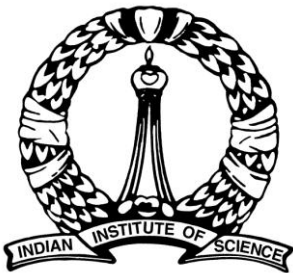


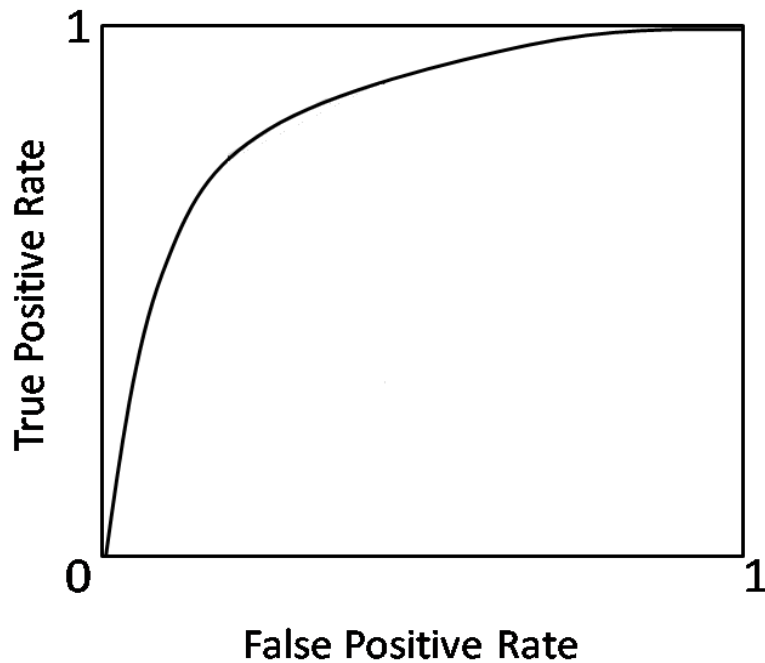
# A Structural SVM Based Approach for Optimizing the Partial AUC

**Harikrishna Narasimhan** and Shivani Agarwal

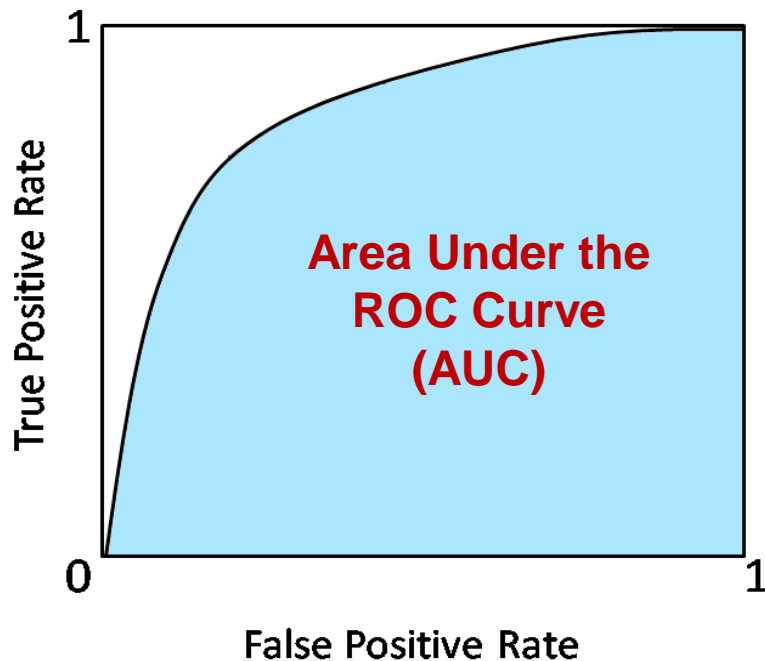


Department of Computer Science and Automation  
Indian Institute of Science, Bangalore

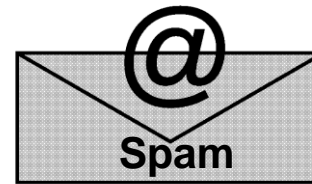
# Receiver Operating Characteristic Curve



# Receiver Operating Characteristic Curve



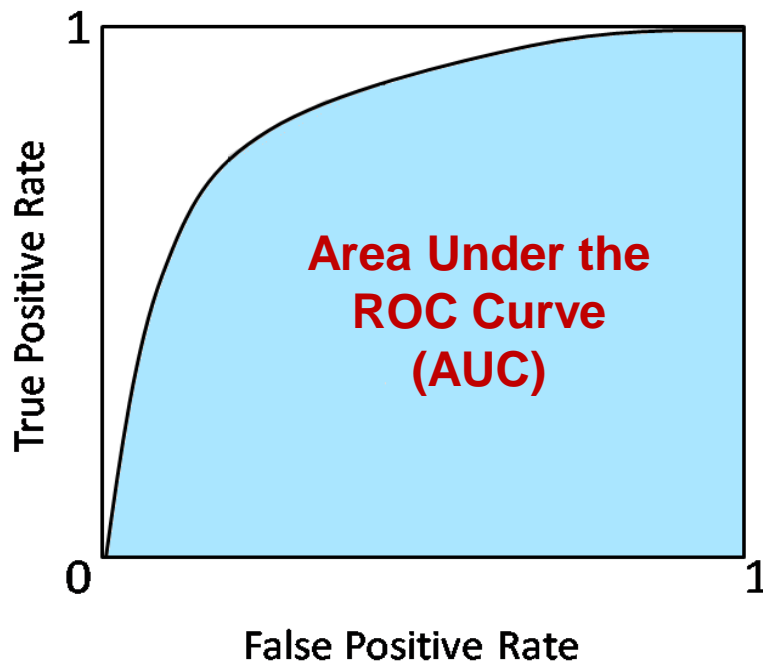
## Binary Classification



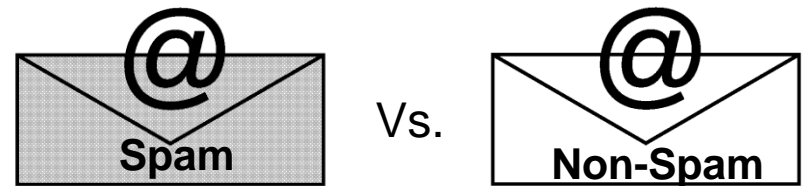
Vs.



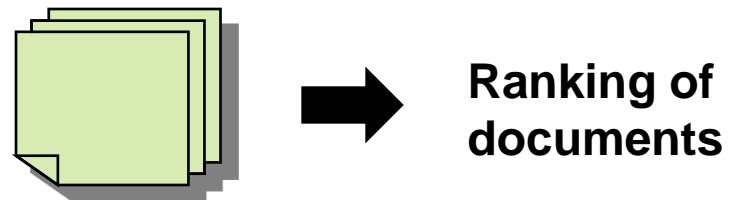
# Receiver Operating Characteristic Curve



