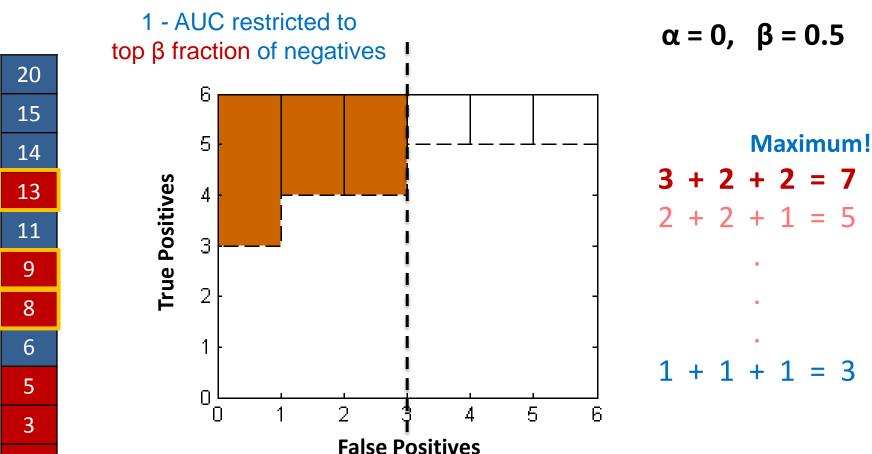
$$3 + 2 + 2 = 7$$

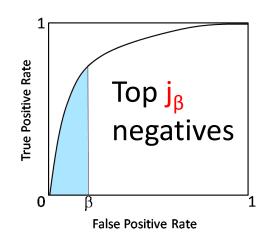
 $2 + 2 + 1 = 5$



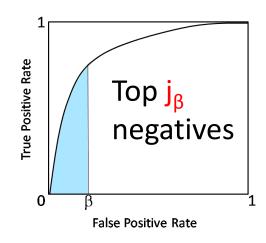


$$3 + 2 + 2 = 7$$
 $2 + 2 + 1 = 5$
 \cdot
 \cdot
 $1 + 1 + 1 = 3$

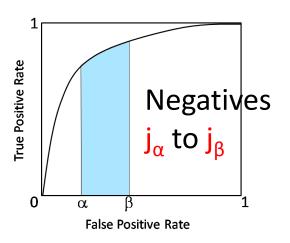




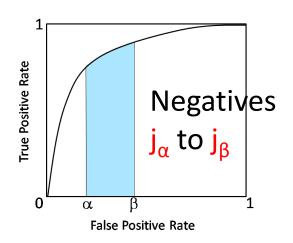
$$(1-pAUC) \propto \max_{\substack{\text{subsets } S \text{ of negatives} \\ \text{of size } j_{\beta}}} \left(1-\text{AUC restricted to negatives in } S\right)$$



$$(1-\text{pAUC}) \propto \max_{\substack{\text{subsets } S \text{ of negatives} \\ \text{of size } j_{\beta}}} \left(\frac{1-\text{AUC restricted to negatives in } S}{1-\text{AUC restricted to negatives in } S} \right)$$



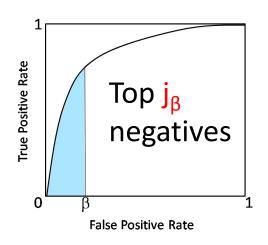
$$(1-pAUC) \propto \max_{\substack{\text{subsets } S \text{ of negatives} \\ \text{of size } j_{\beta}}} \left(1-pAUC \text{ restricted to negatives in } S\right)$$



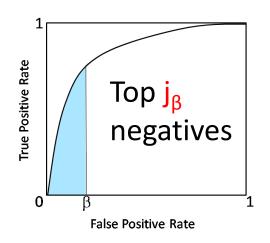
$$(1-\text{pAUC}) \propto \max_{\substack{\text{subsets } S \text{ of negatives} \\ \text{of size } j_{\beta}}} \left(\frac{1-\text{pAUC restricted to negatives in } S}{1-\text{pAUC restricted to negatives in } S}\right)$$

