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
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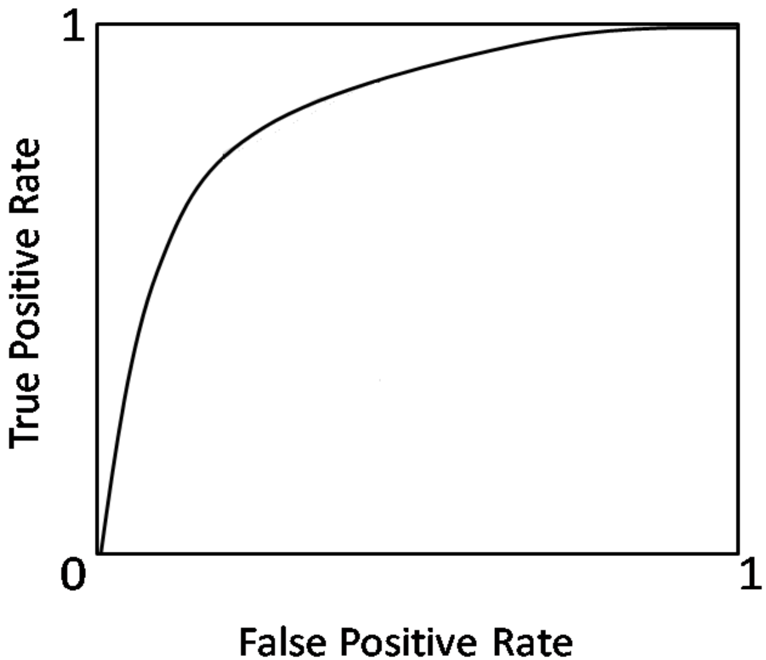
Receiver Operating Characteristic Curve



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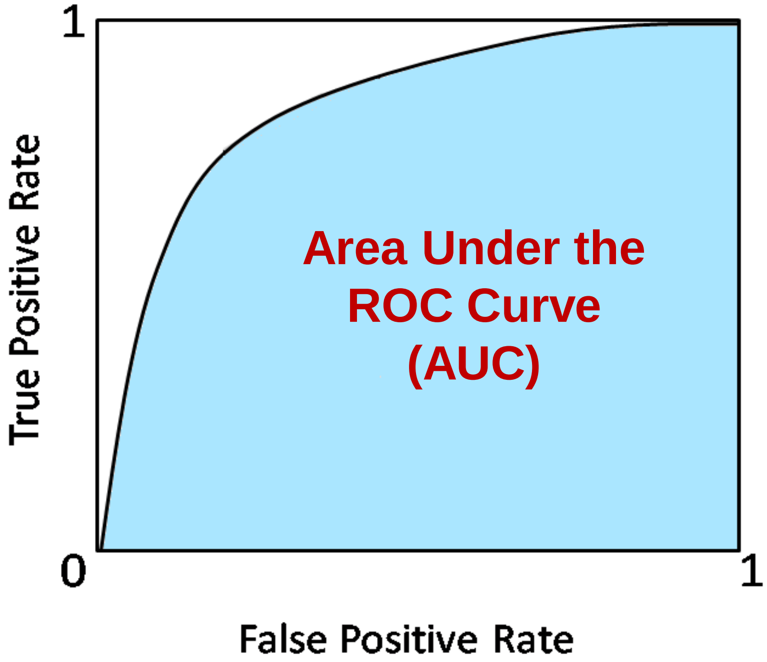
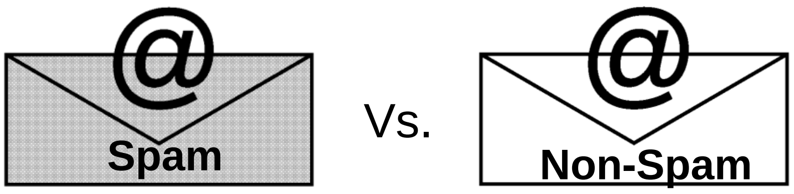


Binary Classification



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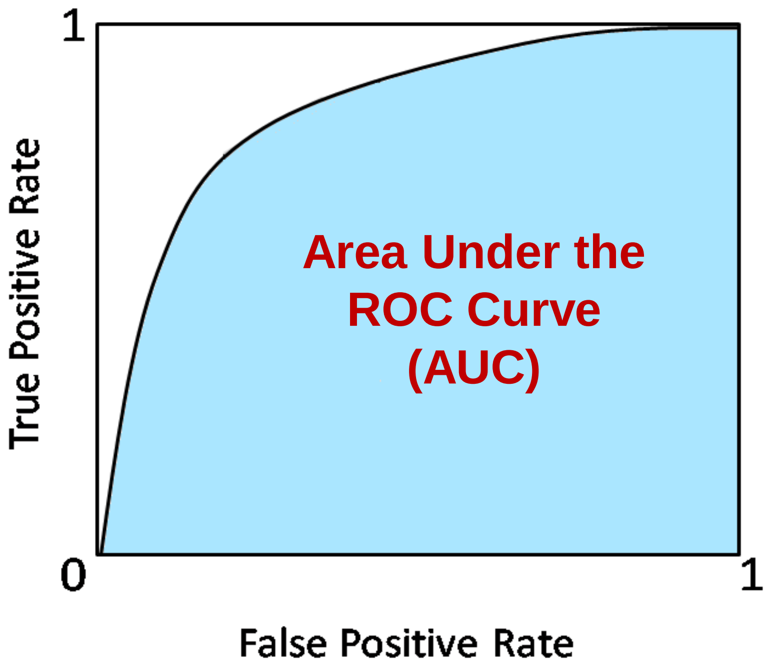

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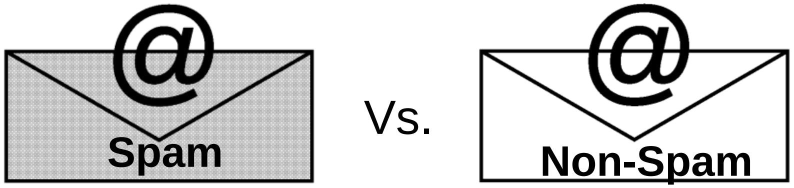
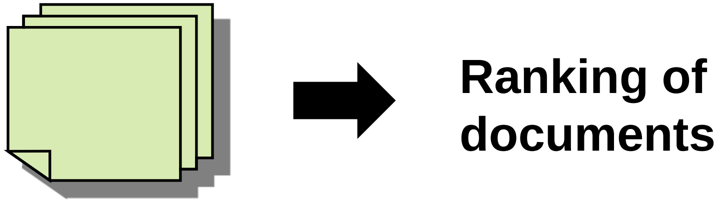
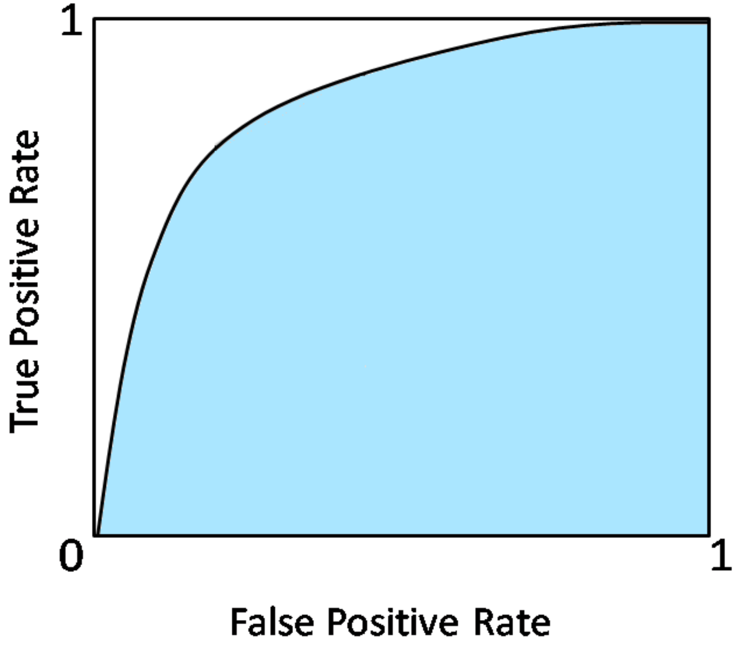


Bipartite Ranking

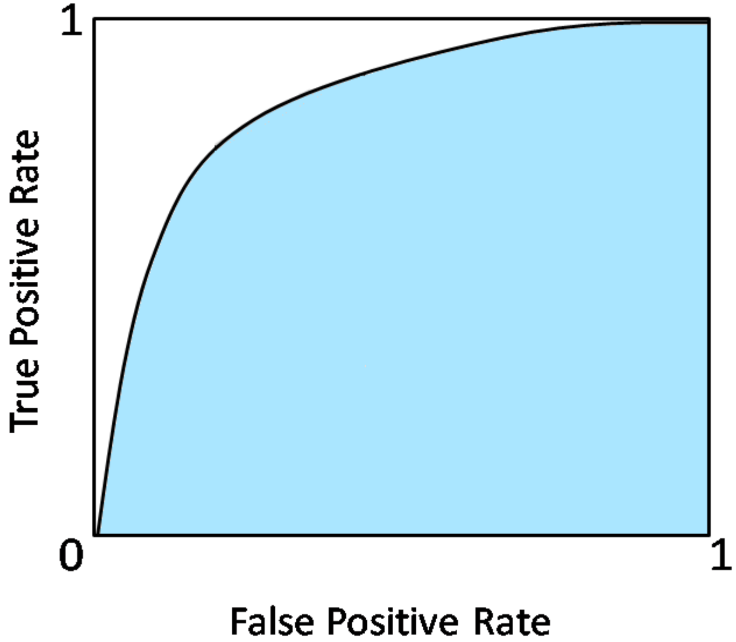


Partial AUC?



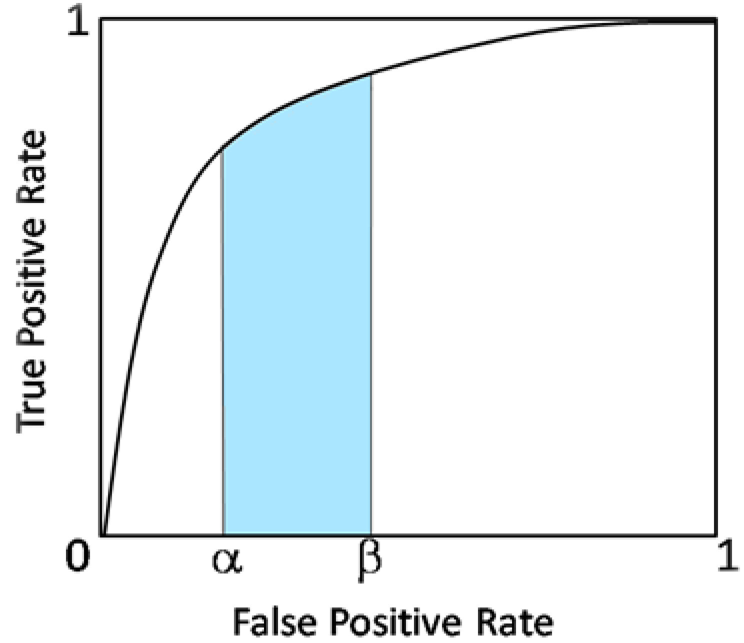
Full AUC

Partial AUC?