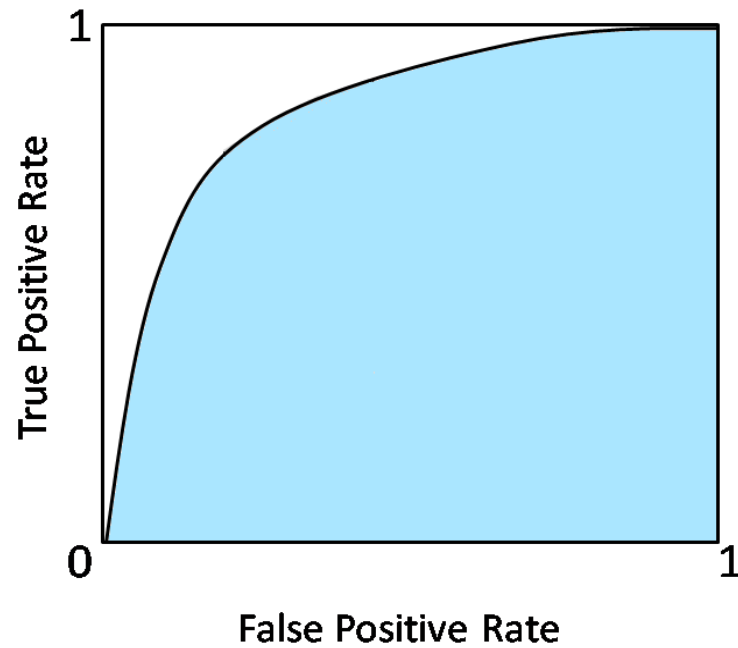
## Binary Classification



## Bipartite Ranking

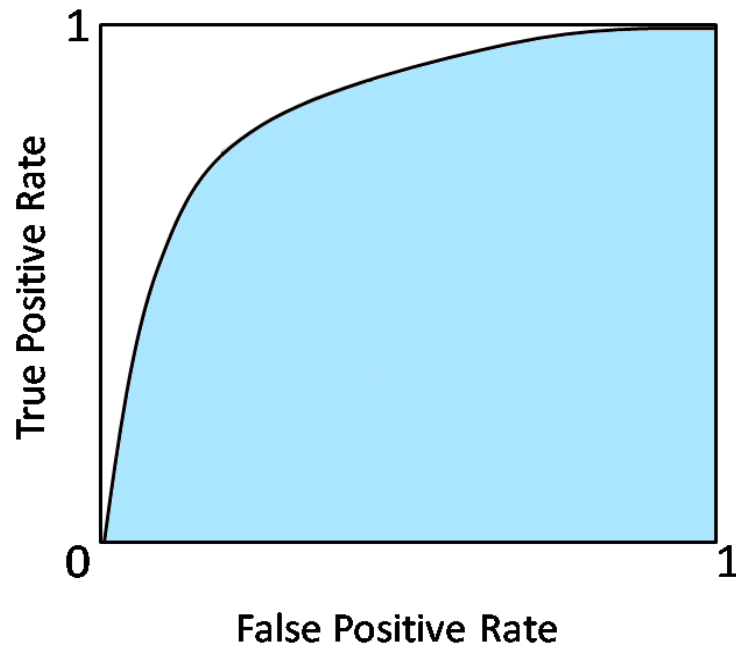


# Partial AUC?



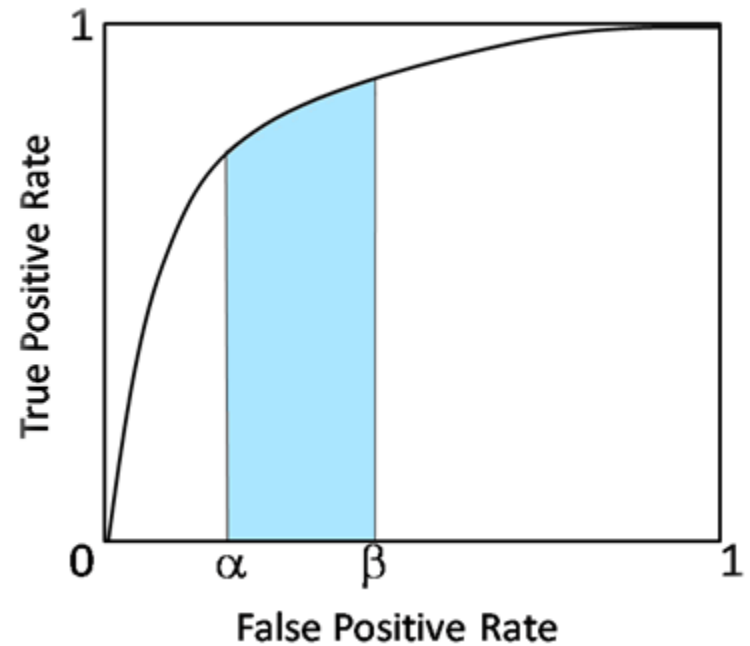
**Full AUC**

# Partial AUC?



**Full AUC**

**Vs**



**Partial AUC**

# Ranking



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learning to rank

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True Positive Rate

1

0

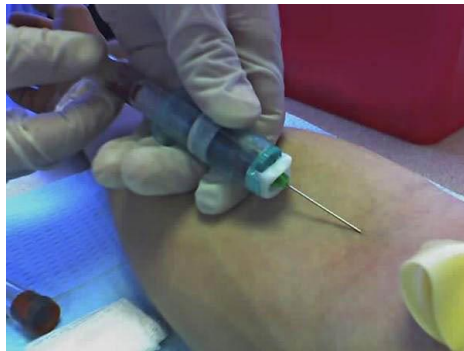
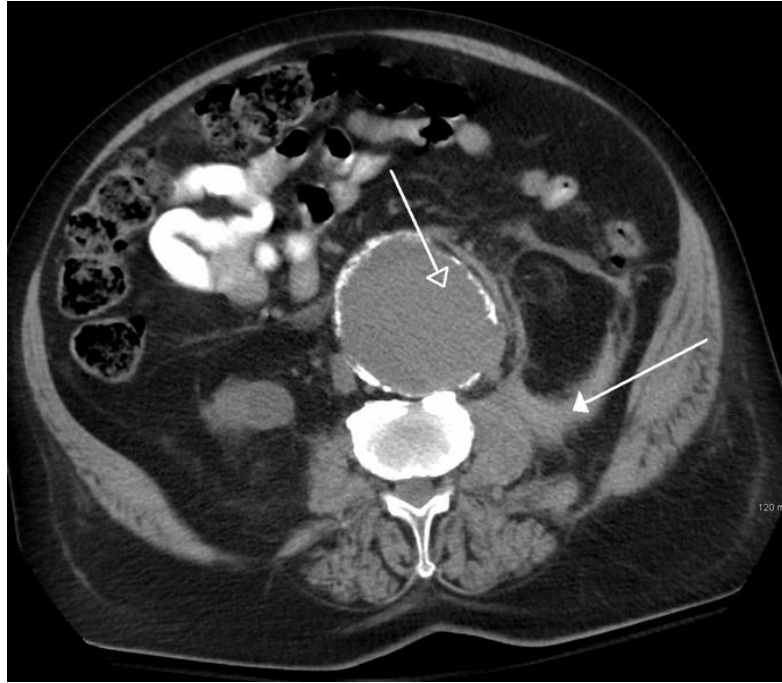
$\beta$

False Positive Rate

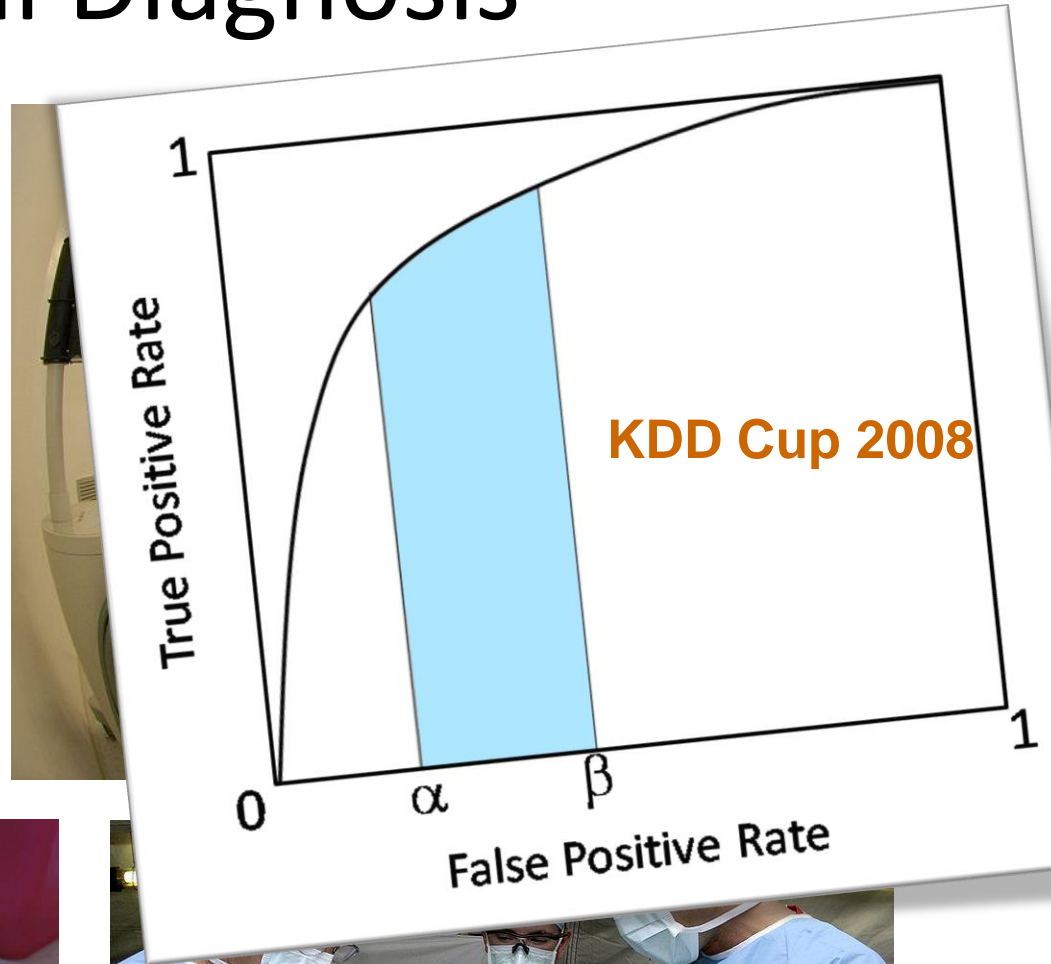
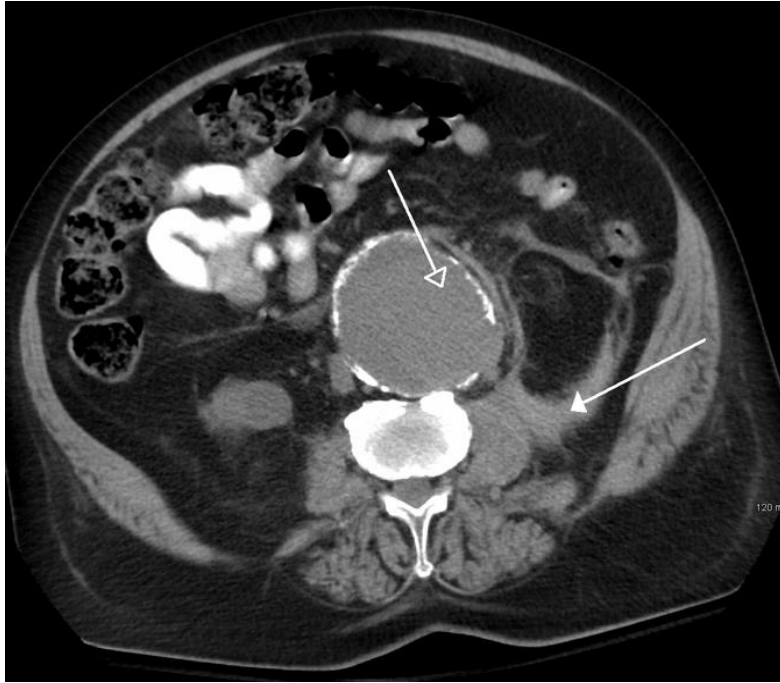
1



