A Structural SVM Based Approach for Optimizing the Partial AUC

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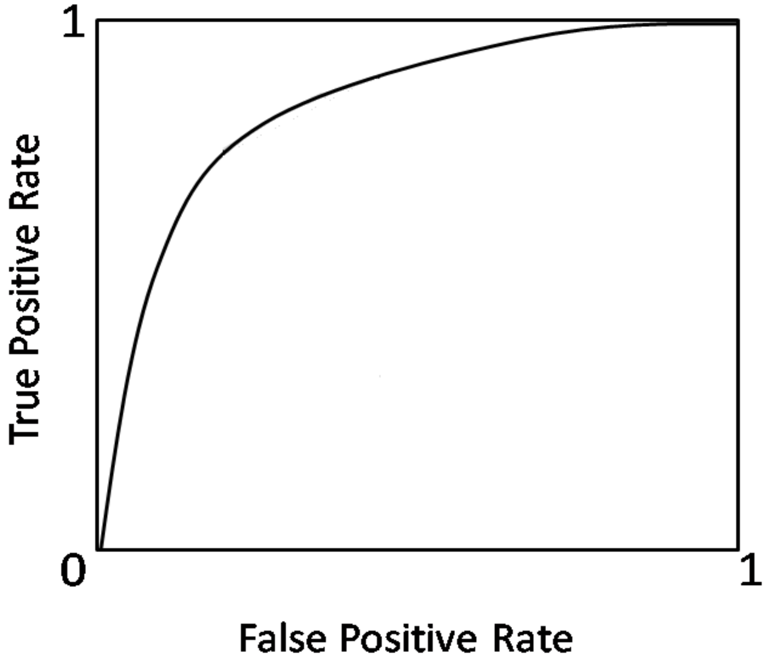
Receiver Operating Characteristic Curve



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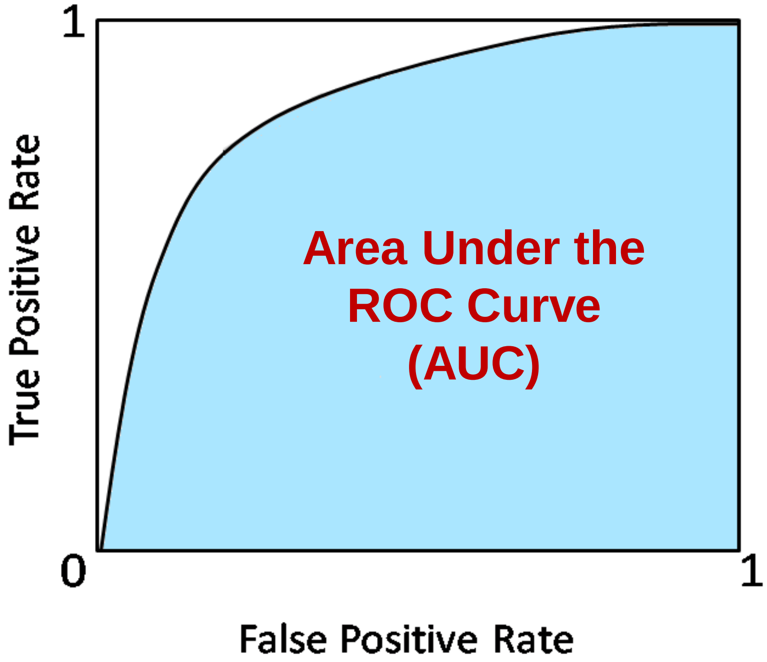
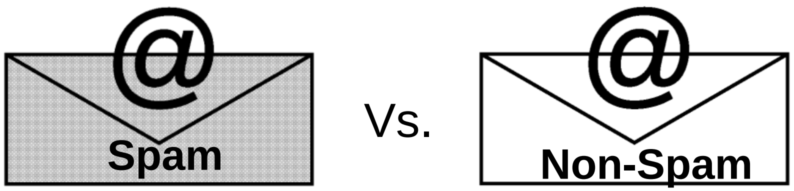