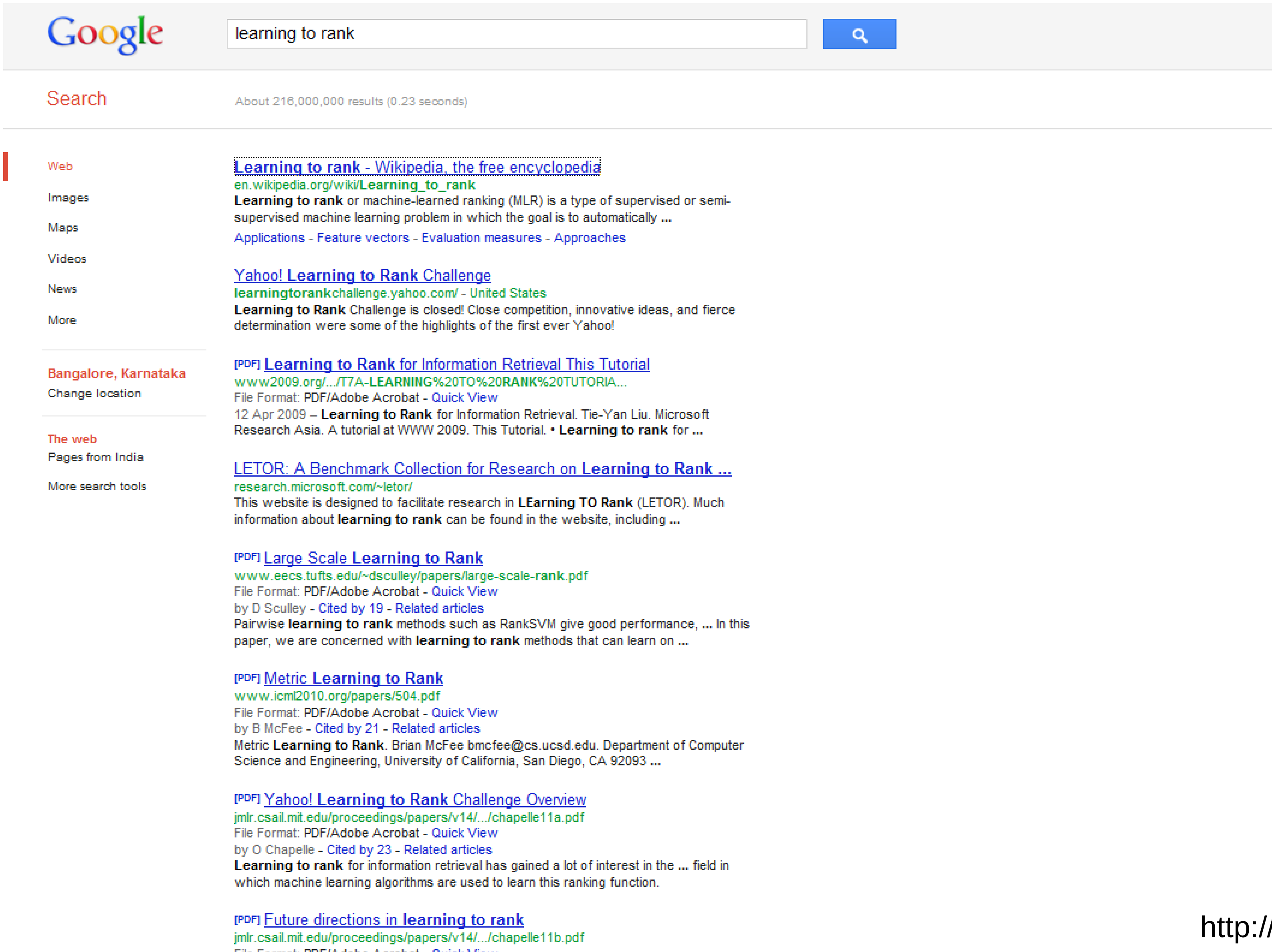
Full AUC

Vs



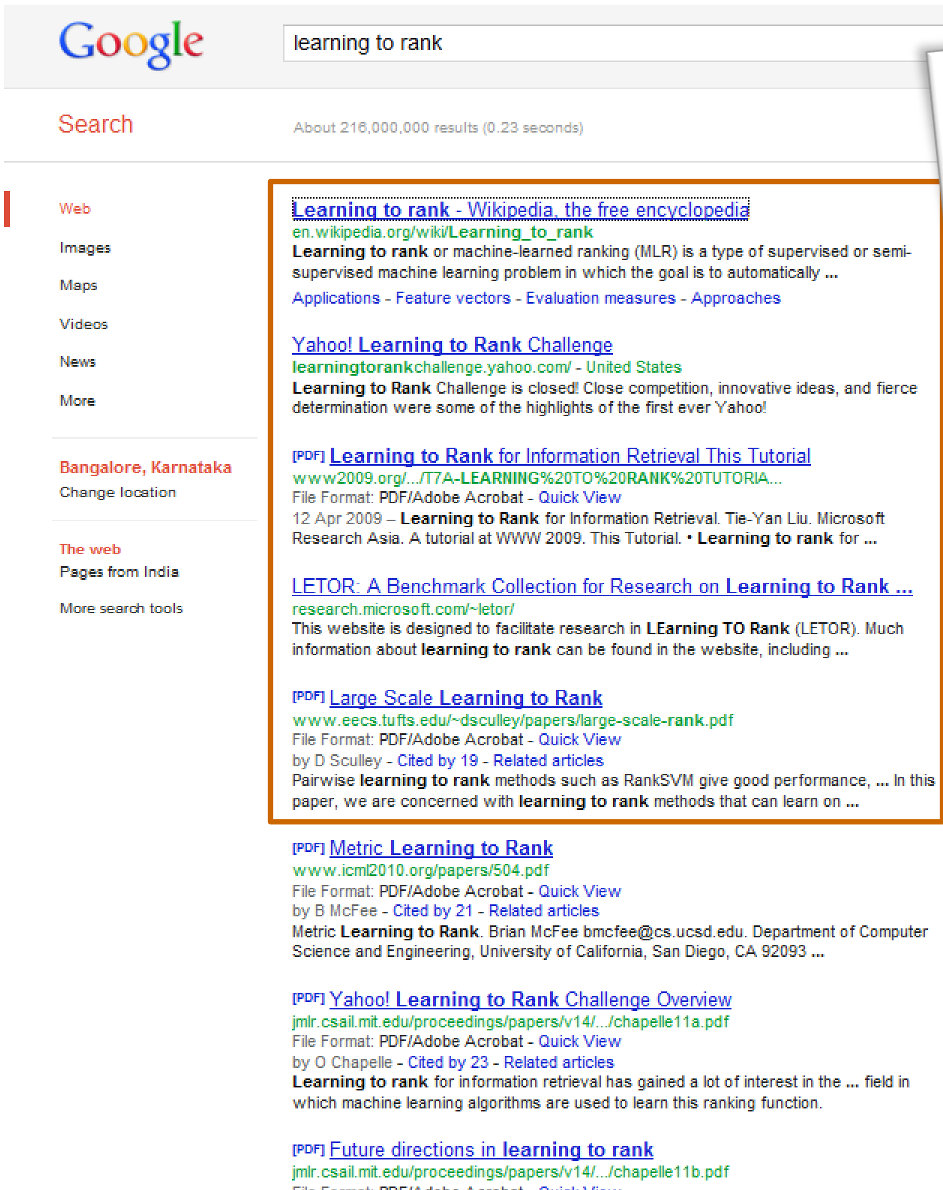
Partial AUC

Ranking



http://www.google.com/

Ranking



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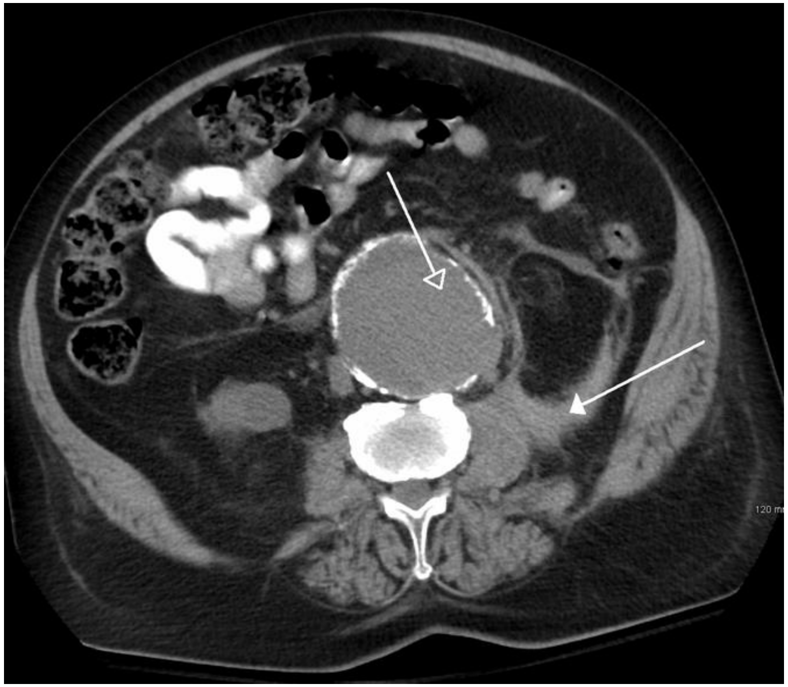
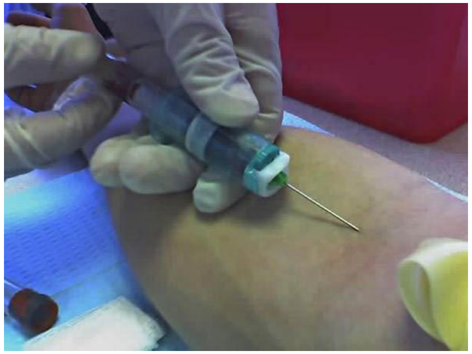
Medical Diagnosis





http://en.wikipedia.org/

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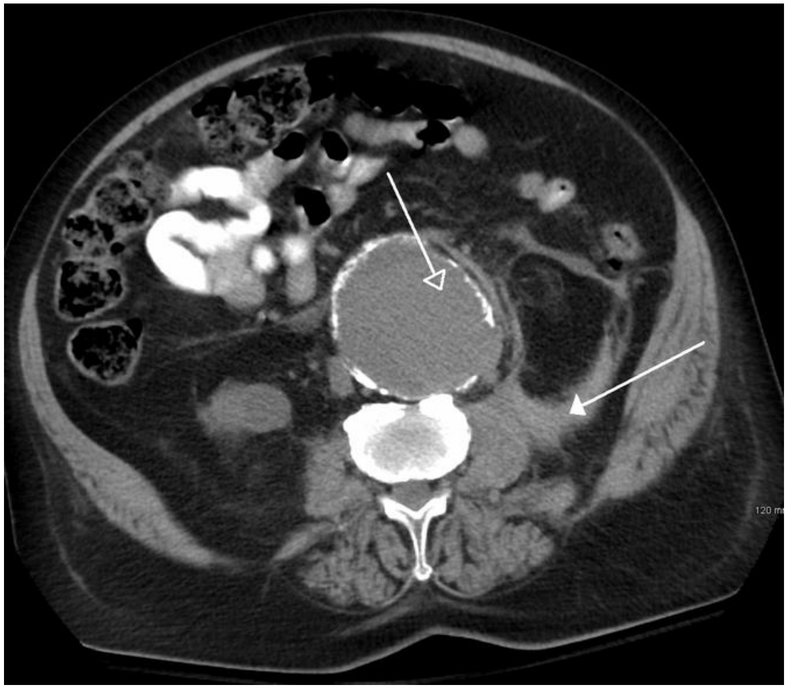

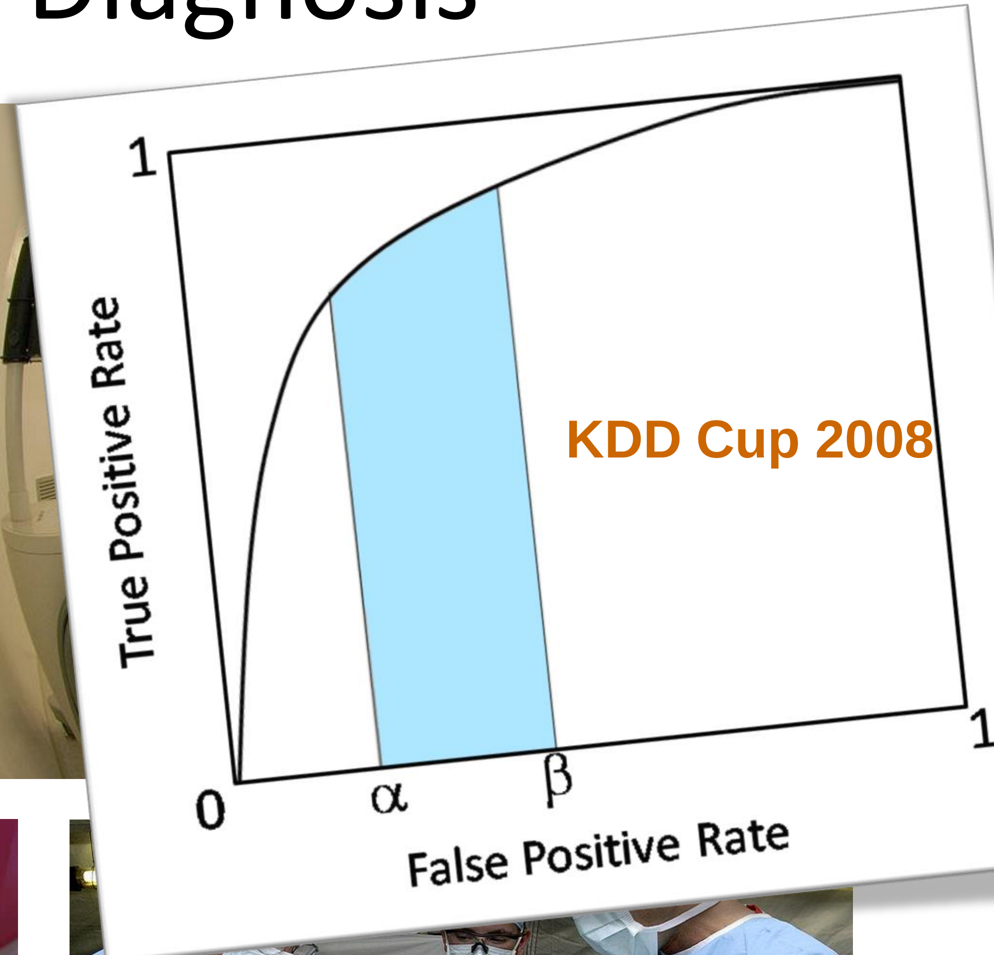

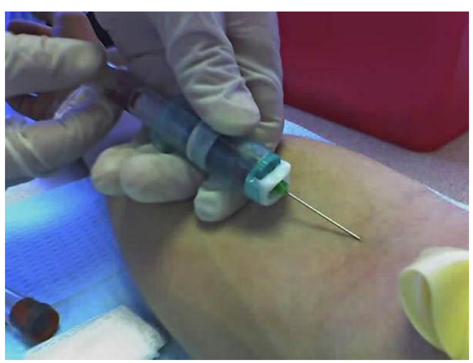

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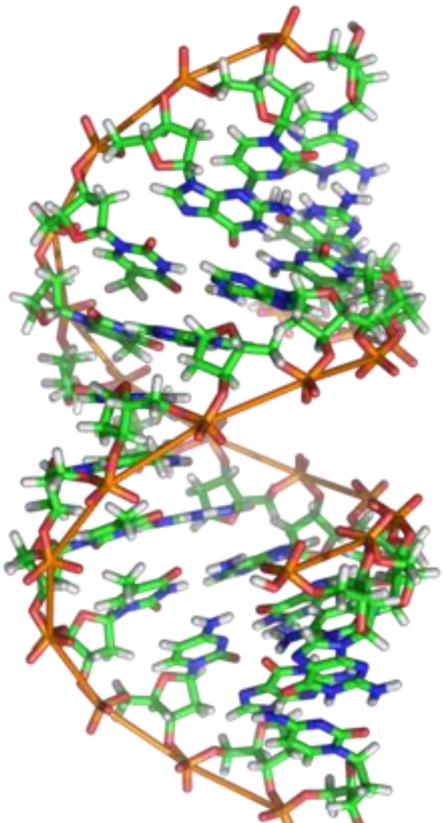
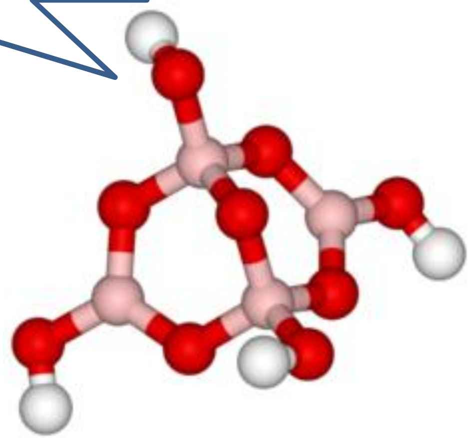
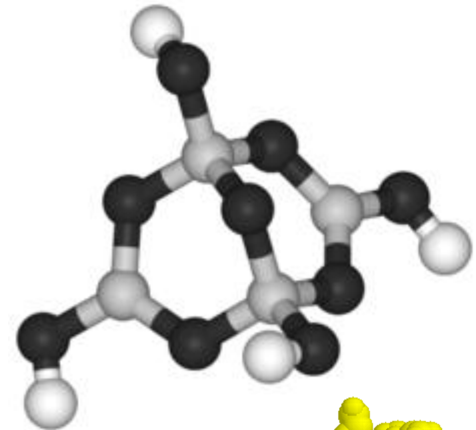
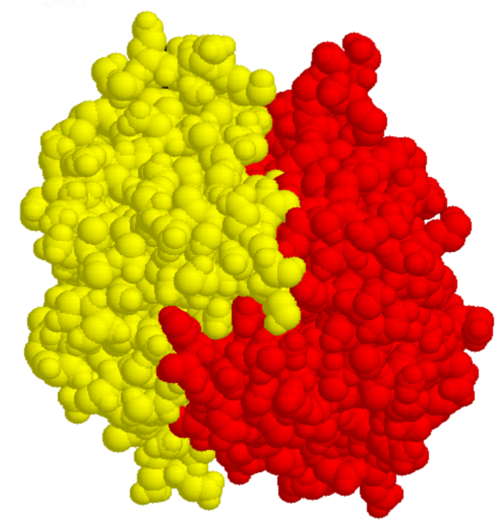
Bioinformatics

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









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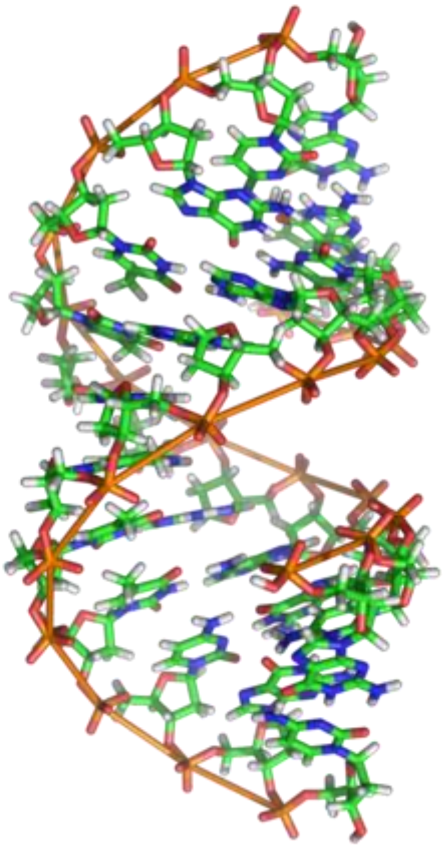