# Medical Diagnosis

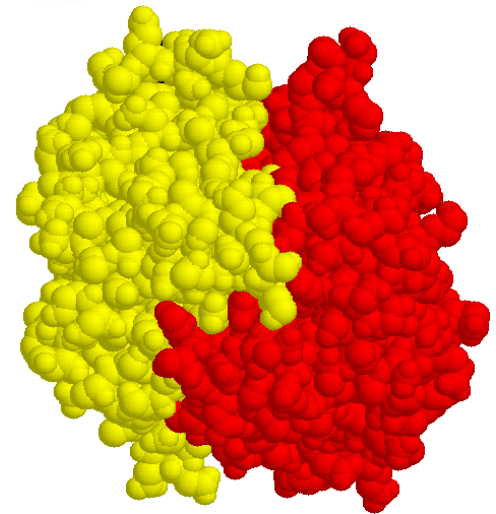
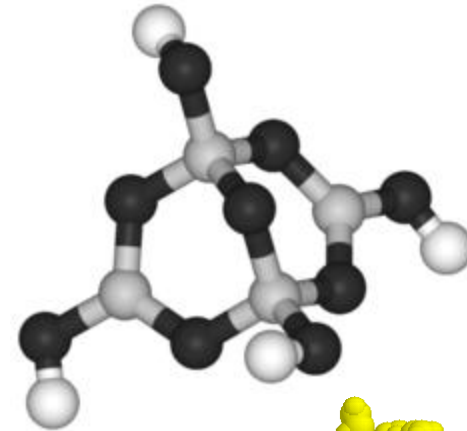
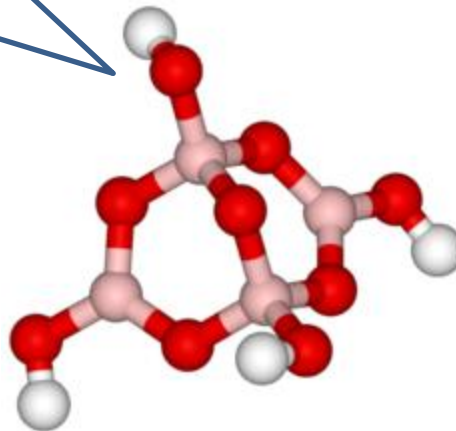
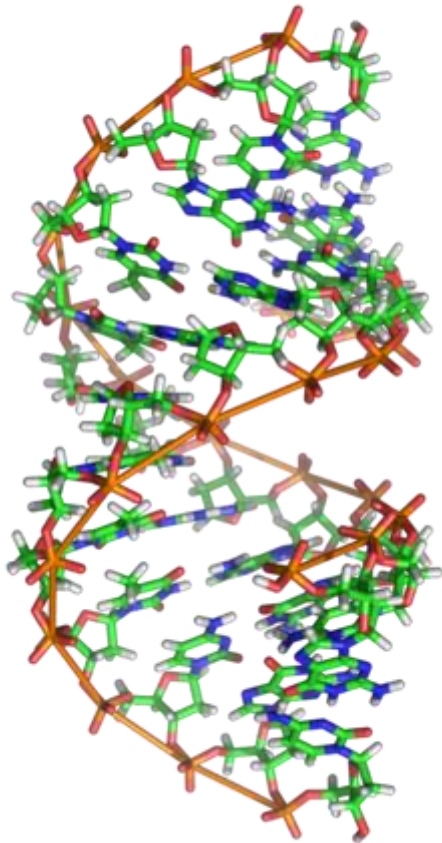


# Medical Diagnosis



# Bioinformatics

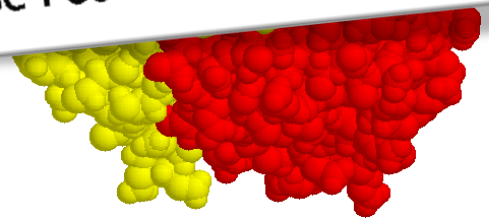
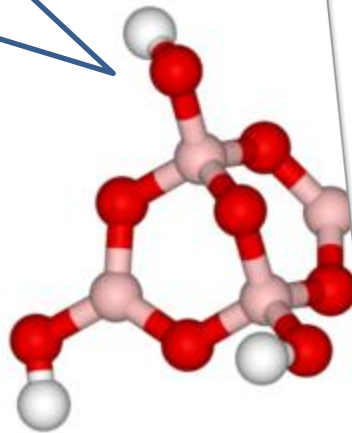
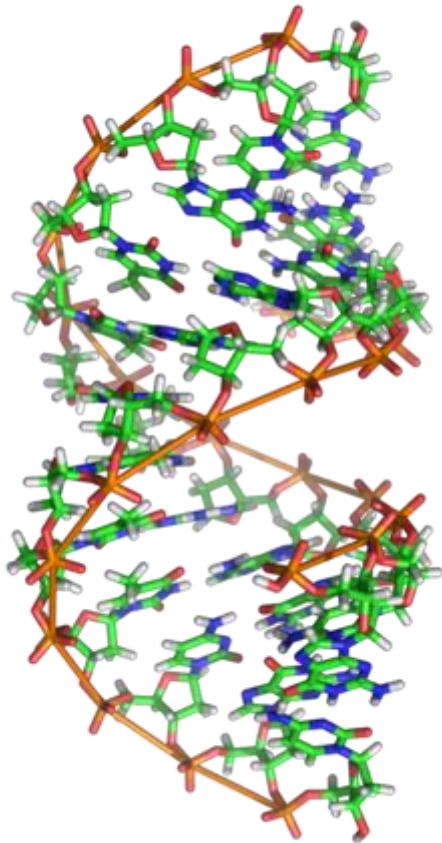
- Drug Discovery
- Gene Prioritization
- Protein Interaction Prediction
- .....





# Bioinformatics

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



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.

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- Improvements over baselines on several real-world applications

# Outline

- Problem Setup
- Structural SVM for Optimizing Partial AUC
- Experiments

# Receiver Operating Characteristic Curve

**Positive Instances**

$x_1^+$

$x_2^+$

$x_3^+$

.....

$x_m^+$

**Negative Instances**

$x_1^-$

$x_2^-$

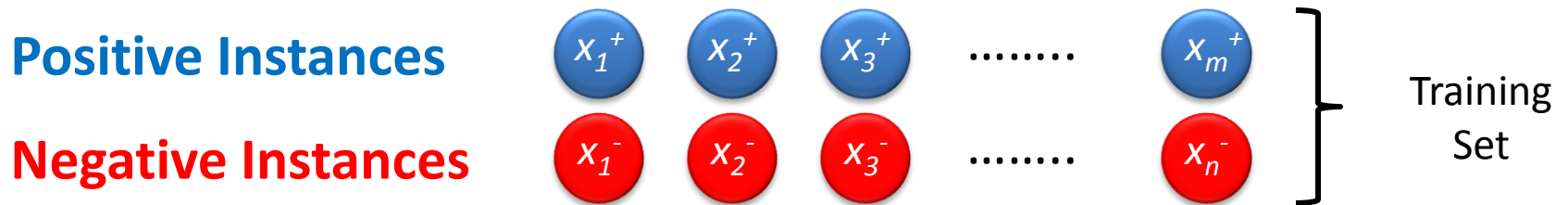
$x_3^-$

.....

$x_n^-$

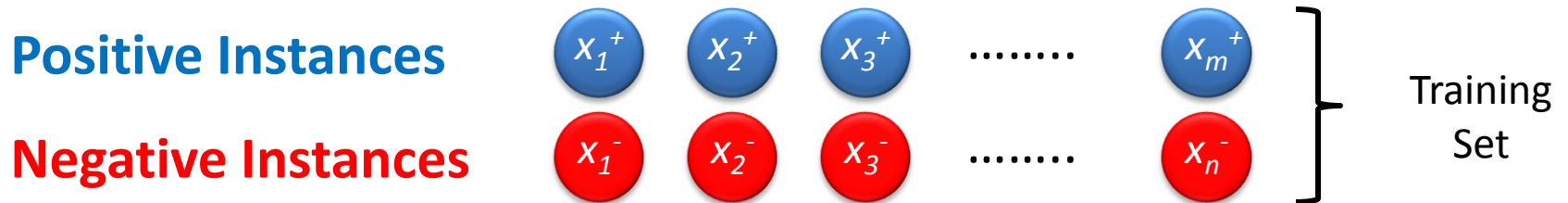
} Training Set

# Receiver Operating Characteristic Curve



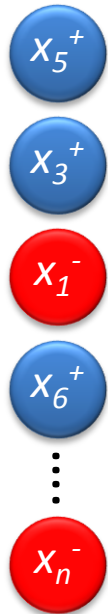
**GOAL?** Learn a scoring function  $f : X \rightarrow \mathbb{R}$

# Receiver Operating Characteristic Curve



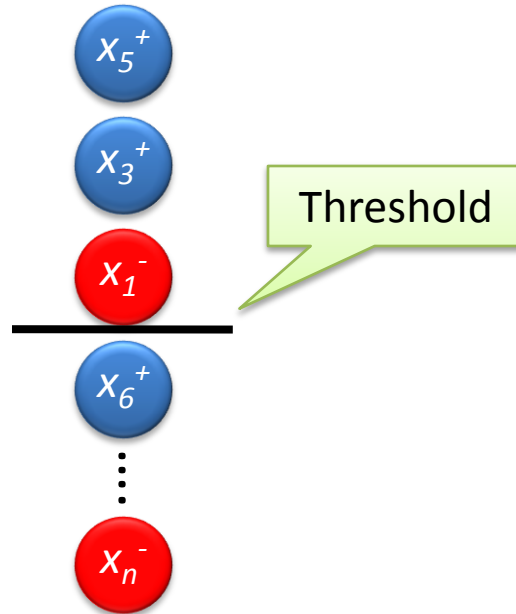
**GOAL?** Learn a scoring function  $f : X \rightarrow \mathbb{R}$