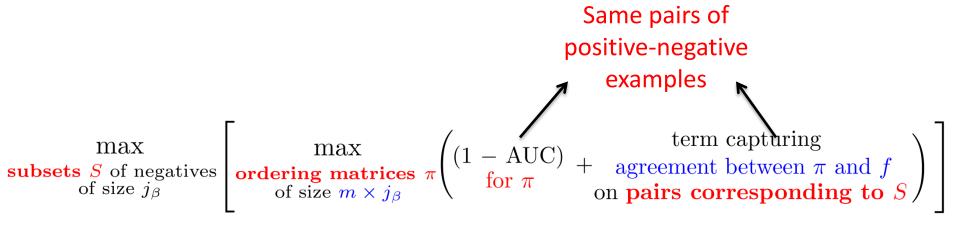
 $\max_{ \substack{ \textbf{subsets} \ S \ \text{of negatives} \\ \text{of size} \ j_{\beta} } }$

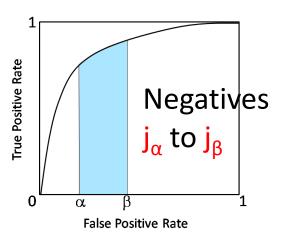
SVMpAUC objective restricted to S



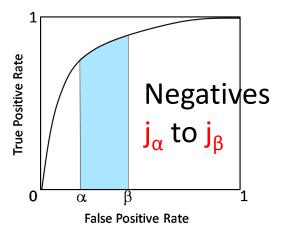
$$\max_{\substack{\text{subsets } S \text{ of negatives} \\ \text{of size } j_{\beta}}} \left[\max_{\substack{\text{ordering matrices } \pi \\ \text{of size } m \times j_{\beta}}} \left((1 - \text{AUC}) + \underset{\text{on pairs corresponding to } S}{\text{term capturing}} \right] \right]$$







```
\max_{\substack{\text{subsets } S \text{ of negatives} \\ \text{of size } j_{\beta}}} \left[ \max_{\substack{\text{ordering matrices } \pi \\ \text{of size } m \times j_{\beta}}} \left( \max_{\substack{\text{for } \pi \\ \text{for } \pi \text{ on pairs corresponding to } S} \right) \right]
```



approx. pair-wise hinge loss + extra term



$$\max_{\substack{\text{subsets } S \text{ of negatives} \\ \text{of size } j_{\beta}}} \begin{bmatrix} \max_{\substack{\text{ordering matrices } \pi \\ \text{of size } m \times j_{\beta}}} \begin{pmatrix} \text{restricted} & \text{term capturing} \\ (1 - \text{pAUC}) + \text{agreement between } \pi \text{ and } f \\ \text{for } \pi & \text{on pairs corresponding to } S \end{pmatrix}$$

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Outline

- Overview of SVMpAUC
- Upper Bound Optimized by SVMpAUC
- Improved Formulation: SVMpAUC-tight
- Optimization Methods
- Experiments

SVMpAUC-tight: Optimization Problem

$$\max_{\substack{\textbf{subsets } S \text{ of negatives} \\ \text{of size } j_{\beta}}} \max_{\substack{\textbf{ordering matrices} \\ \text{of size } m \times j_{\beta}}} \left(\begin{array}{c} \text{restricted} \\ (1-\text{pAUC}) + \text{agreement between } \pi \text{ and } f \\ \text{for } \pi & \text{on pairs corresponding to } S \end{array} \right)$$



+ Regularizer

SVMpAUC-tight: Optimization Problem

$$\max_{\substack{\text{subsets } S \text{ of negatives} \\ \text{of size } j_{\beta}}} \max_{\substack{\text{ordering matrices } \pi \\ \text{of size } m \times j_{\beta}}} \begin{pmatrix} \text{restricted} & \text{term capturing} \\ (1 - \text{pAUC}) + \text{agreement between } \pi \text{ and } f \\ \text{for } \pi & \text{on pairs corresponding to } S \end{pmatrix}$$

exponential in size

+ Regularizer

$$\min_{w,\xi \geq 0} \frac{1}{2} ||w||_2^2 + C\xi$$
s.t. $\forall z \in \mathcal{Z}_{\beta}, \ \pi \in \Pi_{m,j_{\beta}}:$

$$w^{\top} \left(\phi_z(S, \pi^*) - \phi_z(S, \pi)\right) \geq \Delta_{\beta}(\pi^*, \pi) - \xi$$

Quadratic program with an exponential number of constraints

SVMpAUC-tight: Cutting-Plane Solver

$$\min_{w,\xi \ge 0} \frac{1}{2} ||w||_2^2 + C\xi$$

s.t.
$$\forall z \in \mathcal{Z}_{\beta}, \ \pi \in \Pi_{m,j_{\beta}}$$
:

$$w^{ op}ig(\phi_z(S,\pi^*)-\phi_z(S,\pi)ig)\ \geq \Delta_eta(\pi^*,\pi)-\xi$$

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

SVMpAUC-tight: Cutting-Plane Solver

$\min_{w,\xi \ge 0} \frac{1}{2} ||w||_2^2 + C\xi$

s.t. $\forall z \in \mathcal{Z}_{\beta}, \ \pi \in \Pi_{m,j_{\beta}}$:

$$w^{\top} (\phi_z(S, \pi^*) - \phi_z(S, \pi)) \ge \Delta_{\beta}(\pi^*, \pi) - \xi$$