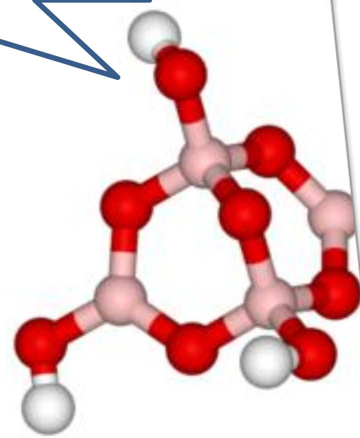

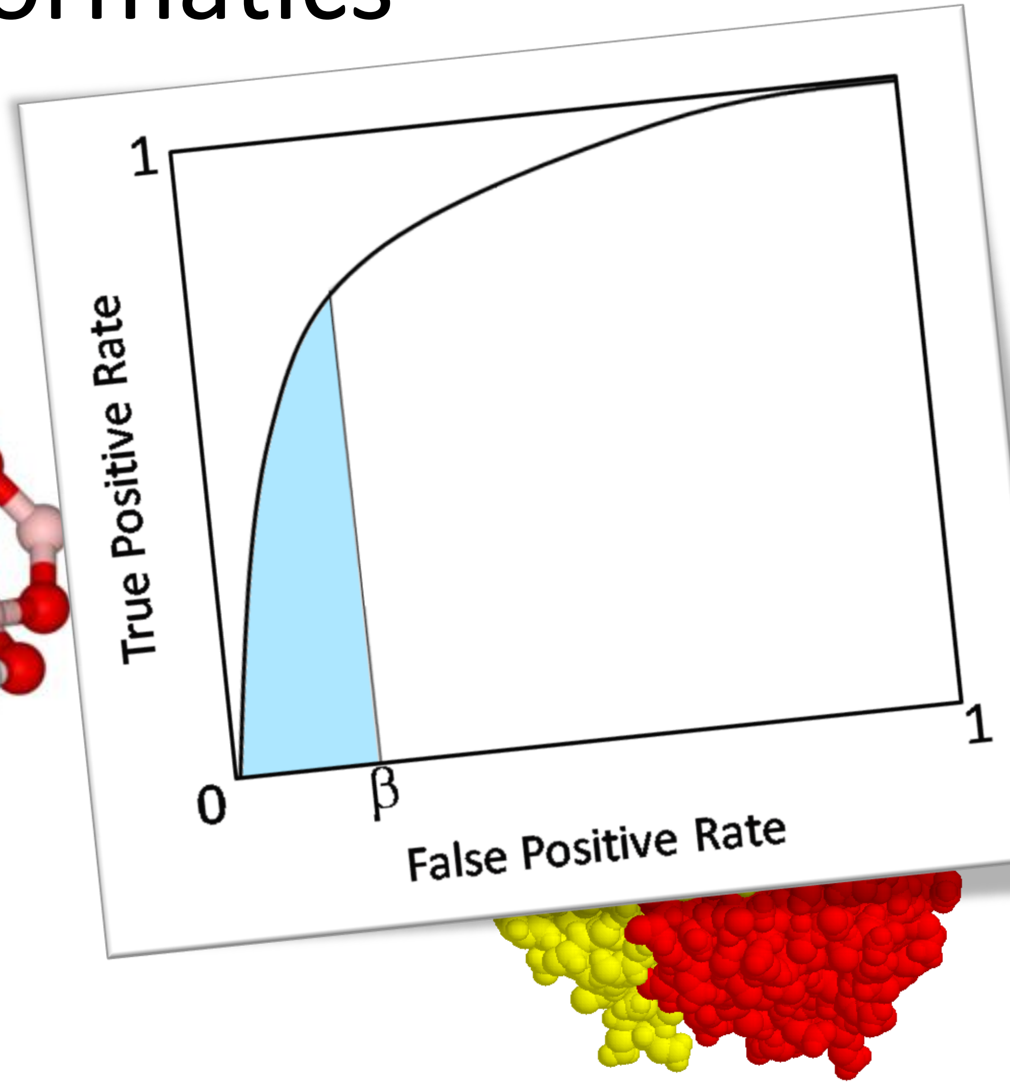

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Partial Area Under the ROC Curve is critical to many applications

SVMpAUC (ICML 2013)

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

SVMpAUC

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

$$\text{s.t.} \quad \forall \pi \in \Pi_{m,n} :$$

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

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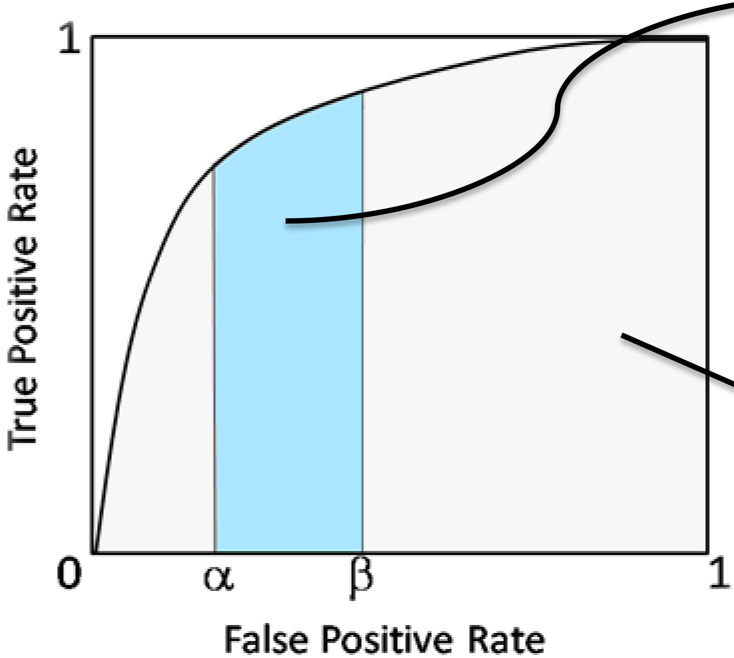


SVM-AUC

Joachims, 2005

Improved Version of SVMpAUC

Tighter upper bound
Improved accuracy
Better runtime guarantee

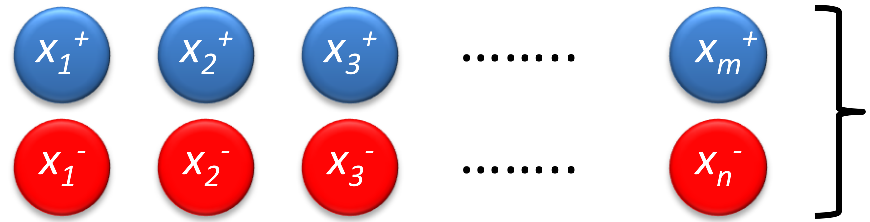
Outline

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

Receiver Operating Characteristic Curve

Positive Instances

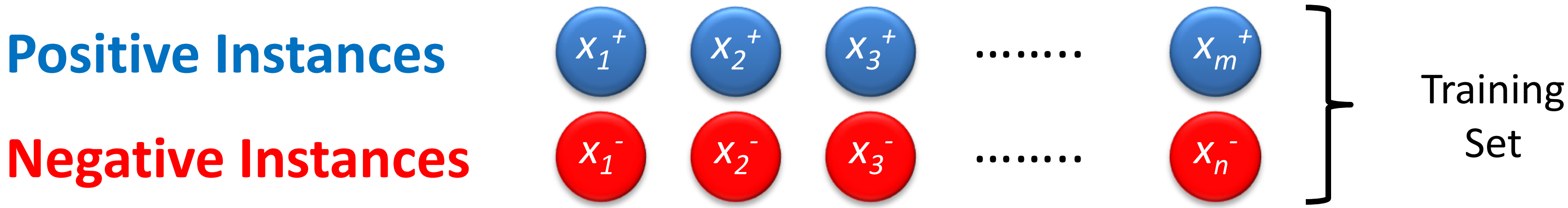
Negative Instances



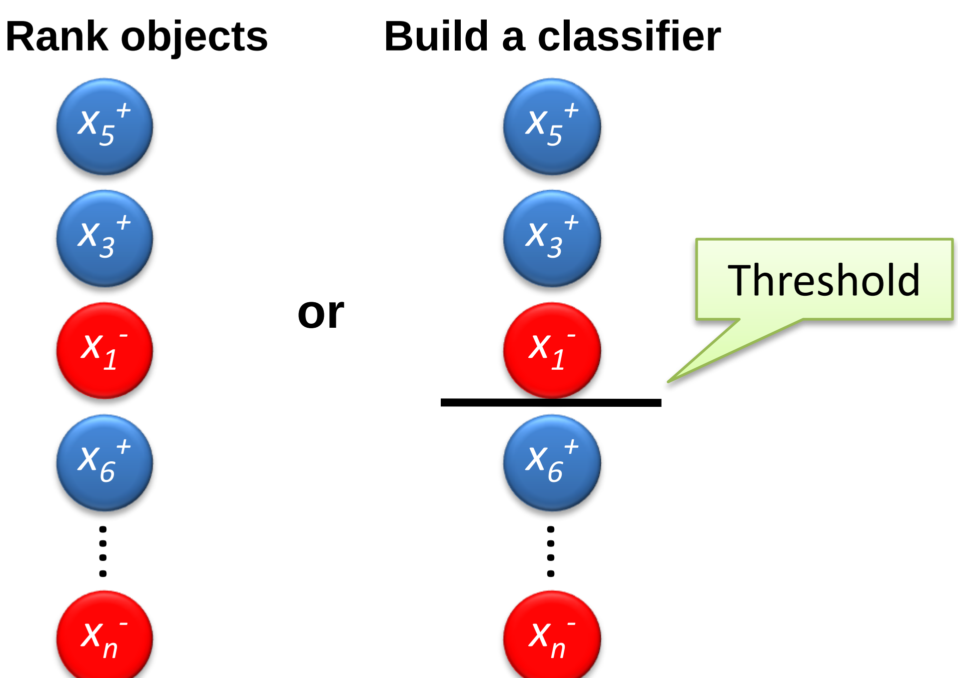
Training Set

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

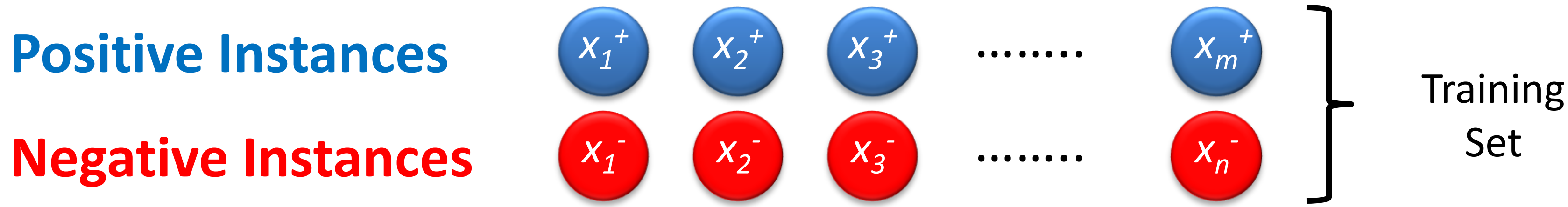
Receiver Operating Characteristic Curve



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



Receiver Operating Characteristic Curve



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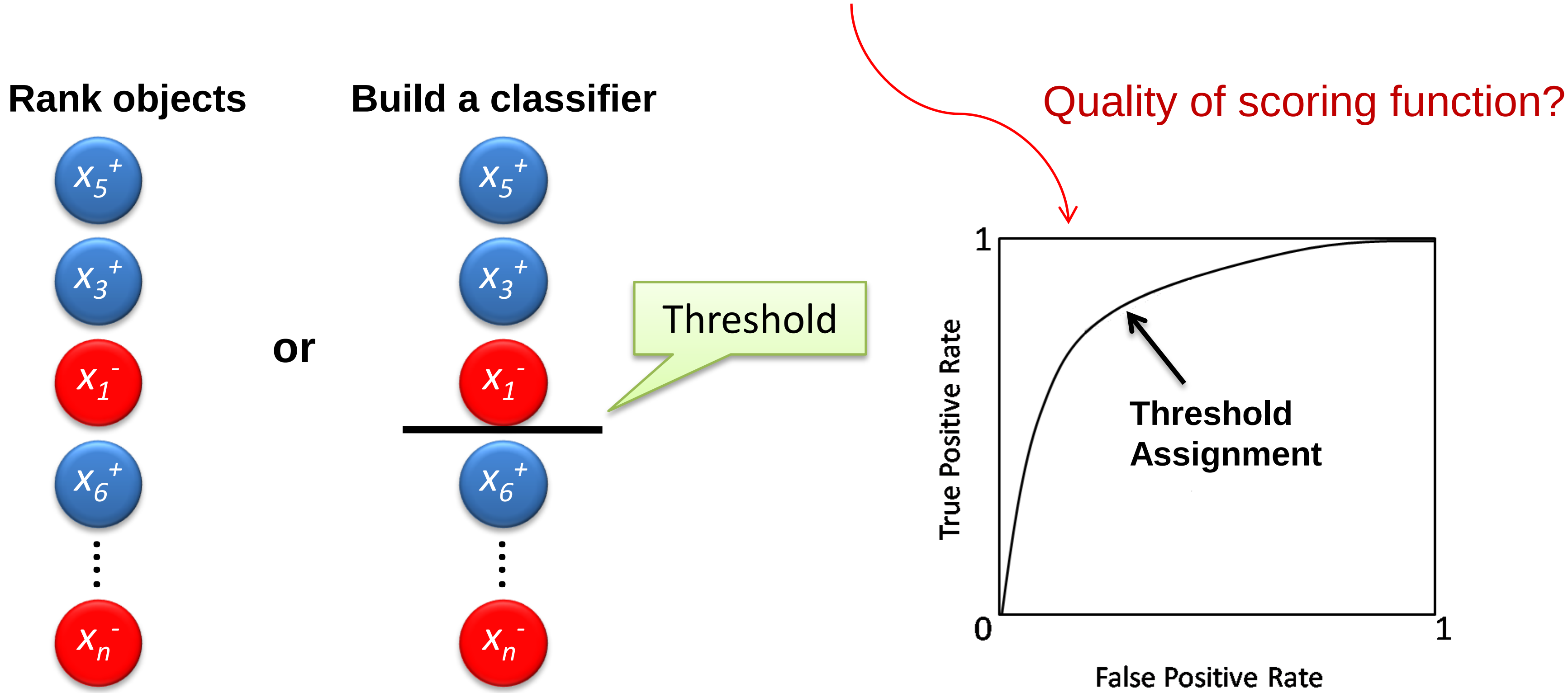
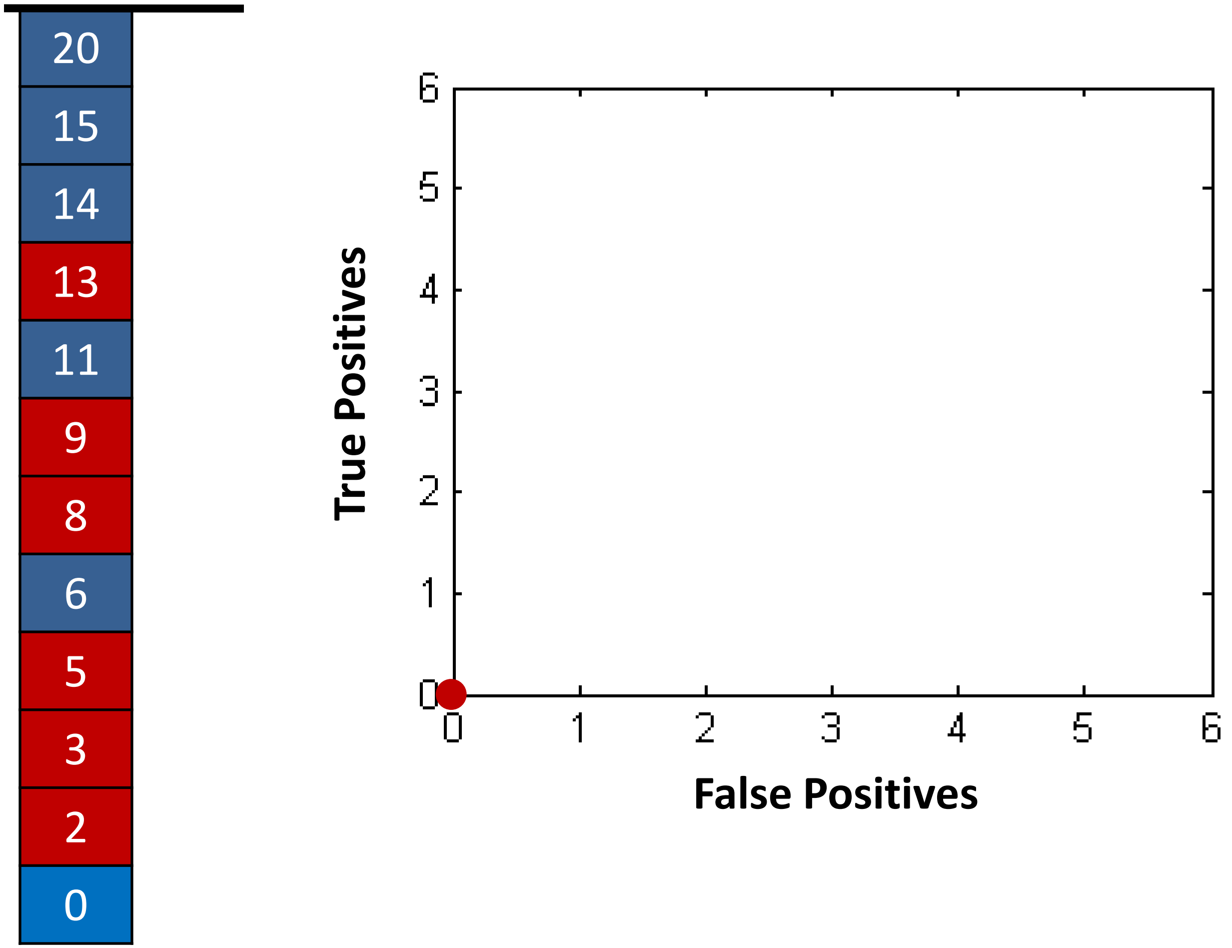