**Rank objects**

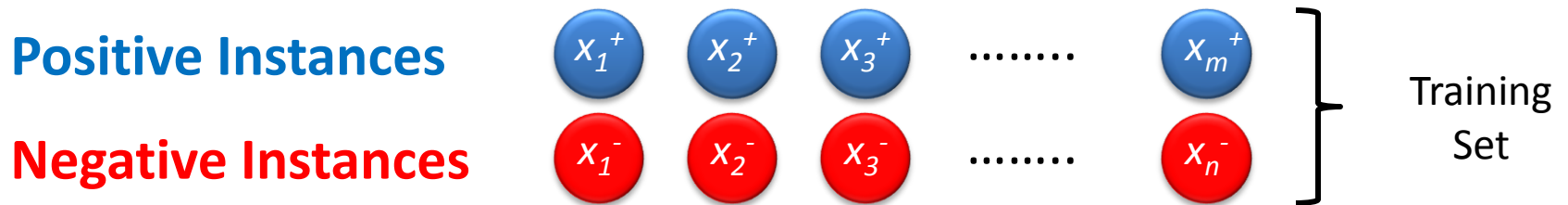


or

**Build a classifier**

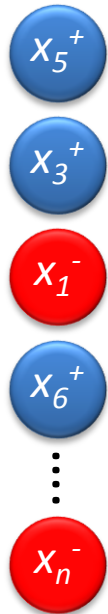


# Receiver Operating Characteristic Curve



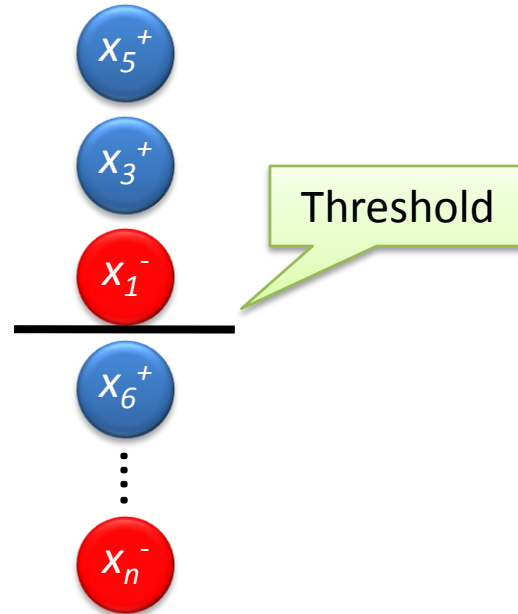
**GOAL?** Learn a scoring function  $f : X \rightarrow \mathbb{R}$

**Rank objects**

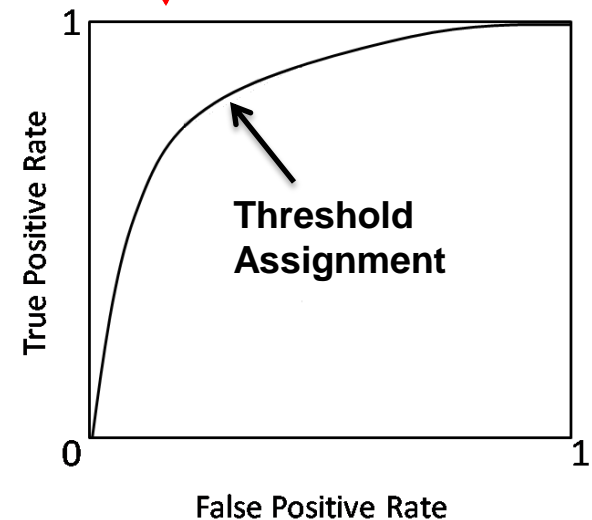


or

**Build a classifier**

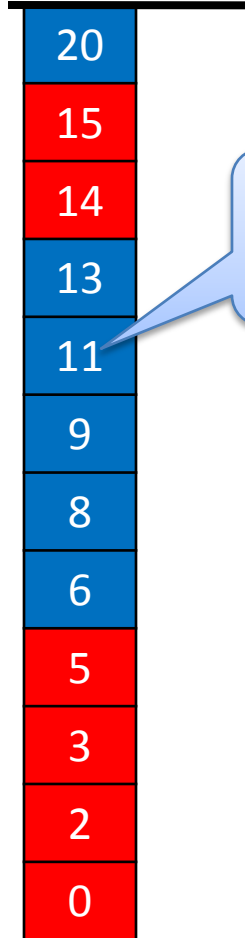


Quality of scoring function?