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

SVMpAUC-tight: Cutting-Plane Solver

Repeat:

$$\min_{w,\xi \ge 0} \; \frac{1}{2} ||w||_2^2 + C\xi$$

s.t. $\forall z \in \mathcal{Z}_{\beta}, \ \pi \in \Pi_{m,j_{\beta}}$:

$$w^{\top} (\phi_z(S, \pi^*) - \phi_z(S, \pi)) \ge \Delta_{\beta}(\pi^*, \pi) - \xi$$

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

Better Runtime Guarantees:

Maximum number of iterations
Time taken per iteration

SVMpAUC-tight: Projected Subgradient Solver

Primal formulation:

$$\min_{w} \left[\max_{z \in \mathcal{Z}_{\beta}, \ \pi \in \Pi_{m,j_{\beta}}} \Delta_{\beta}(\pi^*, \pi) - w^{\top} \left(\phi_{z}(S, \pi^*) - \phi_{z}(S, \pi) \right) \right]$$
s.t.
$$||w||_{2} \leq \lambda$$

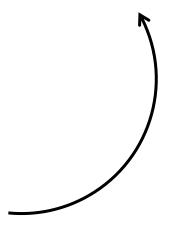
SVMpAUC-tight: Projected Subgradient Solver

Primal formulation:

$$\min_{w} \left[\max_{z \in \mathcal{Z}_{\beta}, \ \pi \in \Pi_{m,j_{\beta}}} \ \Delta_{\beta}(\pi^*, \pi) - w^{\top} (\phi_{z}(S, \pi^*) - \phi_{z}(S, \pi)) \right]$$
s.t.

$$||w||_2 \le \lambda$$

- Compute subgradient and perform update
- 2. Project on to the constraint set.



SVMpAUC-tight: Projected Subgradient Solver

Primal formulation:

$$\min_{w} \left[\max_{z \in \mathcal{Z}_{\beta}, \ \pi \in \Pi_{m,j_{\beta}}} \ \Delta_{\beta}(\pi^*, \pi) - w^{\top} \left(\phi_{z}(S, \pi^*) - \phi_{z}(S, \pi) \right) \right]$$
s.t.

$$||w||_2 \le \lambda$$

Repeat:

- Compute subgradient and perform update
- 2. Project on to the constraint set.

Sparsity-inducing regularizations

LASSO Group LASSO Elastic-Net

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SVMpAUC-tight Vs **SVMpAUC**

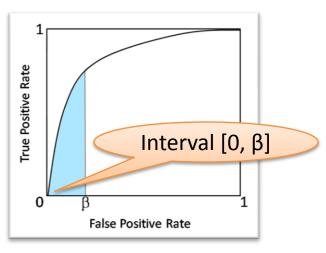
Partial AUC in [0, 0.1]

	Leukemia	PPI	Chem- informatics	KDD Cup 2001	Ovarian Cancer
SVMpAUC-tight	30.44	52.95	65.30	69.91	91.84
SVMpAUC	24.64	51.96	65.28	70.12	91.84
SVMAUC	28.83	39.72	62.78	62.23	92.17

Partial AUC in [0.2s, 0.3s]

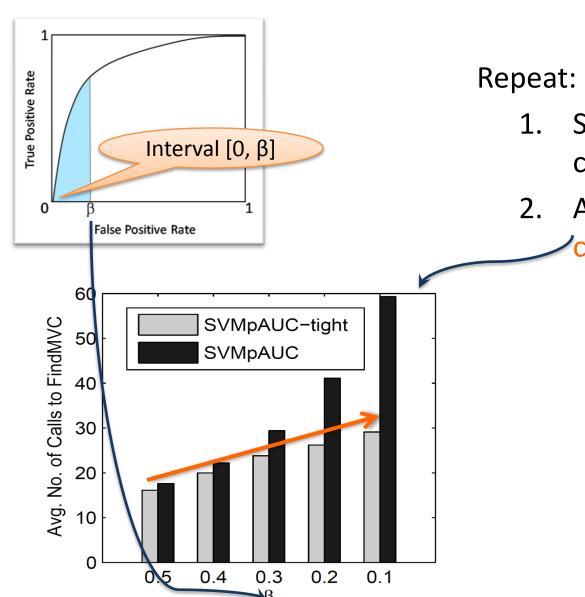
	KDD Cup 2008	
SVMpAUC-tight	53.43	
SVMpAUC	51.89	
SVMAUC	50.66	