Receiver Operating Characteristic Curve
ROC Curve



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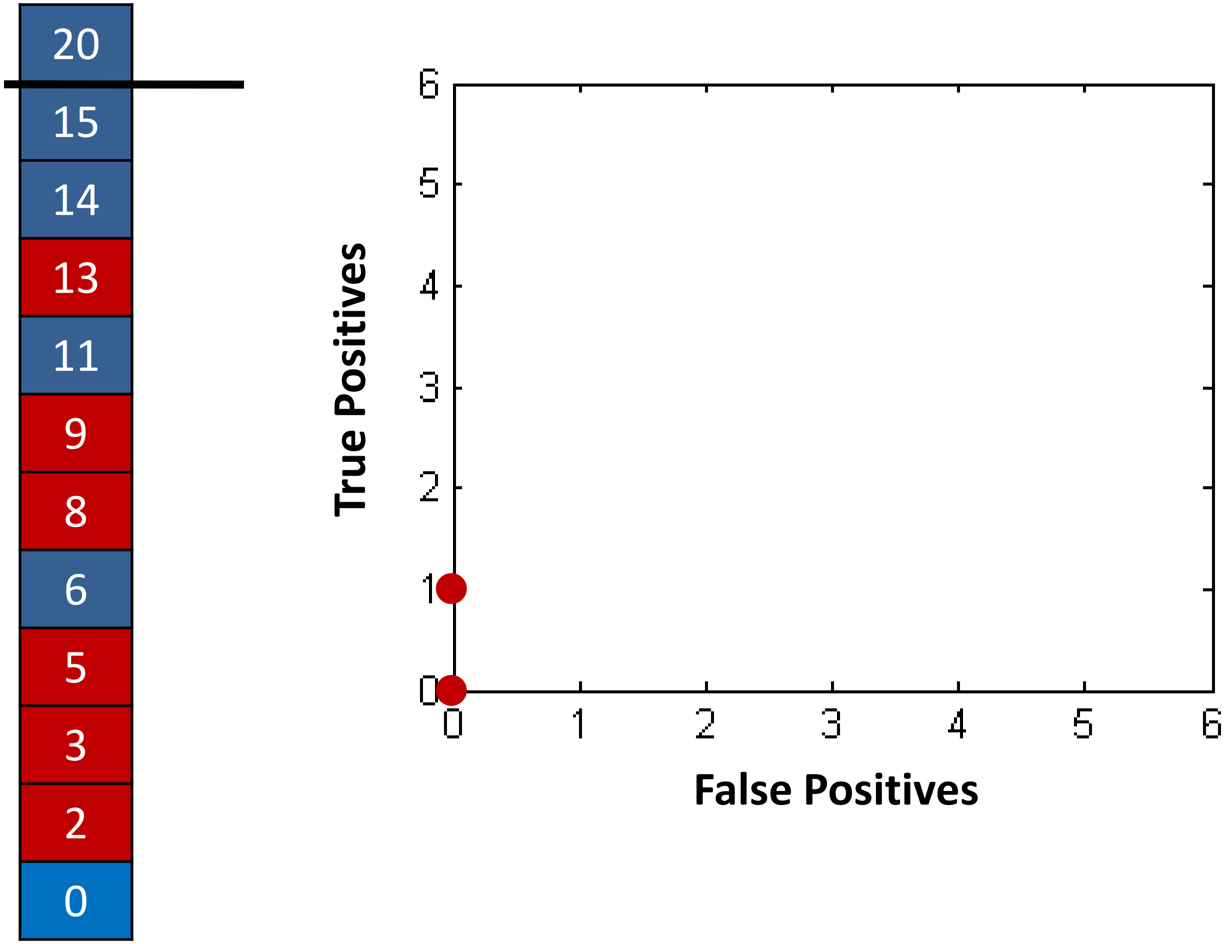
ROC Curve



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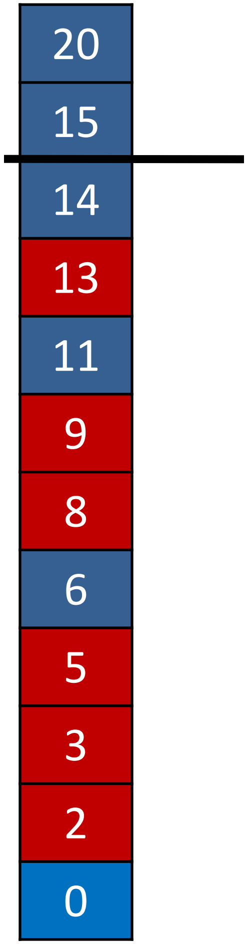

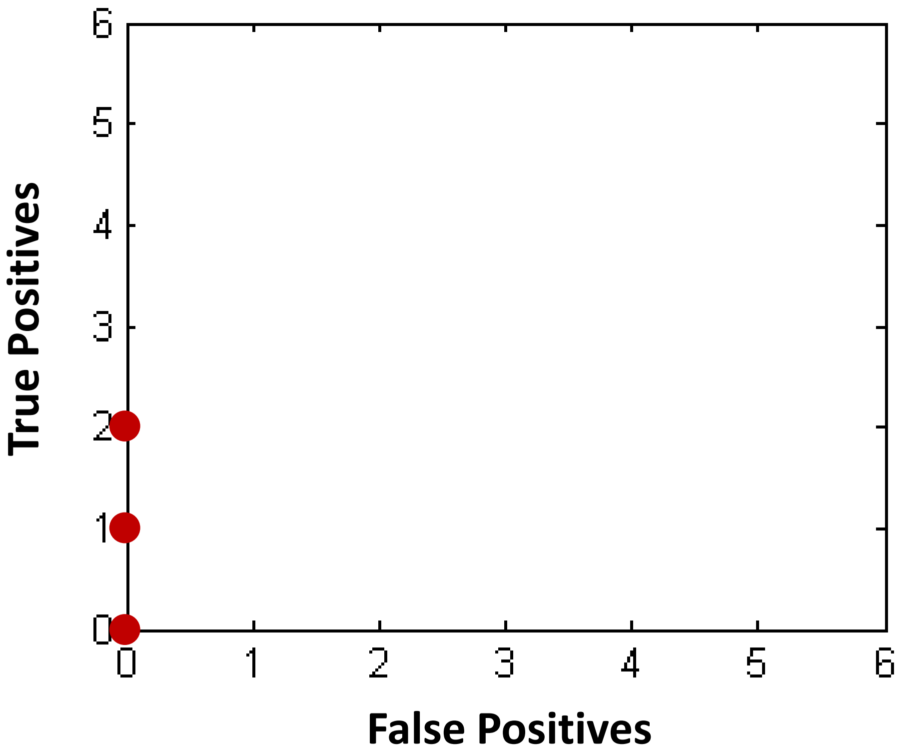

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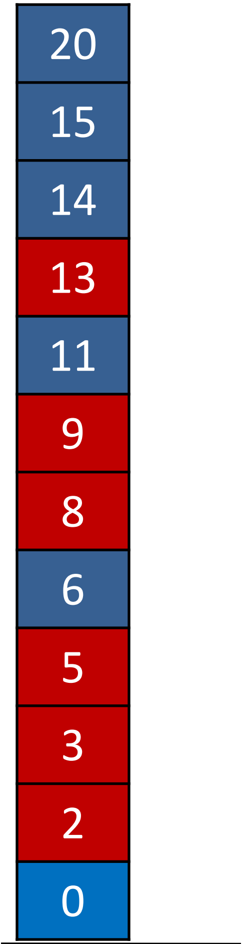

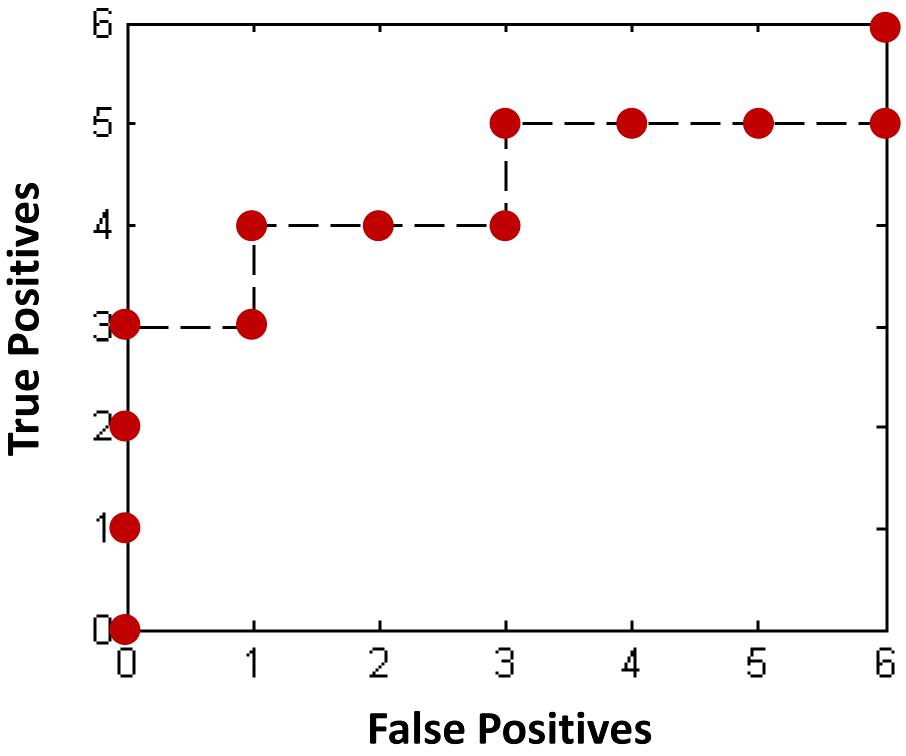

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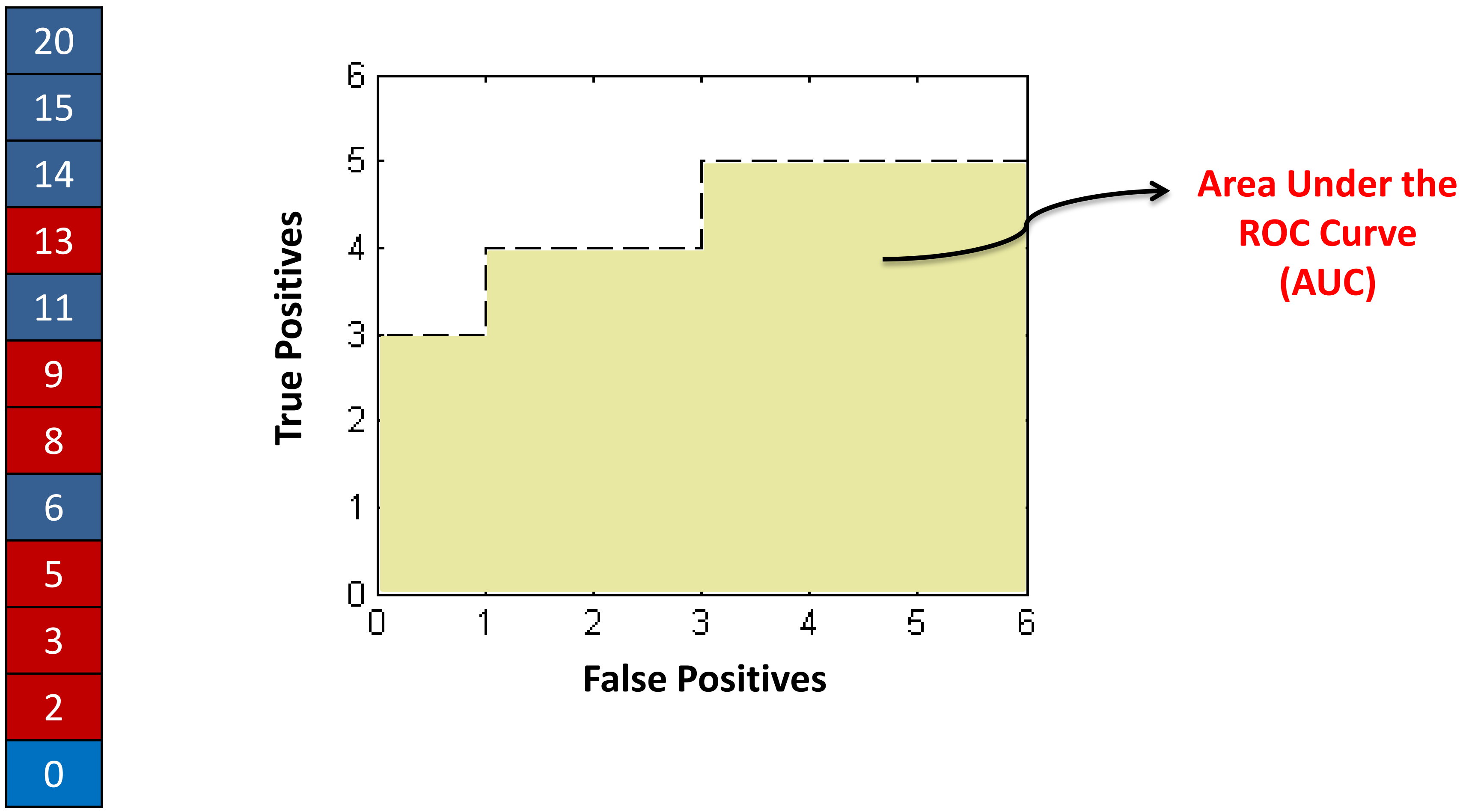