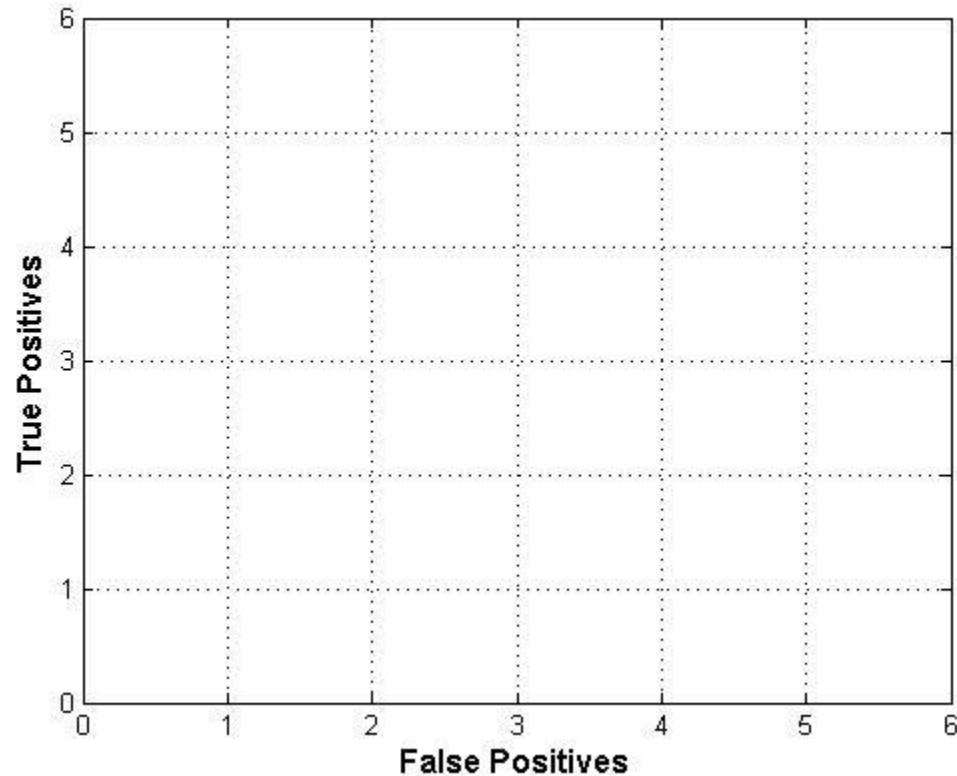


# ROC Curve

## Receiver Operating Characteristic Curve



Scores  
assigned  
by  $f$

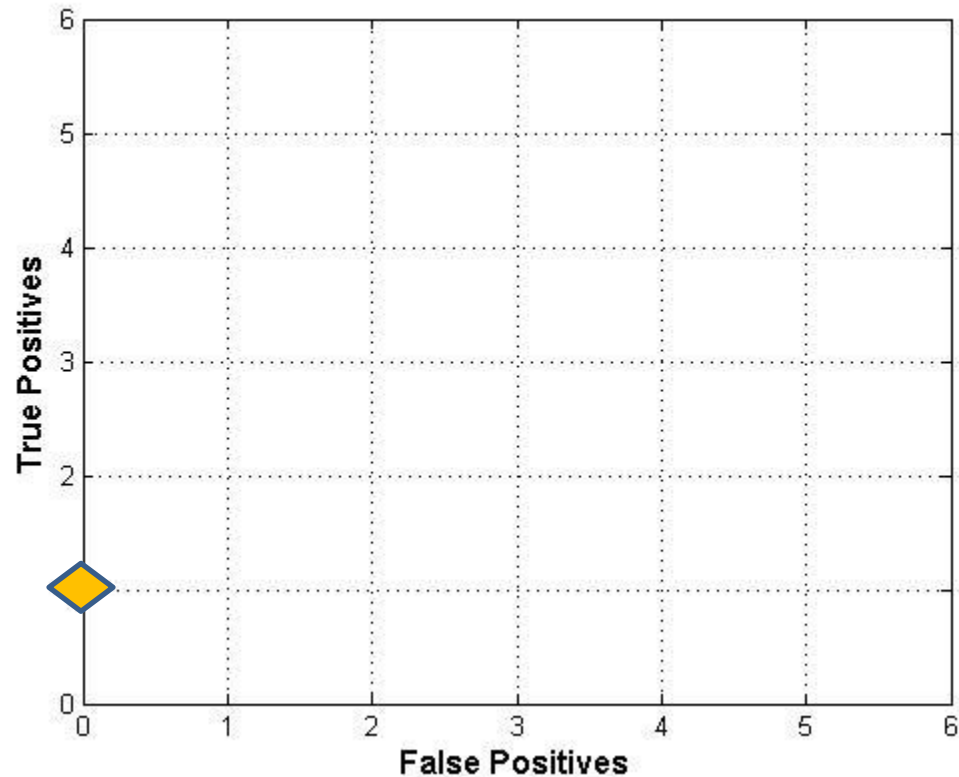




# ROC Curve

Receiver Operating Characteristic Curve

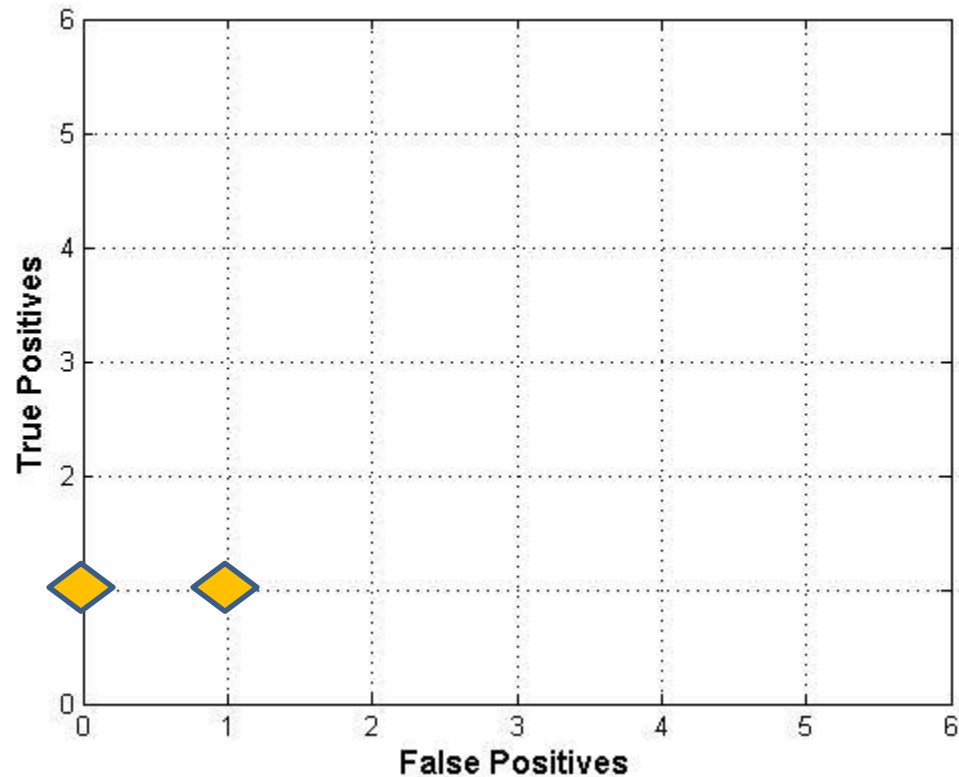
20
15
14
13
11
9
8
6
5
3
2
0



# ROC Curve

Receiver Operating Characteristic Curve

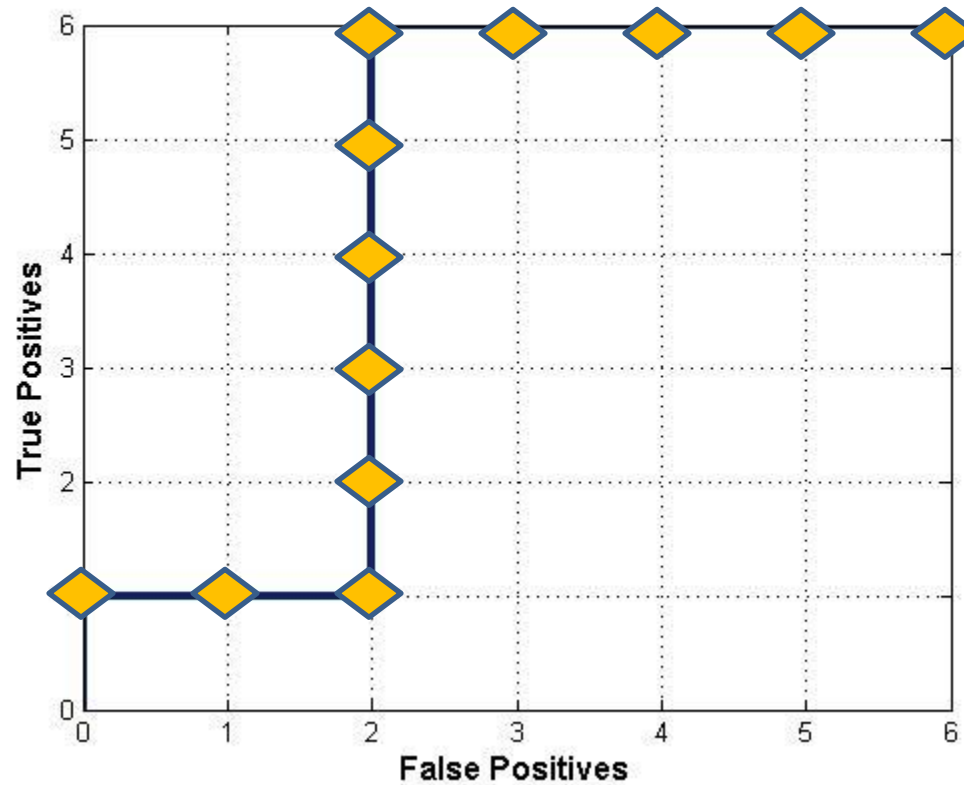
20
15
14
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11
9
8
6
5
3
2
0



# ROC Curve

Receiver Operating Characteristic Curve

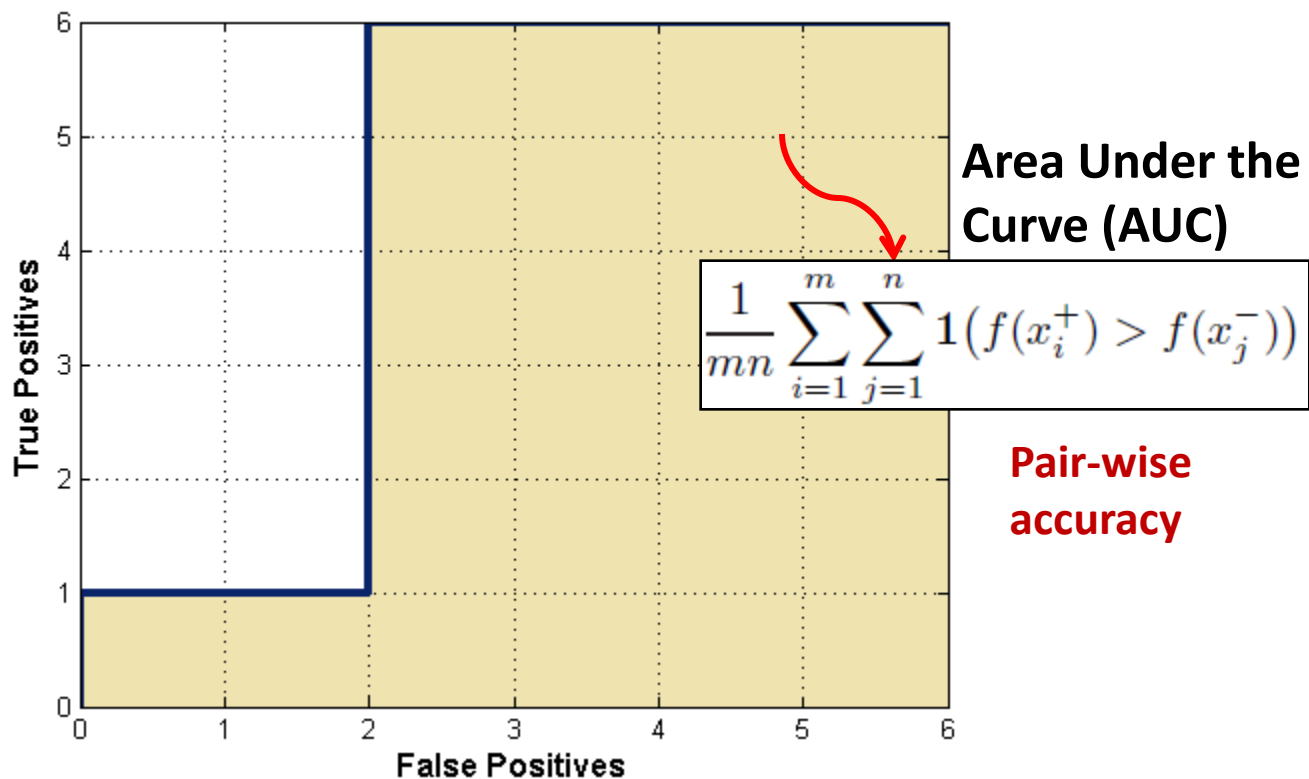
20
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5
3
2
0



# ROC Curve

## Receiver Operating Characteristic Curve

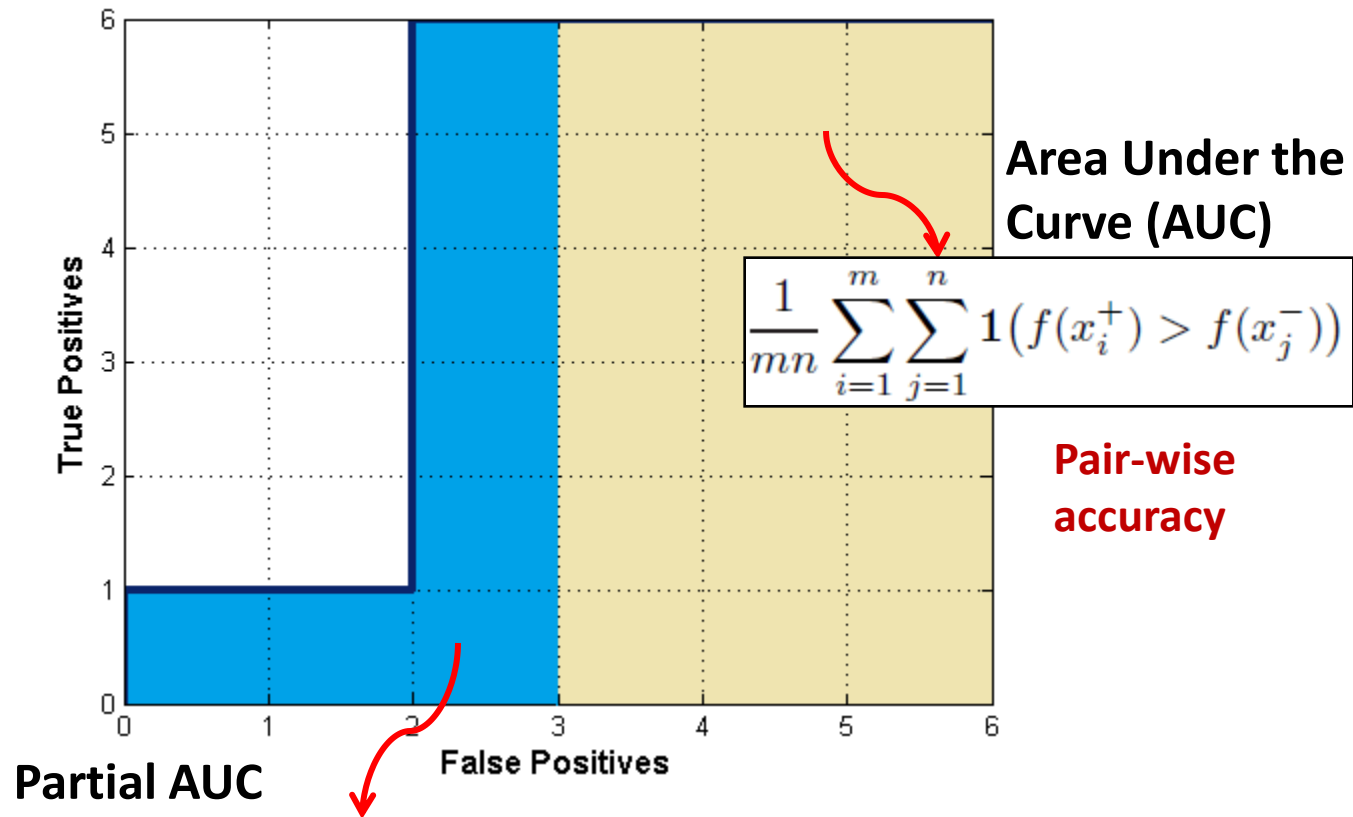
20
15
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2
0



# ROC Curve

## Receiver Operating Characteristic Curve

20
15
14
13
11
9
8
6
5
3
2
0



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

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

# Partial AUC Optimization

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

Discrete and  
Non-differentiable

# Partial AUC Optimization

Minimize:

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

Discrete and  
Non-differentiable



**Convex Upper Bound on “ $1 - \widehat{\text{pAUC}}_f(\alpha, \beta)$ ” + Regularizer**

# Partial AUC Optimization

Minimize:

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

Discrete and  
Non-differentiable



**Convex Upper Bound on “ $1 - \widehat{\text{pAUC}}_f(\alpha, \beta)$ ” + Regularizer**

**Structural SVM**



# Partial AUC Optimization

Minimize:

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**Convex Upper Bound on** “ $1 - \widehat{\text{pAUC}}_f(\alpha, \beta)$ ” **+ Regularizer**

**Structural SVM**

- Extends Joachims' approach for full AUC optimization, but leads to a trickier combinatorial optimization step.