Binary Classification



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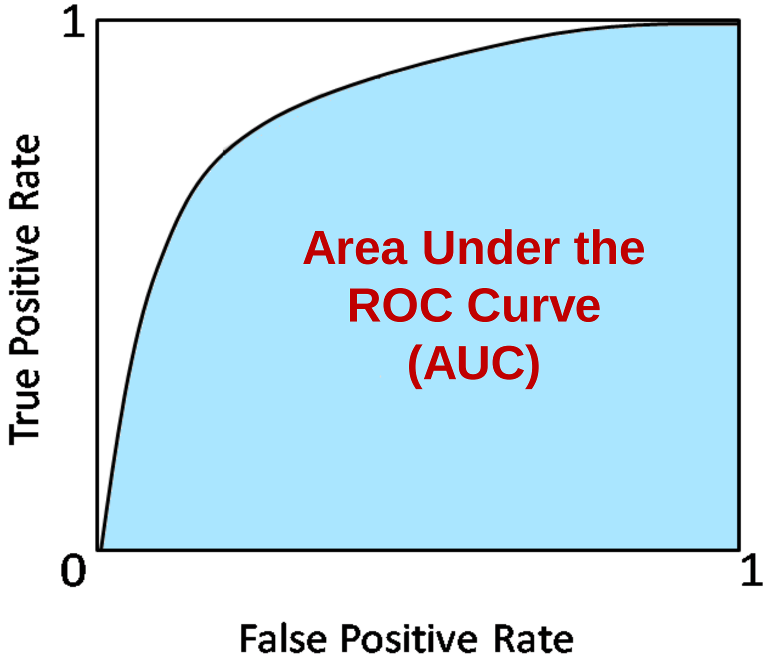

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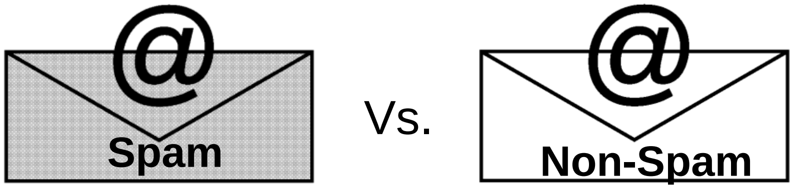
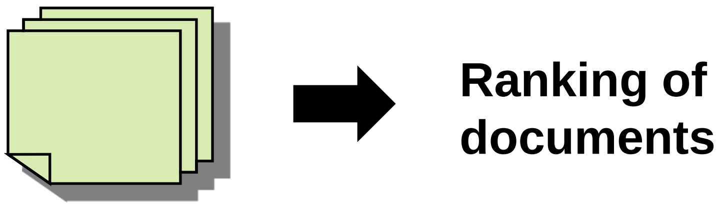
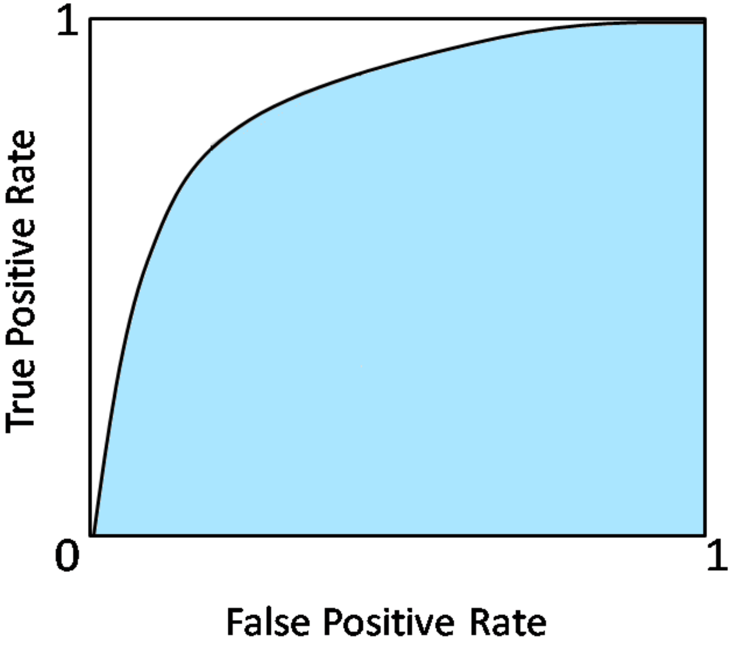