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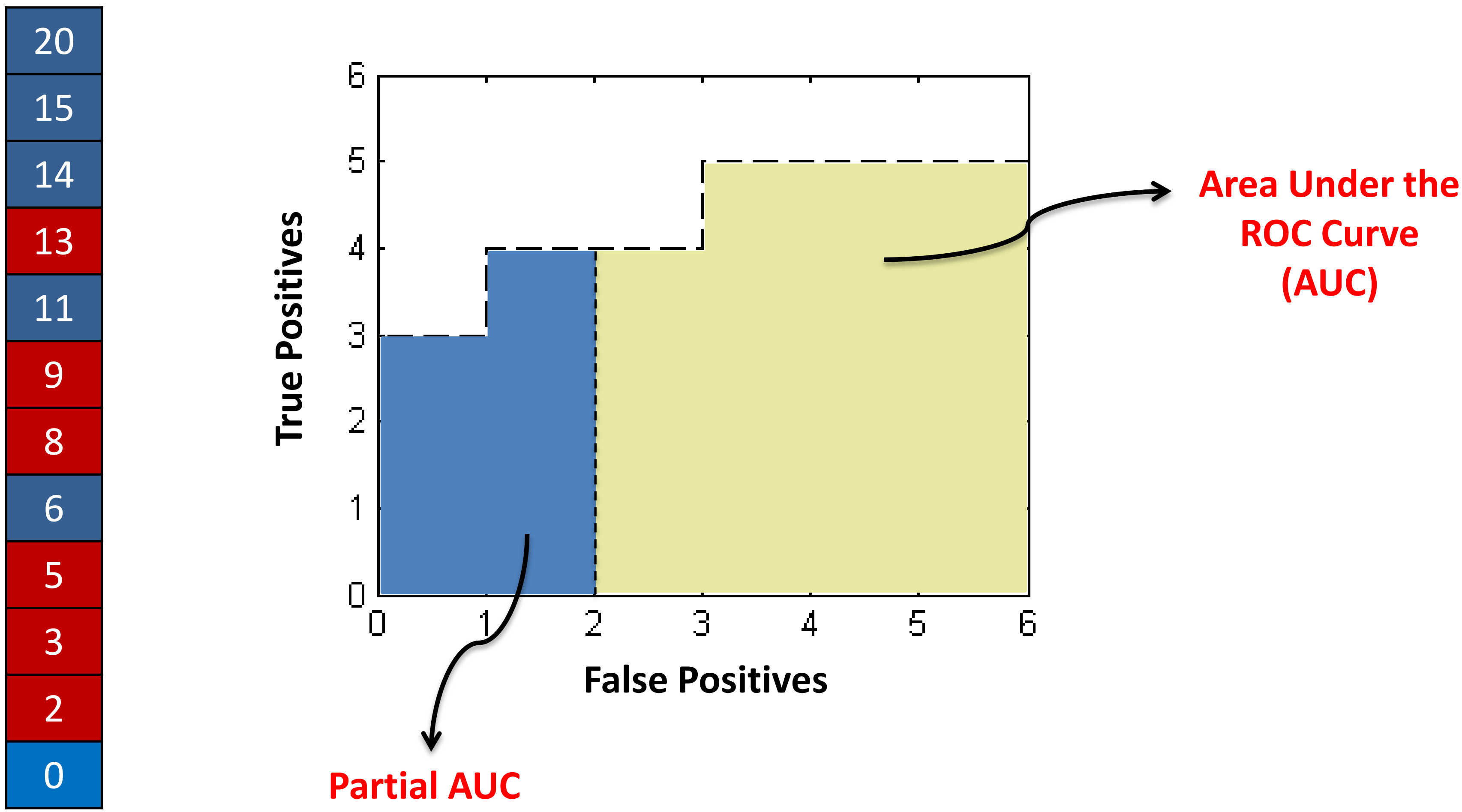

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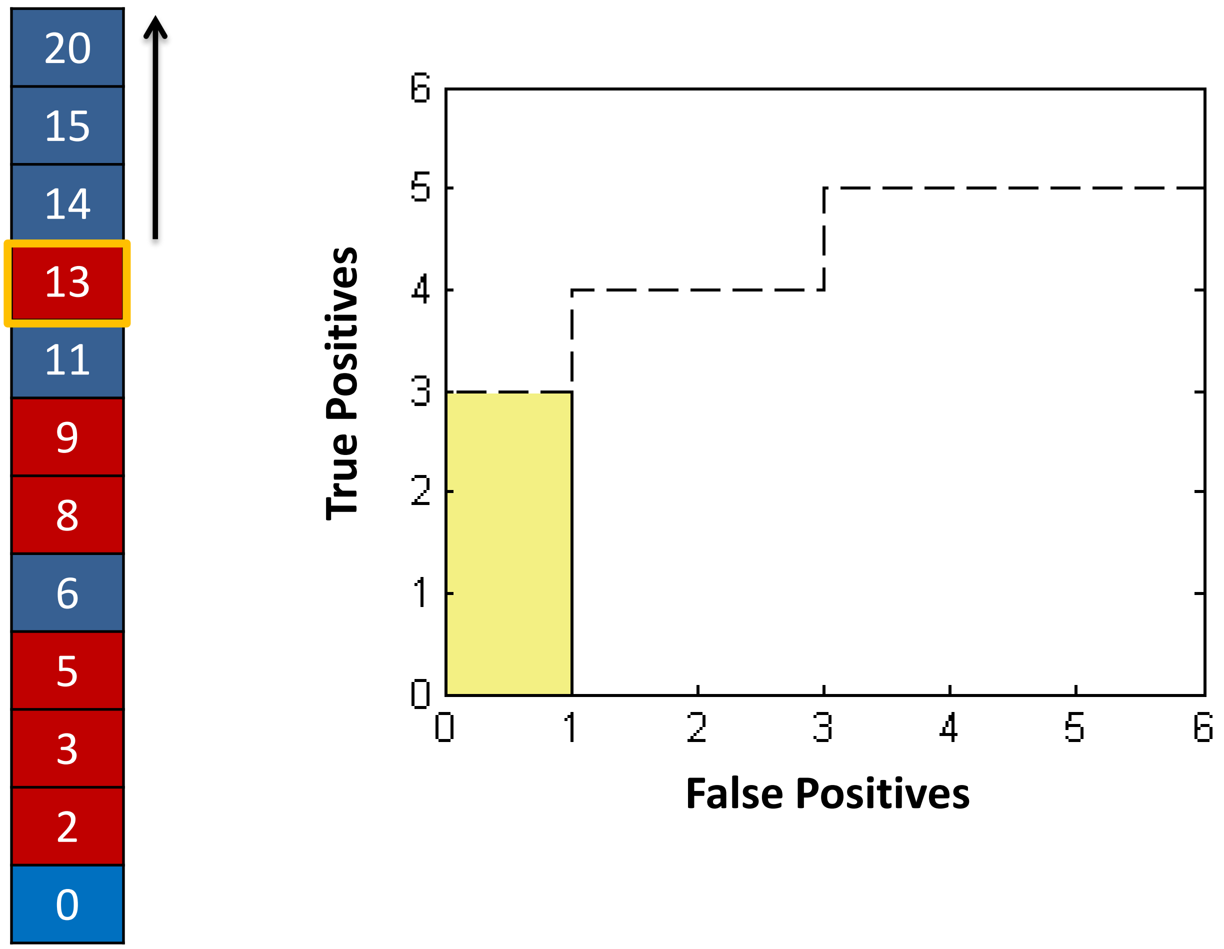

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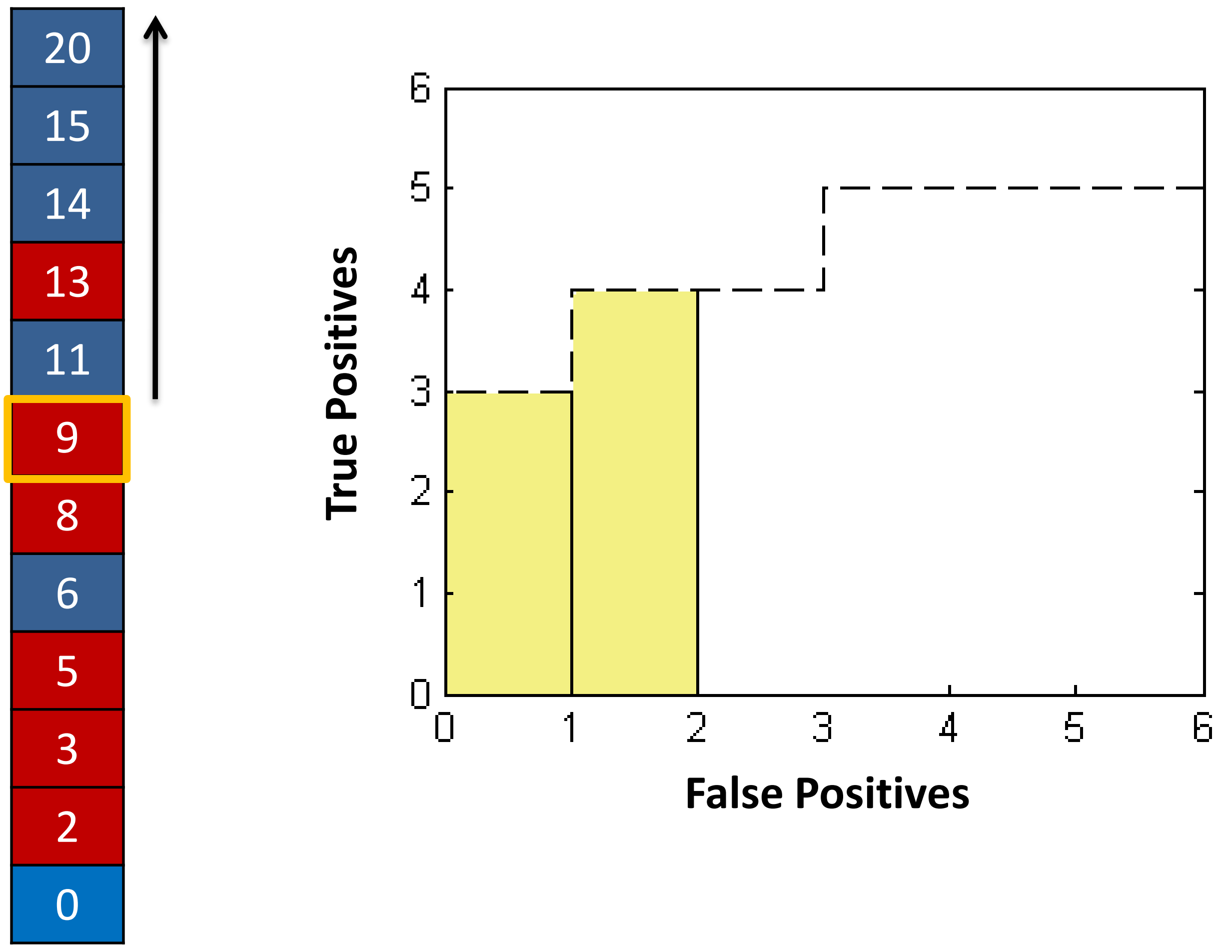

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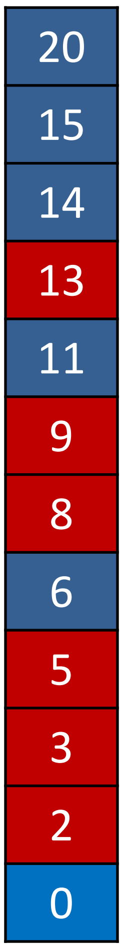

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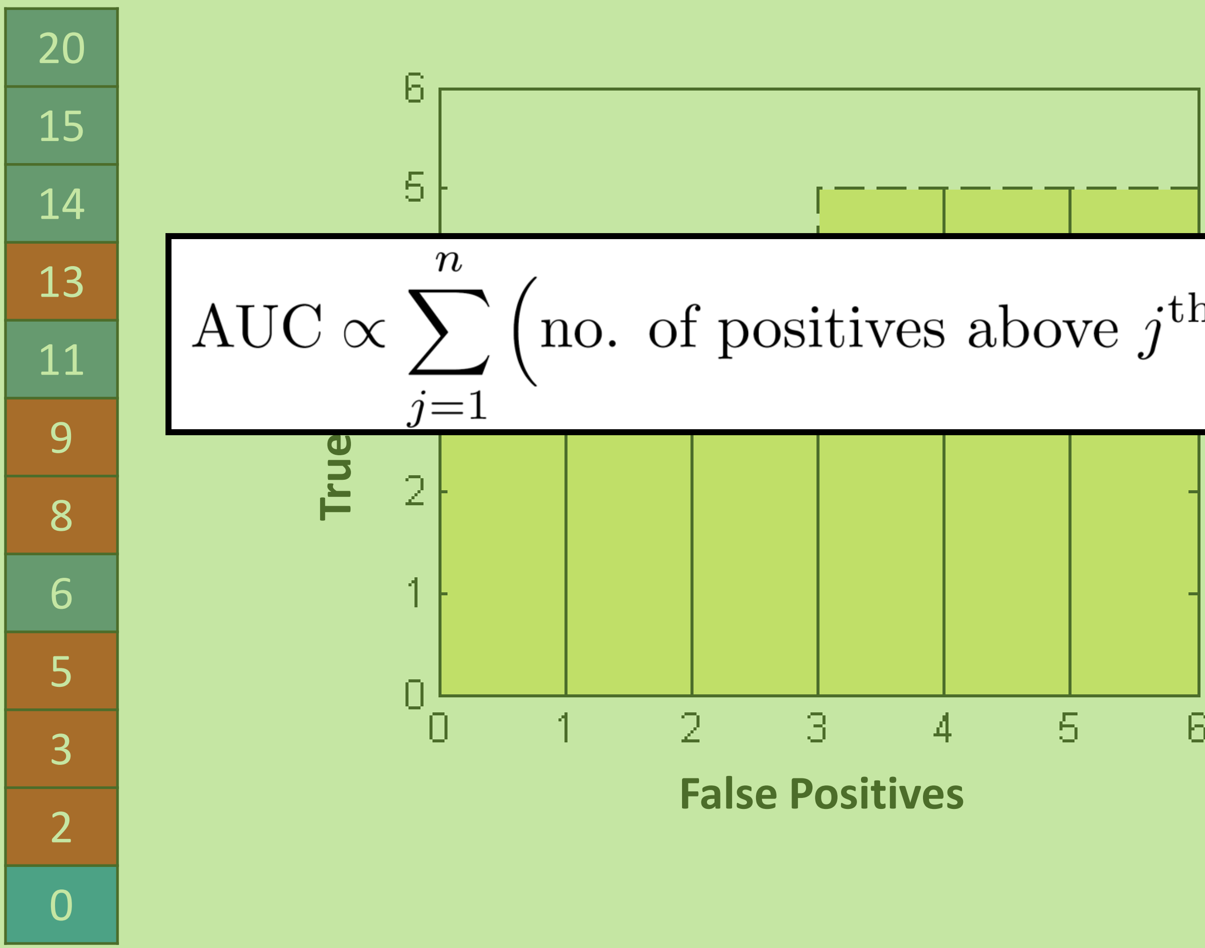


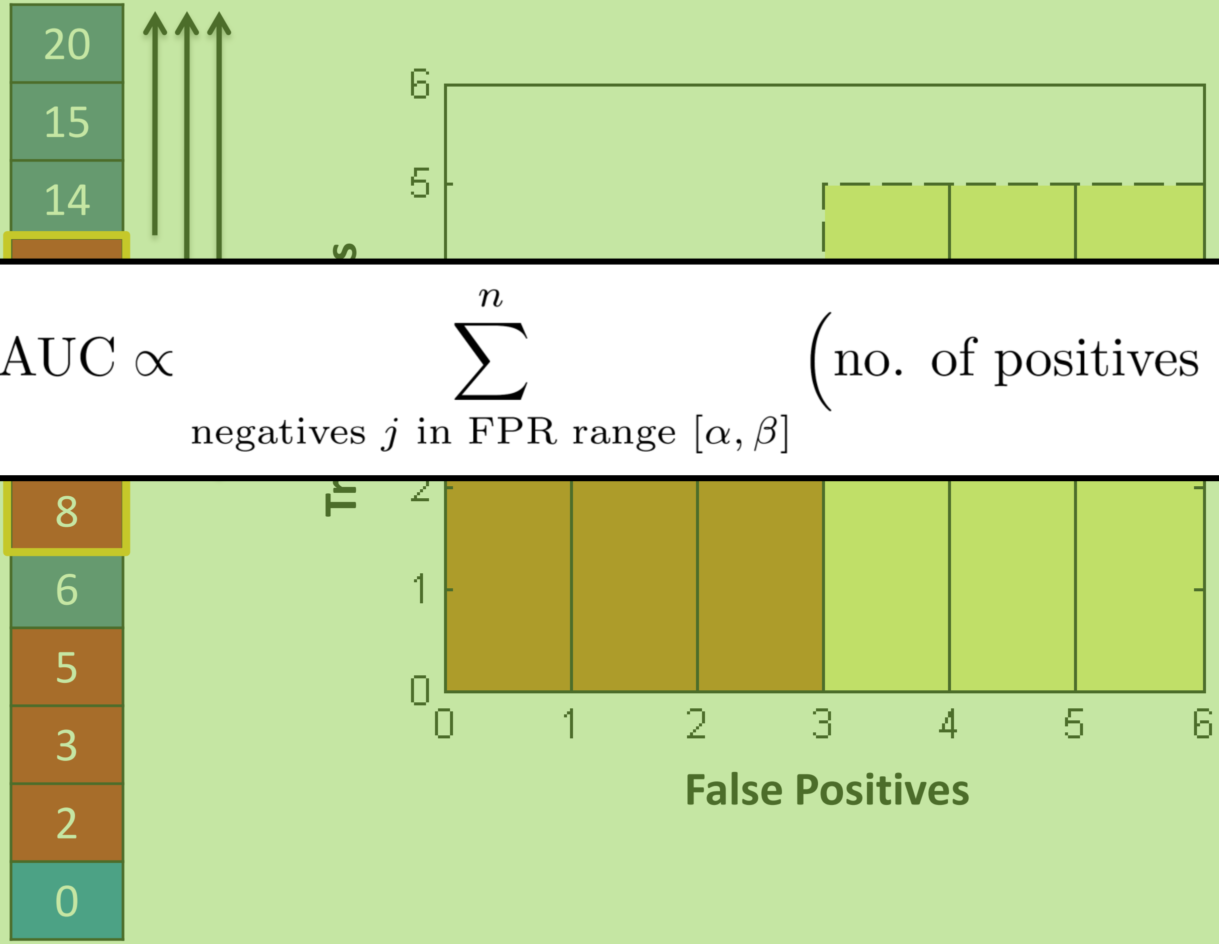
$$\mathrm{AUC} \propto \sum_{j=1}^{n} \left(\text{no. of positives above } j^{\text{th}} \text{ negative} \right)$$

Receiver Operating Characteristic Curve
ROC Curve

β = 0.5

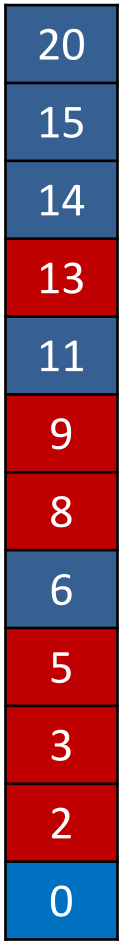
Top 3 negatives!