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**Structural SVM**

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

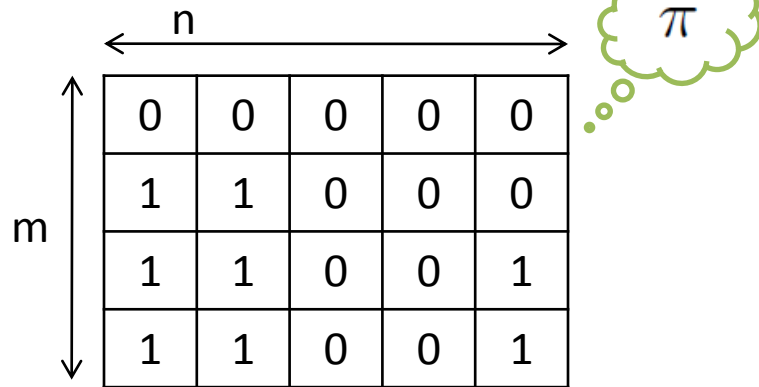
# Outline

- Problem Setup
- Structural SVM for Optimizing Partial AUC
- Experiments

# Structural SVM Based Approach

# Structural SVM Based Approach

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



A diagram illustrating a matrix structure for a Structural SVM. The matrix is 4 rows by 5 columns. The vertical dimension is labeled 'm' and the horizontal dimension is labeled 'n'. The matrix contains binary values (0 and 1). A thought bubble containing the Greek letter  $\pi$  is positioned to the right of the matrix, indicating a permutation or ordering operation.

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

# Structural SVM Based Approach

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

$\leftarrow n \rightarrow$

$\uparrow m \downarrow$

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

$\pi$

compared  
with

0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0

$\pi^*$

**IDEAL**

# Structural SVM Based Approach

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

← n →

m ↑

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

$\pi$

compared with

0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0

$\pi^*$

**IDEAL**

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

s.t.

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

# Structural SVM Based Approach

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

← n

m

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

$\pi$

compared with

0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0

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pAUC Loss



# Structural SVM Based Approach

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

← n

m

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

$\pi$

compared with

0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0

$\pi^*$

IDEAL

Upper Bound on  $(1 - \text{pAUC})$

Regularizer

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

s.t.

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

pAUC Loss

# Structural SVM Based Approach

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

$n$

$m$

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

$\pi$

compared with

0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0

$\pi^*$

IDEAL

Upper Bound on  $(1 - \text{pAUC})$

Regularizer

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

s.t.

pAUC Loss

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

Exponential  
Number of Output  
Matrices!!

# Cutting-plane Solver

Repeat:

1. Solve OP for a subset of constraints.

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

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

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

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Repeat:

$$\begin{aligned} & \min_{w, \xi \geq 0} \frac{1}{2} \|w\|^2 + C\xi \\ \text{s.t. } & \forall \pi \in \mathcal{C} : \\ & w^\top (\phi(S, \pi^*) - \phi(S, \pi)) \geq \Delta_{\text{pAUC}(\alpha, \beta)}(\pi^*, \pi) - \xi \end{aligned}$$

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

# Cutting-plane Solver

Converges in  
**constant** number  
of iterations

Repeat:

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

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

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

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

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**Break down!**

$$\operatorname{argmax}_{\pi} \Delta_{\text{pAUC}(\alpha, \beta)}(\pi^*, \pi) + w^\top (\phi(S, \pi^*) - \phi(S, \pi))$$

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**Break down!**

**Full AUC**

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



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Converges in  
constant number  
of iterations

Repeat:

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

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

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**Break down!**

**Full AUC**

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

**Partial AUC**

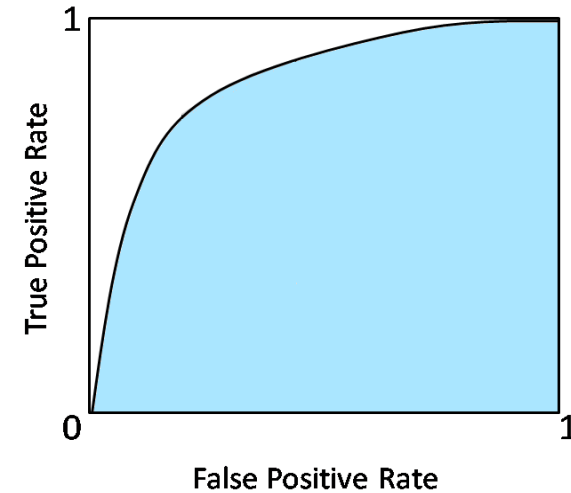
0	1	0	1	0
1	1	0	0	0
1	1	0	0	1
1	1	0	0	1

?

# Trickier Optimization Problem

Full AUC

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

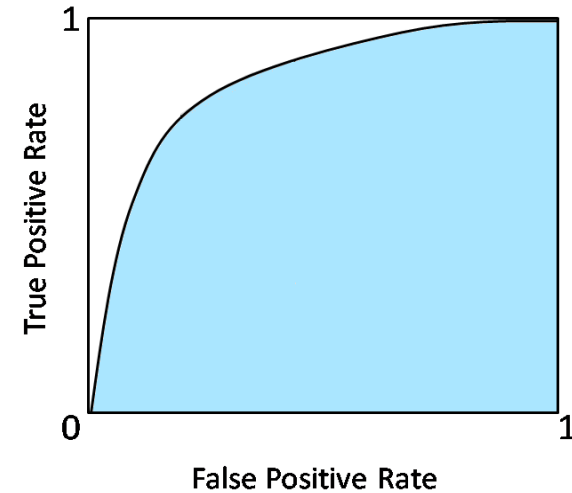


# Trickier Optimization Problem

Full AUC

All Pairs

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

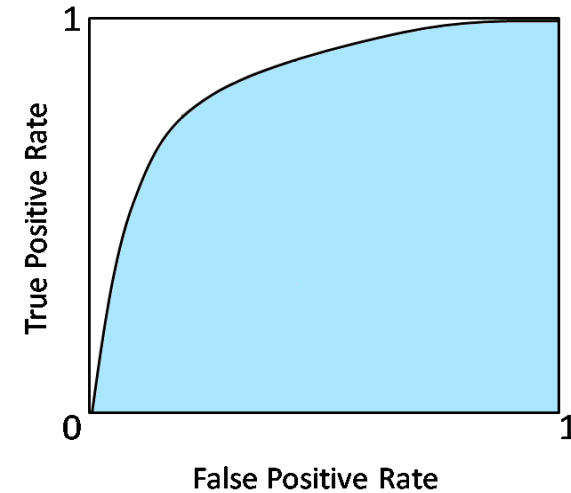


# Trickier Optimization Problem

Full AUC

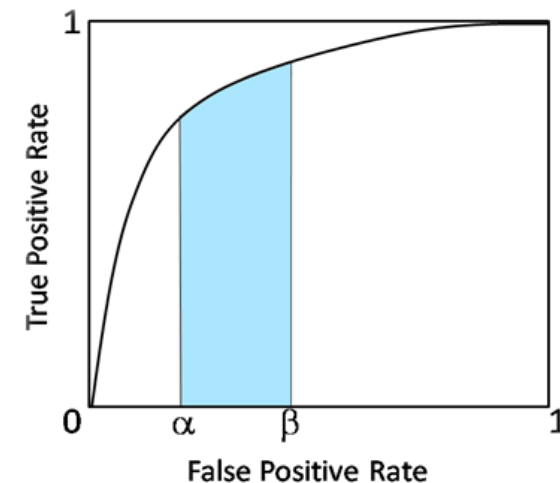
All Pairs

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



Partial AUC

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

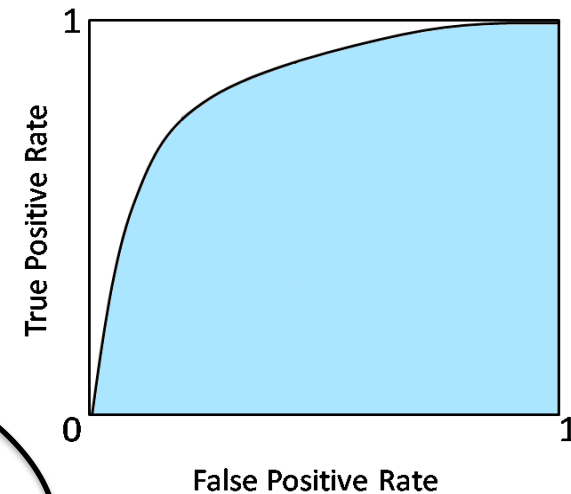


# Trickier Optimization Problem

Full AUC

All Pairs

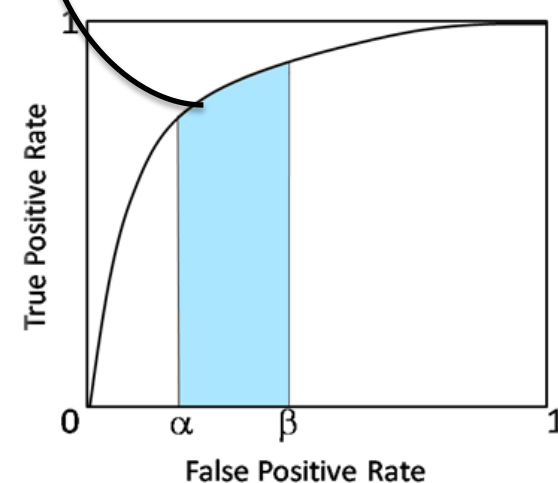
$$\frac{1}{mn} \sum_{i=1}^m \sum_{j=1}^n \mathbf{1}(f(x_i^+) > f(x_j^-))$$