Run-time Analysis



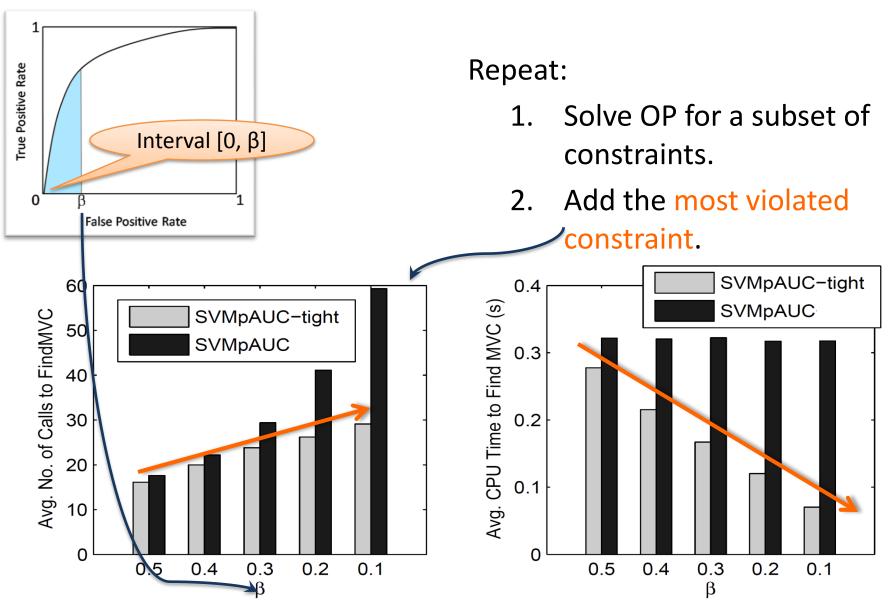
- Solve OP for a subset of constraints.
- Add the most violated constraint.

Run-time Analysis

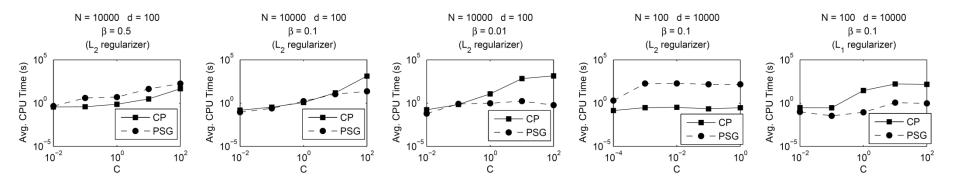


- 1. Solve OP for a subset of constraints.
- Add the most violated constraint.

Run-time Analysis



Cutting-Plane vs. Projected Subgradient



Cutting-plane method is faster on high dimensional data with L2 regularization

Projected subgradient method is faster with L1 regularization

Sparse and Group Sparse Extensions

	pAUC(0, 0.1)			
	Cheminformatics		KDD Cup 2001	
$SVM_{pAUC}^{\ell_2}[0, 0.1]$	63.25	(100)	77.20	(100)
$\mathrm{SVM}_{\mathrm{pAUC}}^{\mathrm{elastic-net}(0.001)}[0, 0.1]$	63.11	(41.5)	77.52	(41.6)
$\mathrm{SVM}_{\mathrm{pAUC}}^{\mathrm{elastic-net}(0.1)}[0, 0.1]$	56.93	(32.24)	71.93	(27.6)
$SVM_{pAUC}^{\ell_1}[0, 0.1]$	53.63	(11.36)	66.22	(10.0)

	pAUC(0, 0.1)	# of groups selected
$SVM_{pAUC}^{\ell_2}[0, 0.1]$	67.09	17
$SVM_{pAUC}^{\ell_1/\ell_2}[0, 0.1]$	65.67	11.3

Sparse models at the cost of decrease in accuracy

Conclusions

- A new support vector algorithm for optimizing partial AUC based on a tight convex upper bound
- Cutting-plane solver with better run-time guarantees
- Experiments on several bioinformatics tasks demonstrate improved accuracy
- Projected subgradient solver allows sparse and group sparse extensions

Questions?