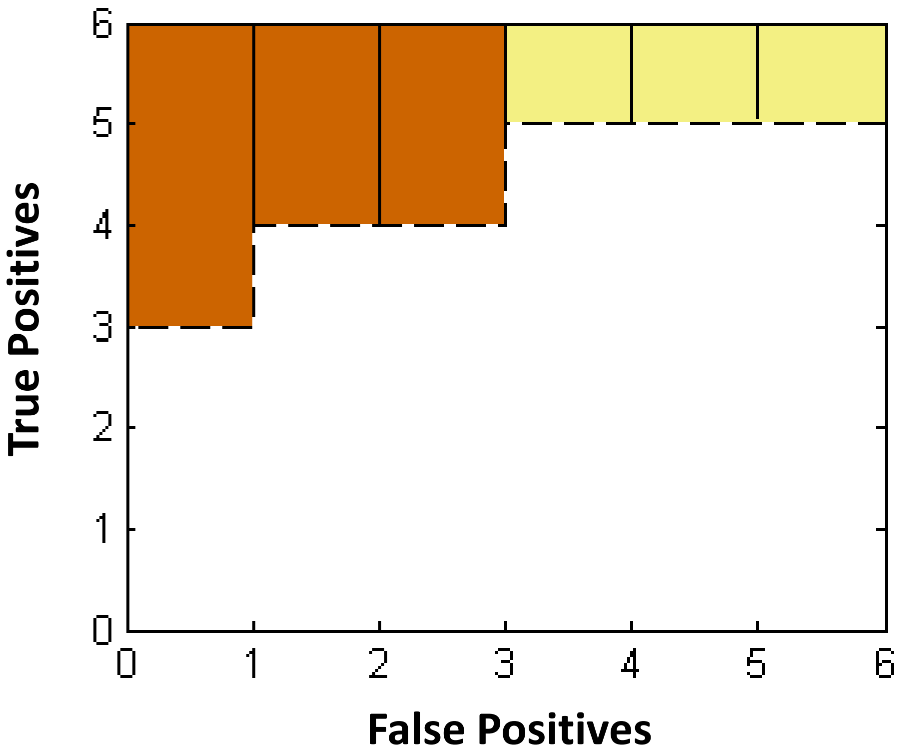
Receiver Operating Characteristic Curve
ROC Curve



$$\text{pAUC} \propto \sum_{\text{negatives } j \text{ in FPR range } [\alpha, \beta]}^{n} \Big(\text{no. of positives above } j^{\text{th}} \text{ negative}\Big)$$

Receiver Operating Characteristic Curve
ROC Curve





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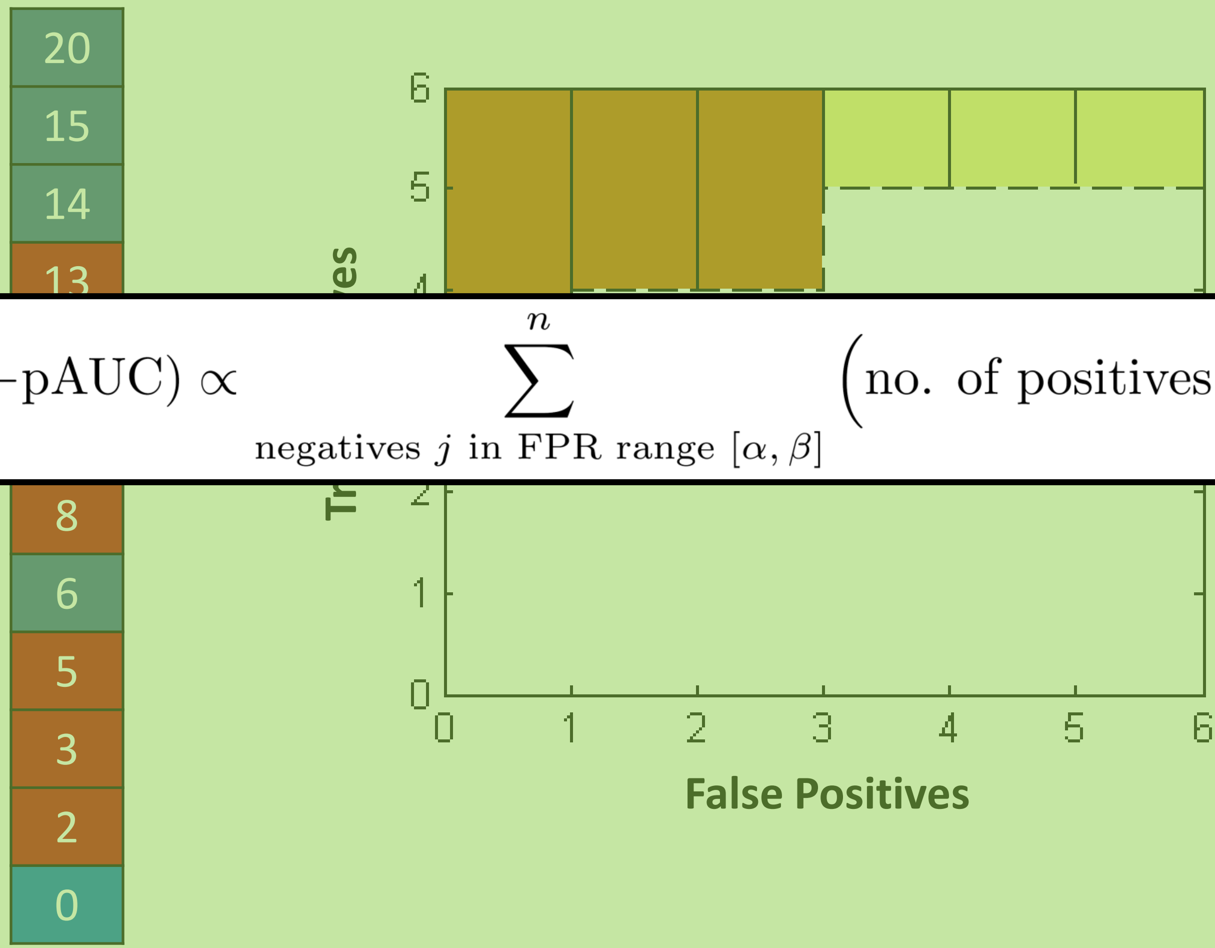


$$(1-\text{pAUC}) \propto \sum_{\text{negatives } j \text{ in FPR range } [\alpha,\beta]}^{n} \Big(\text{no. of positives } \textbf{below } j^{\text{th}} \text{ negative}\Big)$$

(1 – pAUC) for f

Convex Upper Bound

(1 – pAUC) for f

Convex Upper Bound

(1 – pAUC) for f + Regularizer

SVMpAUC (ICML 2013)

SVMpAUC: Structural SVM Approach
Narasimhan and Agarwal, 2013

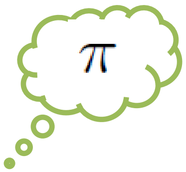
SVMpAUC (ICML 2013)

Ordering of training examples:

n

m

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



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π

Scoring function f

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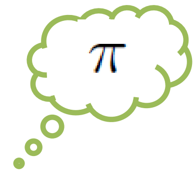

Scoring function f

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

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SVMpAUC (ICML 2013)

Ordering of
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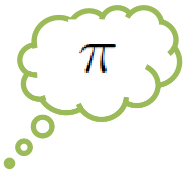

Scoring
function f

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

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Convex Upper Bound

(1 – pAUC) for f + Regularizer

≤

$$\max_{\substack{\textbf{ordering matrices } \pi \\ \text{of size } m \times n}} \left(\underset{\text{for } \pi}{(1 - \text{pAUC})} + \begin{array}{c}\text{term capturing} \\ \text{agreement between } \pi \text{ and } f \\ \text{on all pairs}\end{array} \right)$$

Convex Upper Bound

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≤

$$\max_{\substack{\textbf{ordering matrices } \pi \\ \text{of size } m \times n}} \left(\underset{\text{for } \pi}{(1 - \text{pAUC})} + \begin{array}{c}\text{term capturing} \\ \text{agreement between } \pi \text{ and } f \\ \text{on all pairs}\end{array} \right)$$

How does this upper bound look?

Convex Upper Bound

(1 – pAUC) for f + Regularizer

≤

$$\max_{\substack{\textbf{ordering matrices } \pi \\ \text{of size } m \times n}} \left(\underset{\text{for } \pi}{(1 - \text{pAUC})} + \begin{array}{c}\text{term capturing} \\ \text{agreement between } \pi \text{ and } f \\ \text{on all pairs}\end{array} \right)$$

Can we obtain a tighter upper bound?

Outline

- Overview of SVMpAUC
- Upper Bound Optimized by SVMpAUC
- Improved Formulation: SVMpAUC-tight
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Upper bound we want?

1 - pAUC

$$\propto \sum_{\substack{\text{negatives } j \text{ in} \\ \text{FPR range } [\alpha, \beta]}}^{n} \Big(\text{no. of positives } \textbf{below } j^{\text{th}} \text{ negative}\Big)$$

Upper bound we want?

1 - pAUC

$$\propto \sum_{\substack{\text{negatives } j \text{ in} \\ \text{FPR range } [\alpha,\beta]}}^{n} \sum_{i=1}^{m} \mathbf{1}\left(i^{\text{th}} \text{ positive ranked by } f \text{ below } j^{\text{th}} \text{ negative?}\right)$$

Upper bound we want?

1 - pAUC

$$\propto \sum_{\substack{\text{negatives } j \text{ in} \\ \text{FPR range } [\alpha, \beta]}}^{n} \sum_{i=1}^{m} \mathbf{1}\Big(f(x_i^+) - f(x_j^-) \leq 0\Big)$$

Upper bound we want?

1 - pAUC

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$$\leq \sum_{\substack{\text{negatives } j \text{ in} \\ \text{FPR range } [\alpha, \beta]}}^{n} \sum_{i=1}^{m} \text{hinge-loss}\left(f(x_i^+) - f(x_j^-)\right)$$

pair-wise hinge loss!

Upper optimized by SVMpAUC?

$$\max_{\substack{\textbf{ordering matrices } \pi \\ \text{of size } m \times n}} \left(\begin{array}{c} (1 - \text{pAUC}) \\ \text{for } \pi \end{array} + \begin{array}{c} \text{term capturing} \\ \text{agreement between } \pi \text{ and } f \\ \text{on all pairs} \end{array} \right)$$

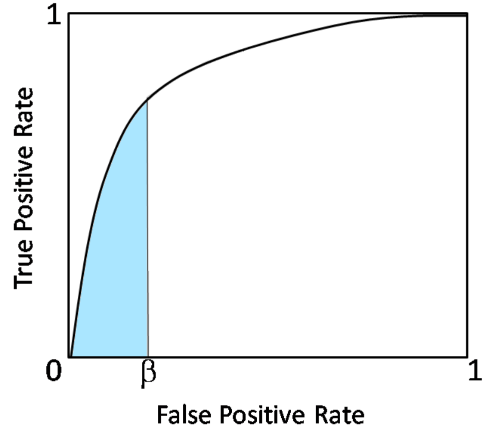
Upper optimized by SVMpAUC?

$$\max_{\substack{\textbf{ordering matrices } \pi \\ \text{of size } m \times n}} \left(\underset{\text{for } \pi}{(1 - \text{pAUC})} + \begin{array}{c}\text{term capturing} \\ \text{agreement between } \pi \text{ and } f \\ \text{on all pairs}\end{array} \right)$$

=

pair-wise hinge loss + extra term

Upper optimized by SVMpAUC?



Subset of pairs of positive-negative examples

$$\max_{\substack{\text{ordering matrices } \pi \\ \text{of size } m \times n}} \left(\underbrace{(1 - \text{pAUC})}_{\text{for } \pi} + \begin{array}{c}\text{term capturing} \\ \text{agreement between } \pi \text{ and } f \\ \text{on } \underline{\text{all pairs}}\end{array} \right)$$

=

pair-wise hinge loss + extra term

Upper optimized by SVMpAUC?

Subset of pairs of positive-negative examples

$$\max_{\substack{\textbf{ordering matrices } \pi \\ \text{of size } m \times n}} \left(\underset{\text{for } \pi}{(1 - \text{pAUC})} + \begin{array}{c}\text{term capturing} \\ \text{agreement between } \pi \text{ and } f \\ \text{on } \underline{\text{all pairs}}\end{array} \right)$$

=

pair-wise hinge loss + ~~extra term~~ ?

Upper optimized by SVMpAUC?

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

Upper optimized by SVMpAUC?

$$\max_{\substack{\textbf{ordering matrices } \pi \\ \text{of size } m \times n}} \left(\underset{\text{for } \pi}{(1 - \text{pAUC})} + \begin{array}{c}\text{term capturing} \\ \text{agreement between } \pi \text{ and } f \\ \text{on all pairs}\end{array} \right)$$

$$\leq$$

pair-wise hinge loss + extra term

Upper optimized by SVMpAUC?

approx. pair-wise hinge loss + extra term

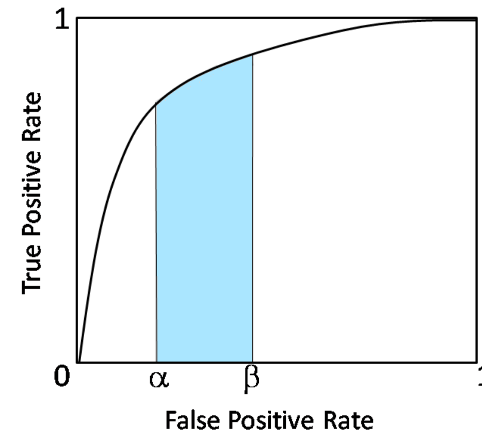
≤

$$\max_{\substack{\text{ordering matrices } \pi \\ \text{of size } m \times n}} \left(\underset{\text{for } \pi}{(1 - \text{pAUC})} + \begin{array}{c}\text{term capturing} \\ \text{agreement between } \pi \text{ and } f \\ \text{on all pairs}\end{array} \right)$$

≤

pair-wise hinge loss + extra term

Upper optimized by SVMpAUC?



approx. pair-wise hinge loss + ~~extra term~~?

$$\leq$$

$$\max_{\substack{\textbf{ordering matrices } \pi \\ \text{of size } m \times n}} \left(\begin{array}{c}(1 - \text{pAUC}) \\ \text{for } \pi\end{array} + \begin{array}{c}\text{term capturing} \\ \text{agreement between } \pi \text{ and } f \\ \text{on all pairs}\end{array} \right)$$

$$\leq$$

pair-wise hinge loss + ~~extra term~~?