Partial AUC

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

Subset of negative instances in the specified FPR range  $[\alpha, \beta]$



# Find Most Violated Constraint

$$\operatorname{argmax}_{\pi} \Delta_{\text{pAUC}(\alpha, \beta)}(\pi^*, \pi) + w^{\top} (\phi(S, \pi^*) - \phi(S, \pi))$$

**Partial AUC**

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

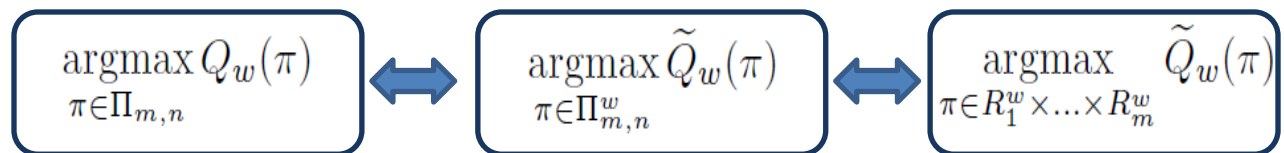
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$$\operatorname{argmax}_{\pi} \Delta_{\text{pAUC}(\alpha, \beta)}(\pi^*, \pi) + w^{\top} (\phi(S, \pi^*) - \phi(S, \pi))$$

**Partial AUC**

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

Equivalent easy-to-solve optimization problem



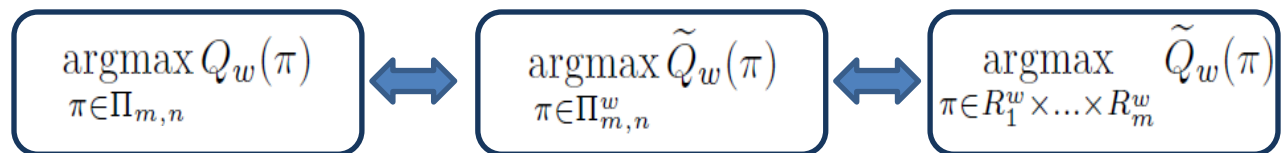
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$$\operatorname{argmax}_{\pi} \Delta_{\text{pAUC}(\alpha, \beta)}(\pi^*, \pi) + w^{\top} (\phi(S, \pi^*) - \phi(S, \pi))$$

**Partial AUC**

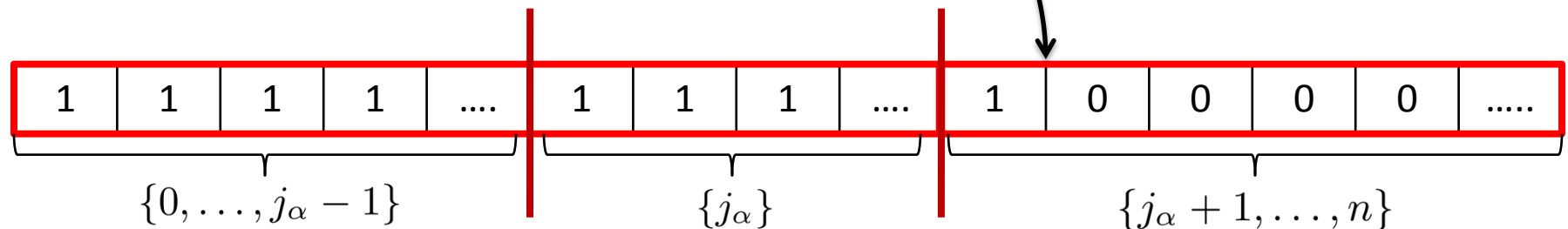
0	1	0	1	0
1	1	0	0	0
1	1	0	0	1
1	1	0	0	1

Equivalent easy-to-solve optimization problem



Divide sorted list of negative examples into 3 parts

$x_i^+$





# Find Most Violated Constraint

$$\operatorname{argmax}_{\pi} \Delta_{\text{pAUC}(\alpha, \beta)}(\pi^*, \pi) + w^{\top} (\phi(S, \pi^*) - \phi(S, \pi))$$

## Partial AUC

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

## Equivalent easy-to-solve optimization problem

$$\operatorname{argmax}_{\pi \in \Pi_{m,n}} Q_w(\pi) \iff \operatorname{argmax}_{\pi \in \Pi_{m,n}^w} \tilde{Q}_w(\pi) \iff \operatorname{argmax}_{\pi \in R_1^w \times \dots \times R_m^w} \tilde{Q}_w(\pi)$$

Divide sorted list of negative examples into 3 parts

$\pi_{i,(j)w}^{(1)} = \begin{cases} 1(w^{\top} x_{i,(j)w}^{\pm} \leq 0), & j \in \{1, \dots, j_{\alpha} - 1\} \\ 0, & j \in \{j_{\alpha}, \dots, n\} \end{cases}$ 
 $\pi_{i,(j)w}^{(2)} = \begin{cases} 1, & j \in \{1, \dots, j_{\alpha}\} \\ 0, & j \in \{j_{\alpha} + 1, \dots, n\} \end{cases}$ 
 $\pi_{i,(j)w}^{(3)} = \begin{cases} 1, & j \in \{1, \dots, j_{\alpha} + 1\} \\ 1(w^{\top} x_{i,(j)w}^{\pm} \leq 1), & j \in \{j_{\alpha} + 2, \dots, j_{\beta}\} \\ 1(w^{\top} x_{i,(j)w}^{\pm} \leq n\beta - j_{\beta}), & j = j_{\beta} + 1 \\ 1(w^{\top} x_{i,(j)w}^{\pm} \leq 0), & j \in \{j_{\beta} + 2, \dots, n\} \end{cases}$

$x_i^+$

**Closed-form solution**

1	1	1	1	....	1	1	1	....	1	0	0	0	0	....
{0, ..., j <sub>α</sub> - 1}					{j <sub>α</sub> }				{j <sub>α</sub> + 1, ..., n}					

# Find Most Violated Constraint

$$\operatorname{argmax} \Delta_{\text{pAUC}(\alpha, \beta)}(\pi^*, \pi) + w^\top (\phi(S, \pi^*) - \phi(S, \pi))$$

1: Inputs:  $S = (S_+, S_-)$ ,  $\alpha$ ,  $\beta$ ,  $w$

2: For  $i = 1, \dots, m$  do

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

$$\pi_{i, (j)_w}^{(1)} = \begin{cases} 1(w^\top x_{i, (j)_w}^\pm \leq 0), & j \in \{1, \dots, j_\alpha - 1\} \\ 0, & j \in \{j_\alpha, \dots, n\} \end{cases}$$

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

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

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

$$\pi_{i, (j)_w}^{(3)} = \begin{cases} 1, & j \in \{1, \dots, j_\alpha + 1\} \\ 1(w^\top x_{i, (j)_w}^\pm \leq 1), & j \in \{j_\alpha + 2, \dots, j_\beta\} \\ 1(w^\top x_{i, (j)_w}^\pm \leq n\beta - j_\beta), & j = j_\beta + 1 \\ 1(w^\top x_{i, (j)_w}^\pm \leq 0), & j \in \{j_\beta + 2, \dots, n\} \end{cases}$$

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

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

8: End For

9: Output:  $\bar{\pi}$

Equivalent to solve optimization problem

$$\operatorname{argmax}_{\pi \in \Pi_{m,n}^w} \tilde{Q}_w(\pi)$$

$$\operatorname{argmax}_{\pi \in R_1^w \times \dots \times R_m^w} \tilde{Q}_w(\pi)$$

Closed-form

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

$$\pi_{i, (j)_w}^{(3)} =$$

$$\begin{cases} 1(w^\top x_{i, (j)_w}^\pm \leq 0), & j \in \{j_\beta + 2, \dots, n\} \end{cases}$$

1	0	0	0	0	.....
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$\{j_\alpha + 1, \dots, n\}$

$\{0, \dots, j_\alpha - 1\}$

$\{j_\alpha\}$

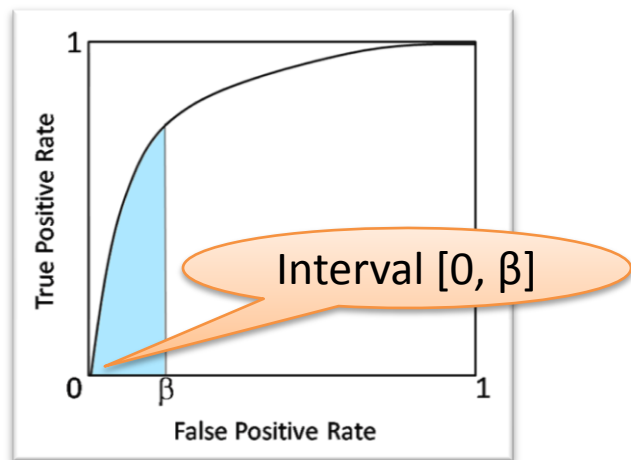
# Outline

- Problem Setup
- Structural SVM for Optimizing Partial AUC
- Experiments

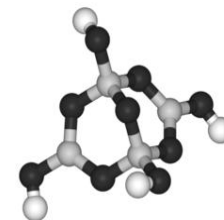
# Experimental Results

## 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 *
$Greedy\text{-}Heuristic[0, 0.1]$	8.33 *

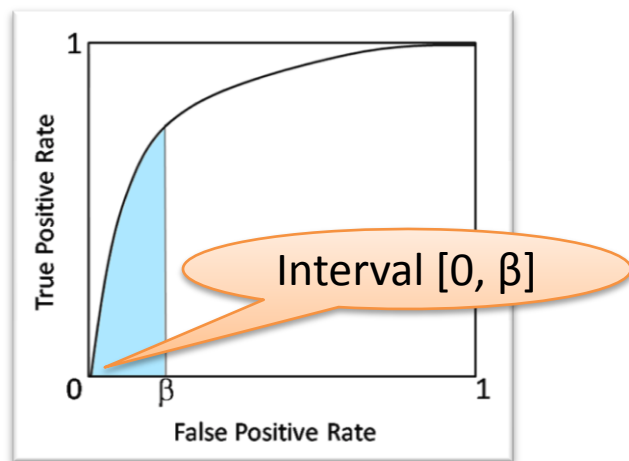
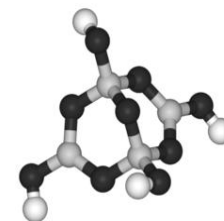


# Experimental Results

## Drug Discovery

50 active compounds / 2092 inactive compounds

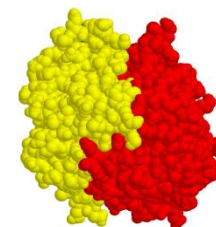
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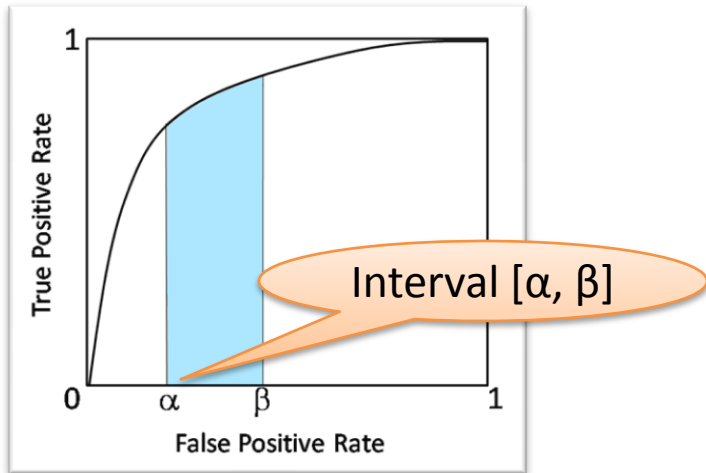
## Protein-Protein Interaction Prediction

$\sim 3 \times 10^3$  interacting pairs /  $\sim 2 \times 10^5$  non-interacting pairs

	pAUC(0, 0.1)
<b>SVM<sub>pAUC</sub>[0,0.1]</b>	<b>51.79</b>
SVM <sub>AUC</sub>	39.72 *
ASVM[0,0.1]	44.51 *
pAUCBoost[0,0.1]	48.65 *
Greedy-Heuristic[0,0.1]	47.33 *



# Experimental Results



## KDD Cup 2008

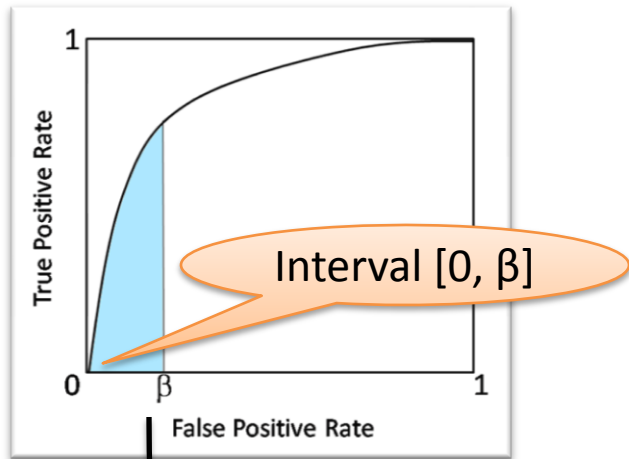
### Breast Cancer Detection

~600 malignant ROIs /  $\sim 10^5$  benign ROIs

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

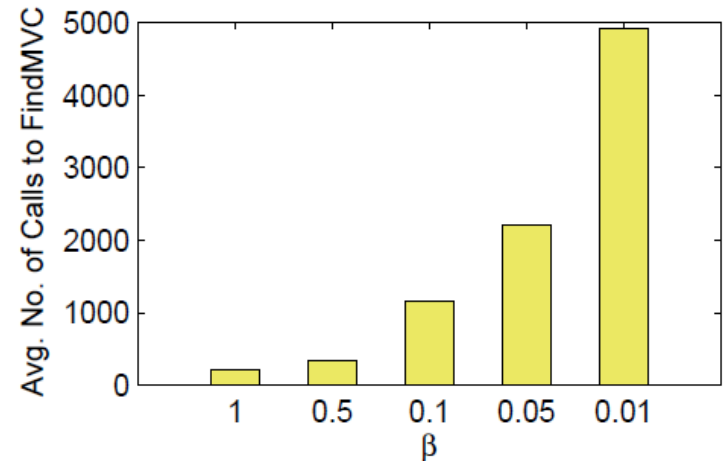
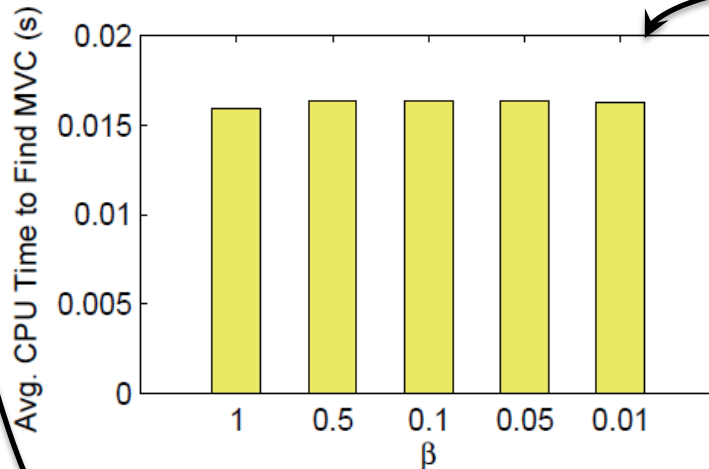
# Experimental Results

## RunTime Analysis



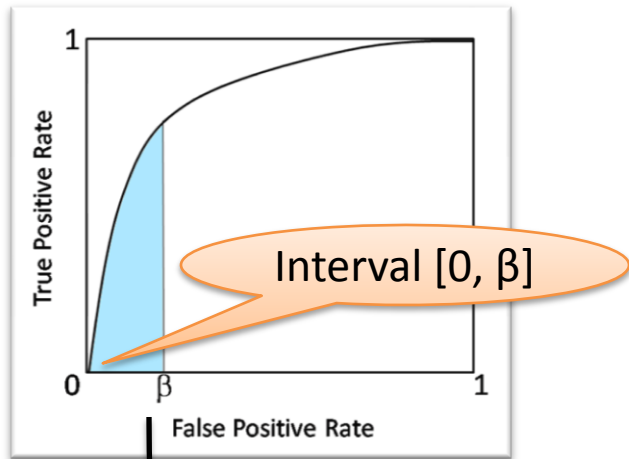
Repeat:

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



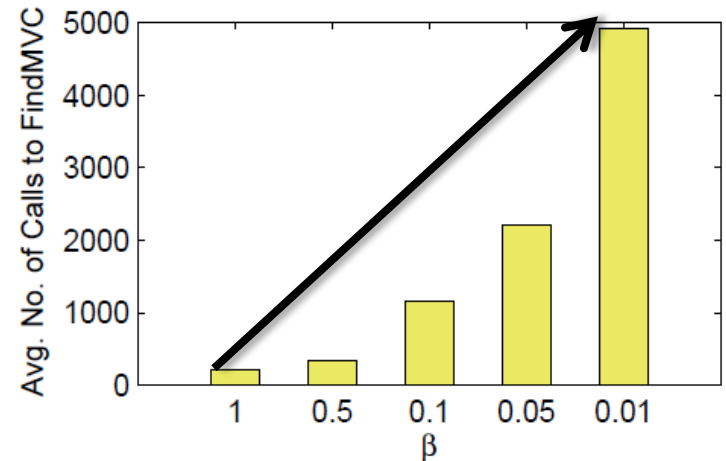
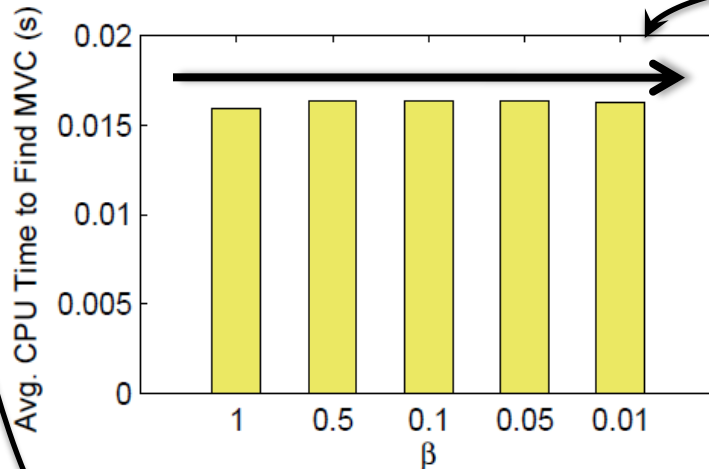
# Experimental Results

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Repeat:

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- Follow up: Improved algorithm that optimizes a tighter upper bound on the partial AUC loss

Narasimhan, H. and Agarwal, S.  $\text{SVM}_{\text{pAUC}}^{\text{tight}}$ : A new support vector method for optimizing partial AUC based on a tight convex upper bound. In *Proceedings of the ACM SIGKDD Conference on Knowledge, Discovery and Data Mining (KDD)*, 2013. To appear.

Questions?