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- Overview of SVMpAUC
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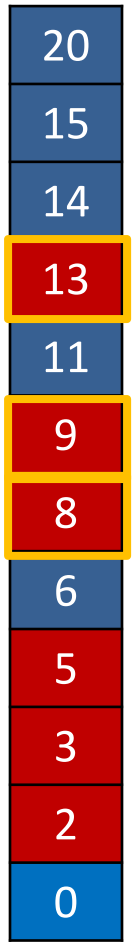
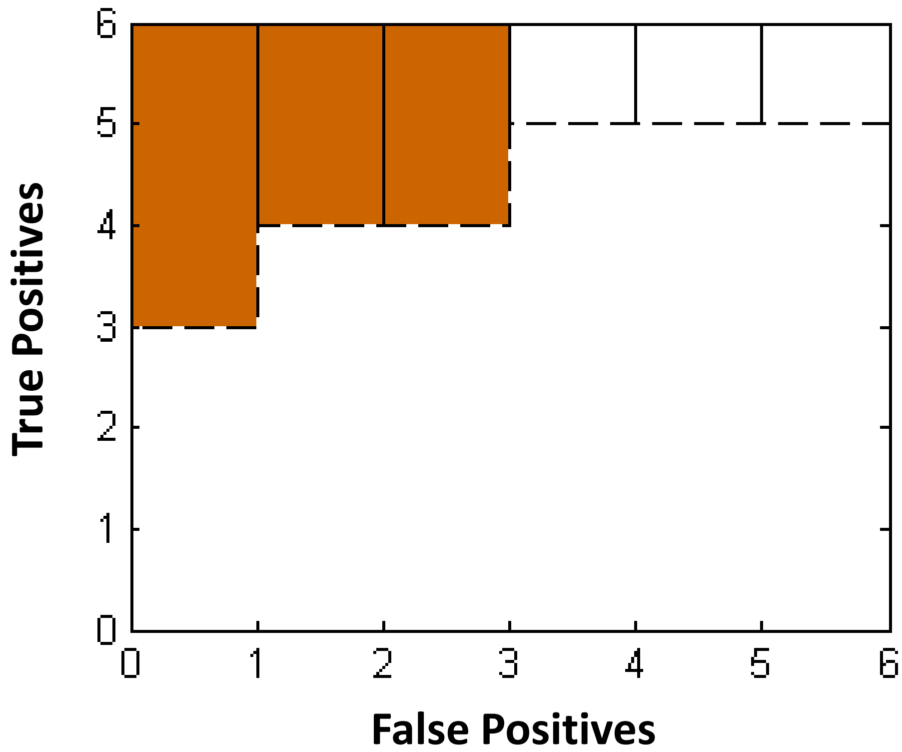
Rewriting the Partial AUC Loss

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

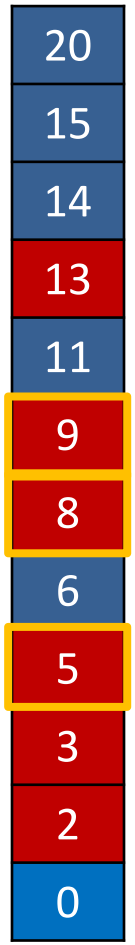


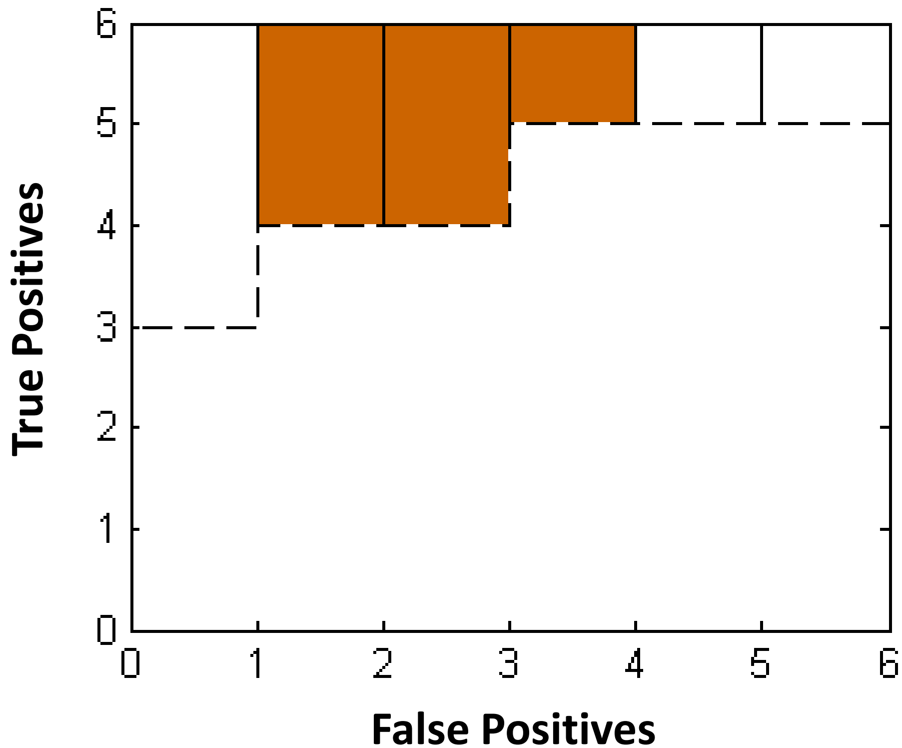


$3 + 2 + 2 = 7$

Rewriting the Partial AUC Loss

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



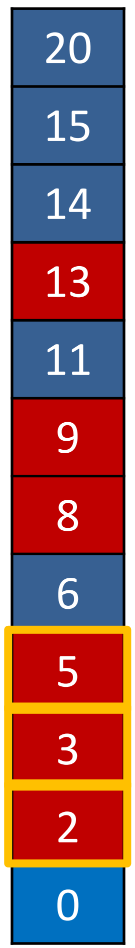


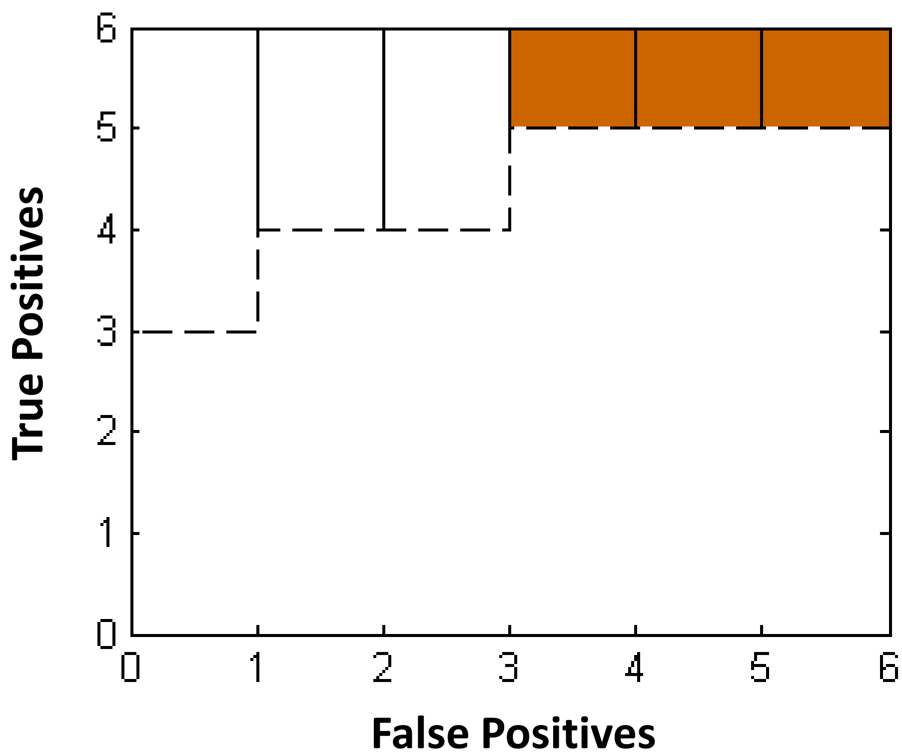
$3 + 2 + 2 = 7$

$2 + 2 + 1 = 5$

Rewriting the Partial AUC Loss

α = 0, β = 0.5





3 + 2 + 2 = 7

2 + 2 + 1 = 5

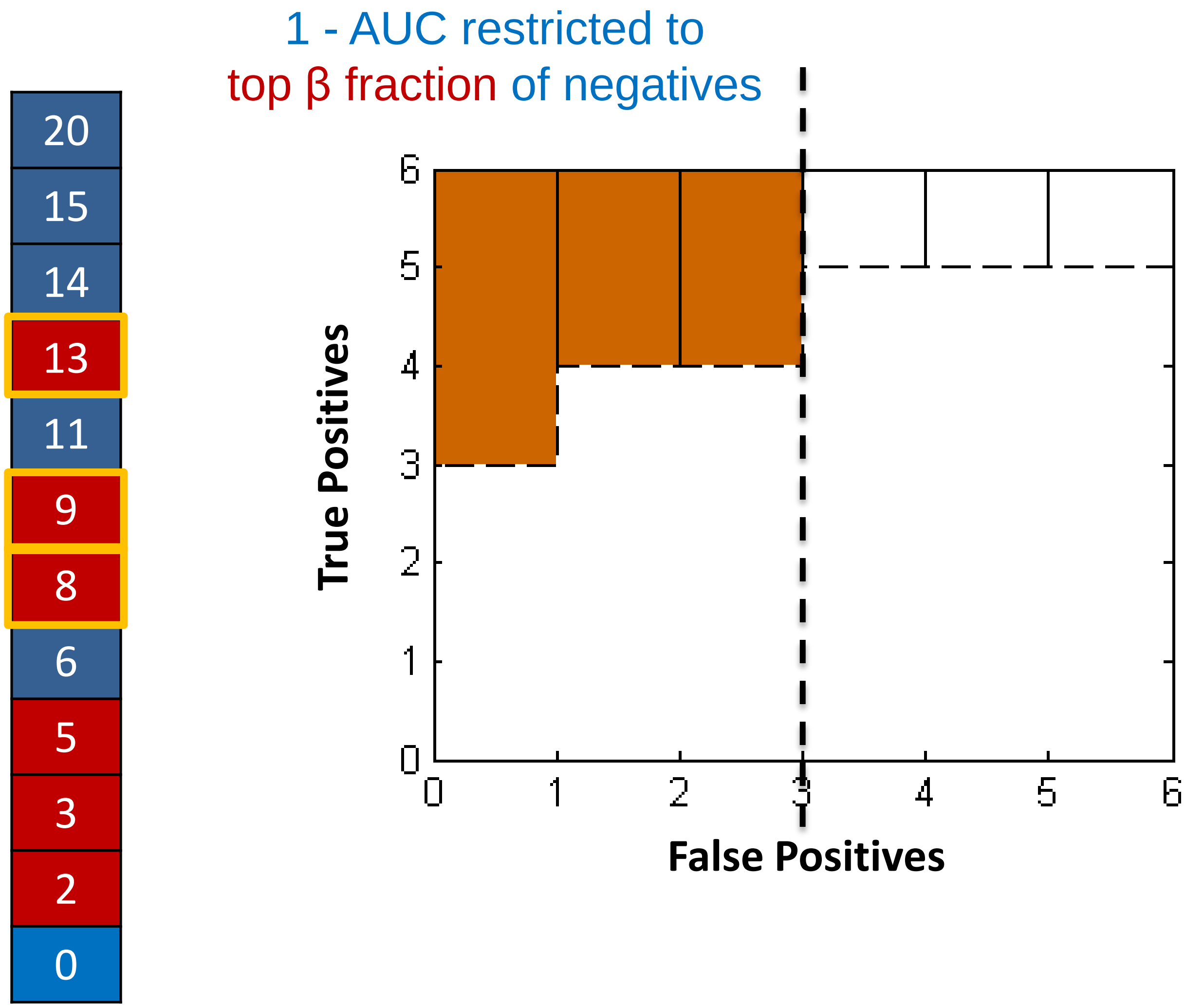
.

.

.

1 + 1 + 1 = 3

Rewriting the Partial AUC Loss



α = 0, β = 0.5

Maximum!

3 + 2 + 2 = 7

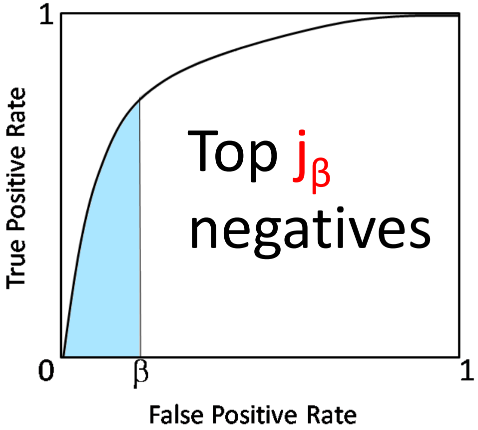
2 + 2 + 1 = 5

.

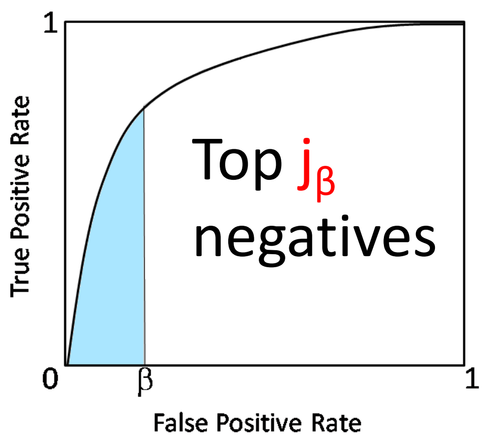
.

.

1 + 1 + 1 = 3

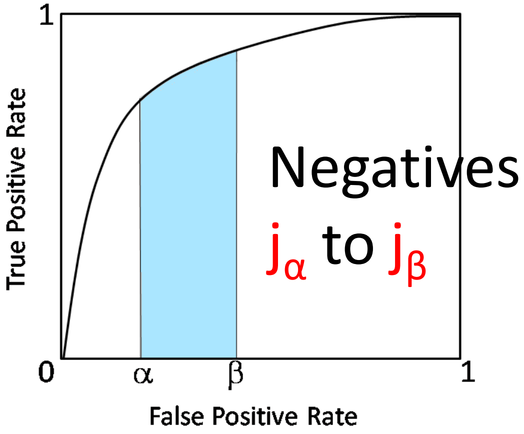


$$(1-\text{pAUC}) \propto \max_{\substack{\text{subsets } S \text{ of negatives} \\ \text{of size } j_\beta}} \left(1-\text{AUC restricted to negatives in } S\right)$$

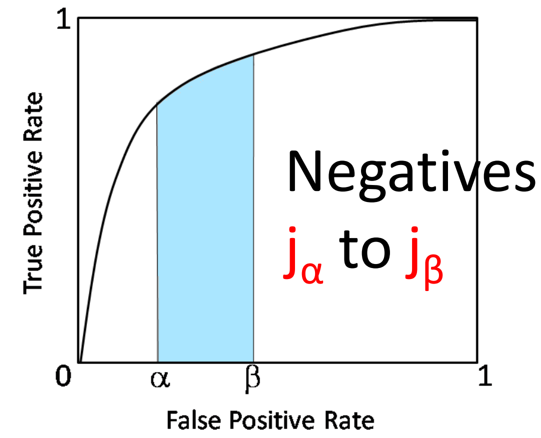


SVM-AUC

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



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



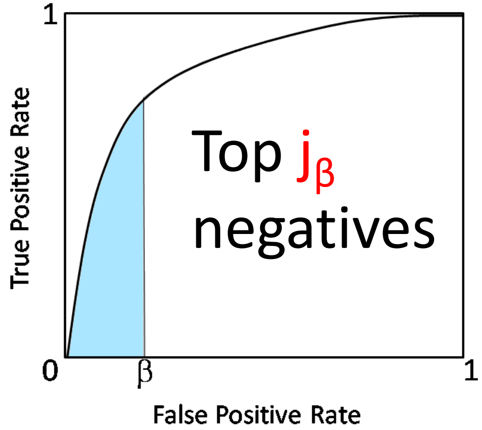
Truncated SVMpAUC

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

SVMpAUC-tight: Improved Formulation

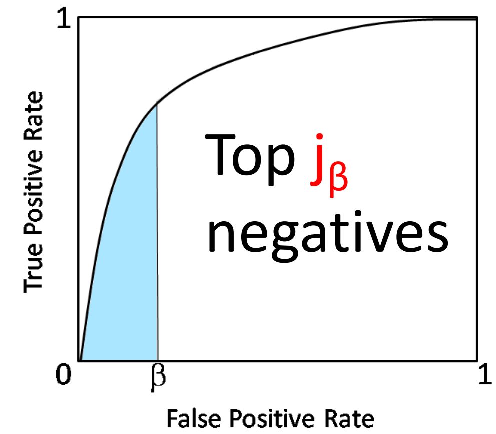
$$\max_{\substack{\textbf{subsets } S \text{ of negatives} \\ \text{of size } j_\beta}} \Big[\text{ SVMpAUC objective restricted to } S \Big]$$

SVMpAUC-tight: Improved Formulation



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

SVMpAUC-tight: Improved Formulation



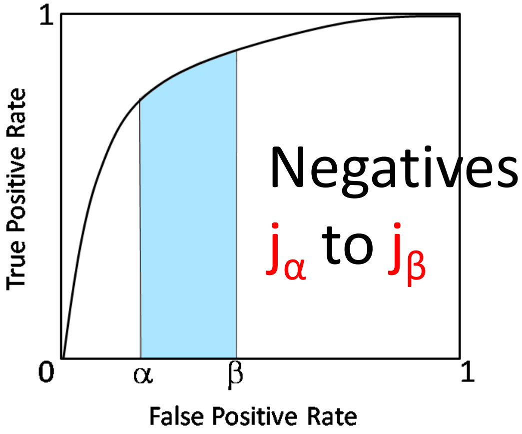
Same pairs of positive-negative examples

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

=

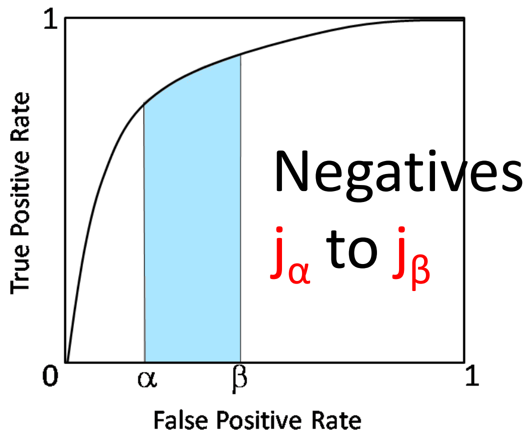
pair-wise hinge loss + ~~extra term~~

SVMpAUC-tight: Improved Formulation



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

SVMpAUC-tight: Improved Formulation



approx. pair-wise hinge loss + ~~extra term~~

≤

$$\max_{\substack{\textbf{subsets } S \text{ of negatives} \\ \text{of size } j_\beta}} \left[\max_{\substack{\textbf{ordering matrices } \pi \\ \text{of size } m \times j_\beta}} \left(\underset{\text{for } \pi}{\overset{\text{restricted}}{(1 - \text{pAUC})}} + \underset{\text{on } \textbf{pairs corresponding to } S}{\overset{\text{term capturing}}{\text{agreement between } \pi \text{ and } f}} \right) \right]$$

≤

pair-wise hinge loss + ~~extra term~~

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SVMpAUC-tight: Optimization Problem

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

exponential in size

\+ Regularizer

SVMpAUC-tight: Optimization Problem

$$\max_{\substack{\textbf{subsets } S \text{ of negatives} \\ \text{of size } j_\beta}} \; \max_{\substack{\textbf{ordering matrices } \pi \\ \text{of size } m \times j_\beta}} \left(\underset{\text{for } \pi}{\overset{\text{restricted}}{(1 - \text{pAUC})}} + \underset{\text{on } \textbf{pairs corresponding to } S}{\overset{\text{term capturing}}{\text{agreement between } \pi \text{ and } f}} \right)$$

exponential in size

\+ Regularizer

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

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

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

Quadratic program with an exponential number of constraints

SVMpAUC-tight: Cutting-Plane Solver

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

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

$$w^\top \big(\phi_z(S,\pi^*) - \phi_z(S,\pi)\big) \;\geq \Delta_\beta(\pi^*,\pi) - \xi$$

Repeat:

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

SVMpAUC-tight: Cutting-Plane Solver

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

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

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

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Repeat:

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

Better Runtime Guarantees:

Maximum number of iterations

Time taken per iteration

SVMpAUC-tight: Projected Subgradient Solver

Primal formulation:

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

$$\text{s.t.}$$

$$||w||_2 \leq \lambda$$

SVMpAUC-tight: Projected Subgradient Solver

Primal formulation:

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

$$\text{s.t.}$$

$$||w||_2 \leq \lambda$$

Repeat:

1. 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.

$$||w||_2 \leq \lambda$$

Sparsity-inducing regularizations

LASSO
Group LASSO
Elastic-Net

Repeat:

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

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SVMpAUC-tight Vs **SVMpAUC**

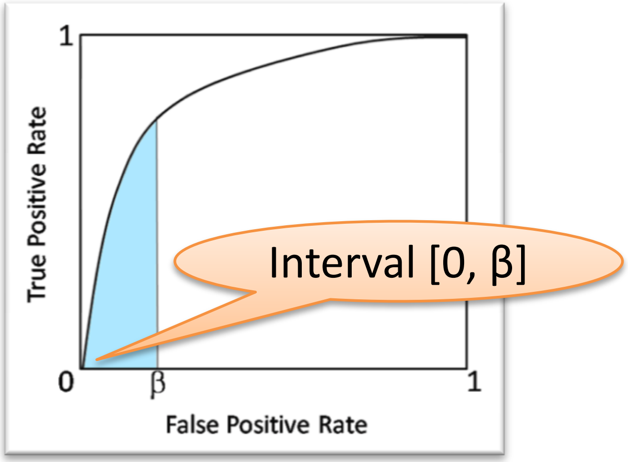
Partial AUC in [0, 0.1]

	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

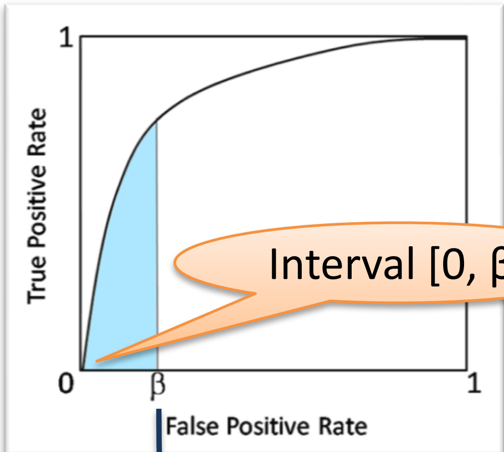
Run-time Analysis



Repeat:

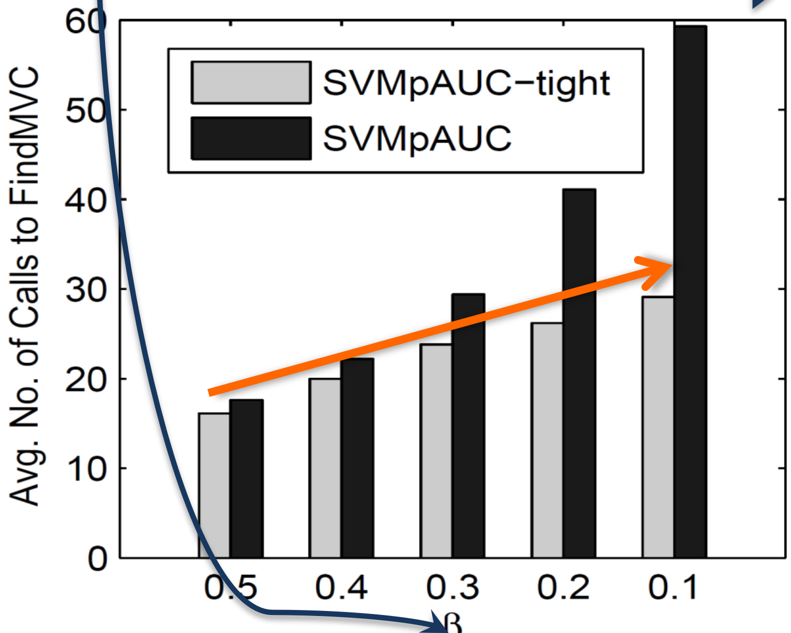
1. Solve OP for a subset of constraints.
2. Add the most violated constraint.

Run-time Analysis

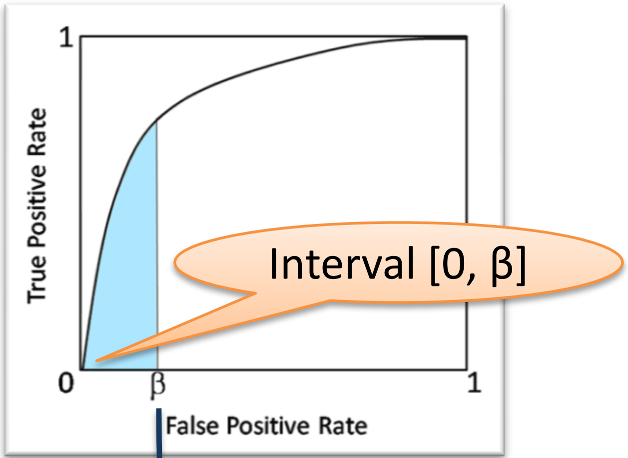


Repeat:

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



Run-time Analysis



Repeat:

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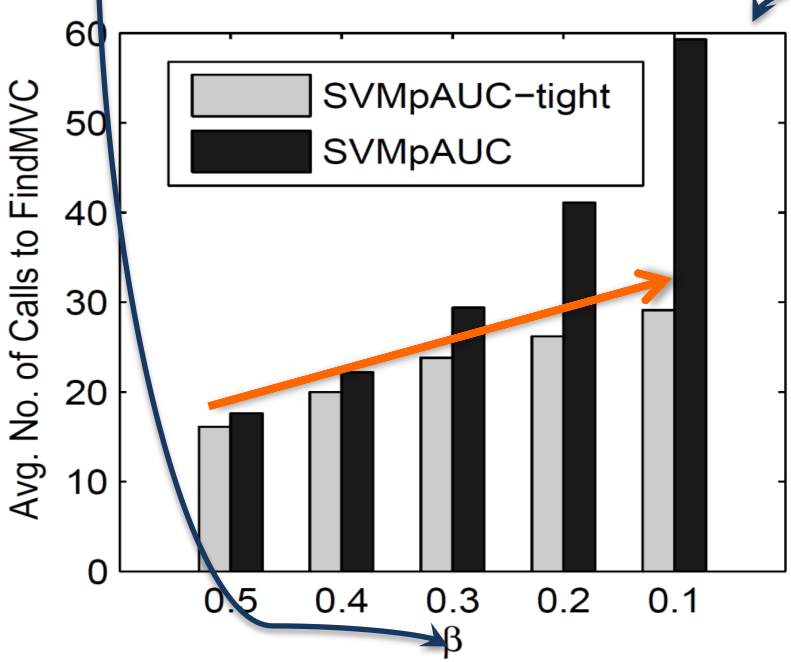
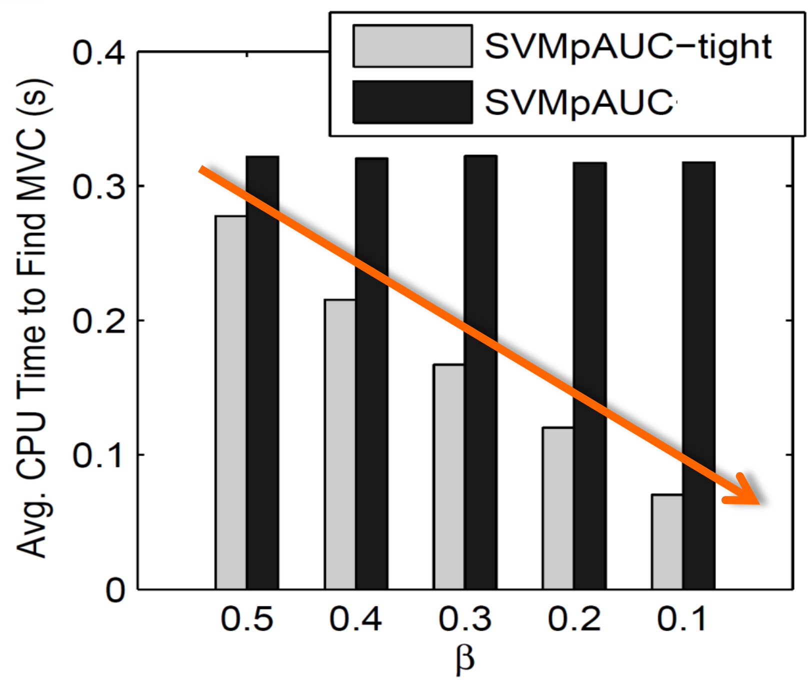
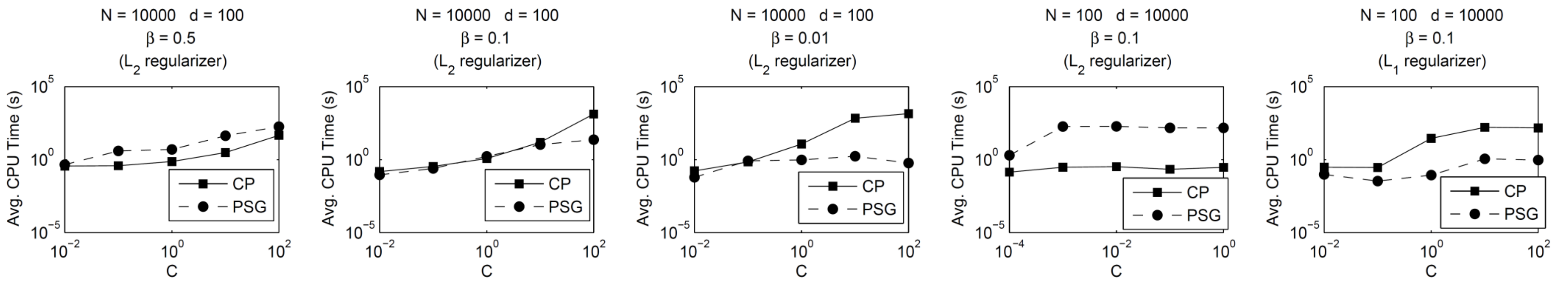




Cutting-Plane vs. Projected Subgradient



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	
$\text{SVM}^{\ell 2}_{\text{pAUC}}[0, 0.1]$	**63.25**	(100)	77.20	(100)
$\text{SVM}^{\text{elastic-net}(0.001)}_{\text{pAUC}}[0, 0.1]$	63.11	(41.5)	**77.52**	(41.6)
$\text{SVM}^{\text{elastic-net}(0.1)}_{\text{pAUC}}[0, 0.1]$	56.93	(32.24)	71.93	(27.6)
$\text{SVM}^{\ell 1}_{\text{pAUC}}[0, 0.1]$	53.63	(**11.36**)	66.22	(**10.0**)

	pAUC(0, 0.1)	# of groups selected
$\text{SVM}^{\ell 2}_{\text{pAUC}}[0, 0.1]$	**67.09**	17
$\text{SVM}^{\ell 1/\ell 2}_{\text{pAUC}}[0, 0.1]$	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?