Bipartite Ranking

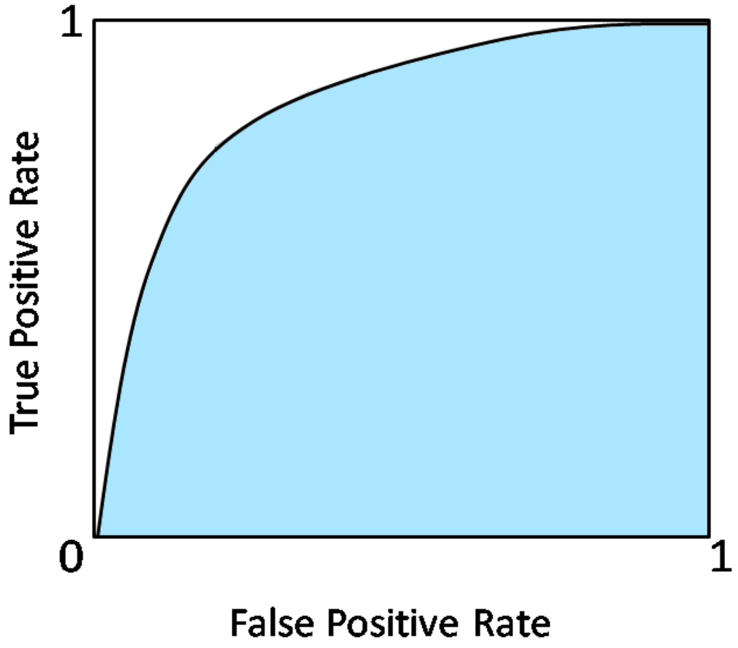


Partial AUC?



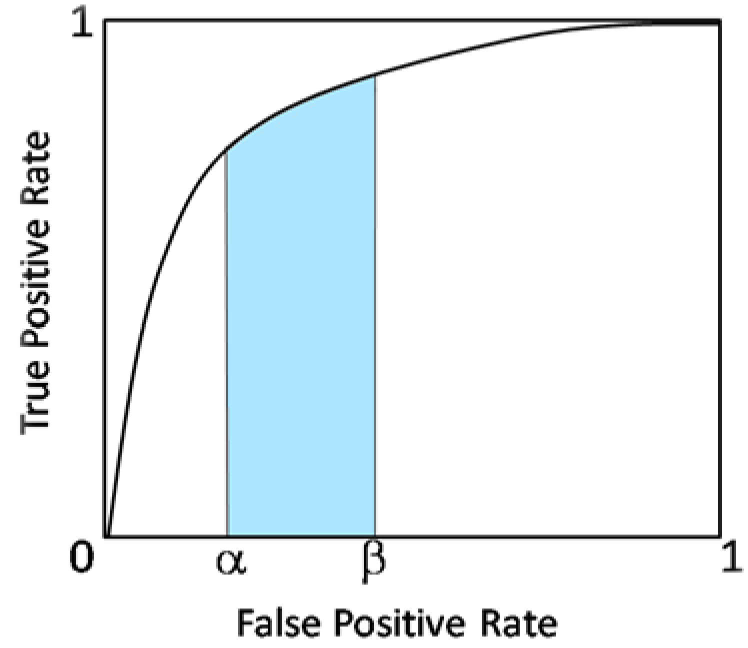
Full AUC

Partial AUC?



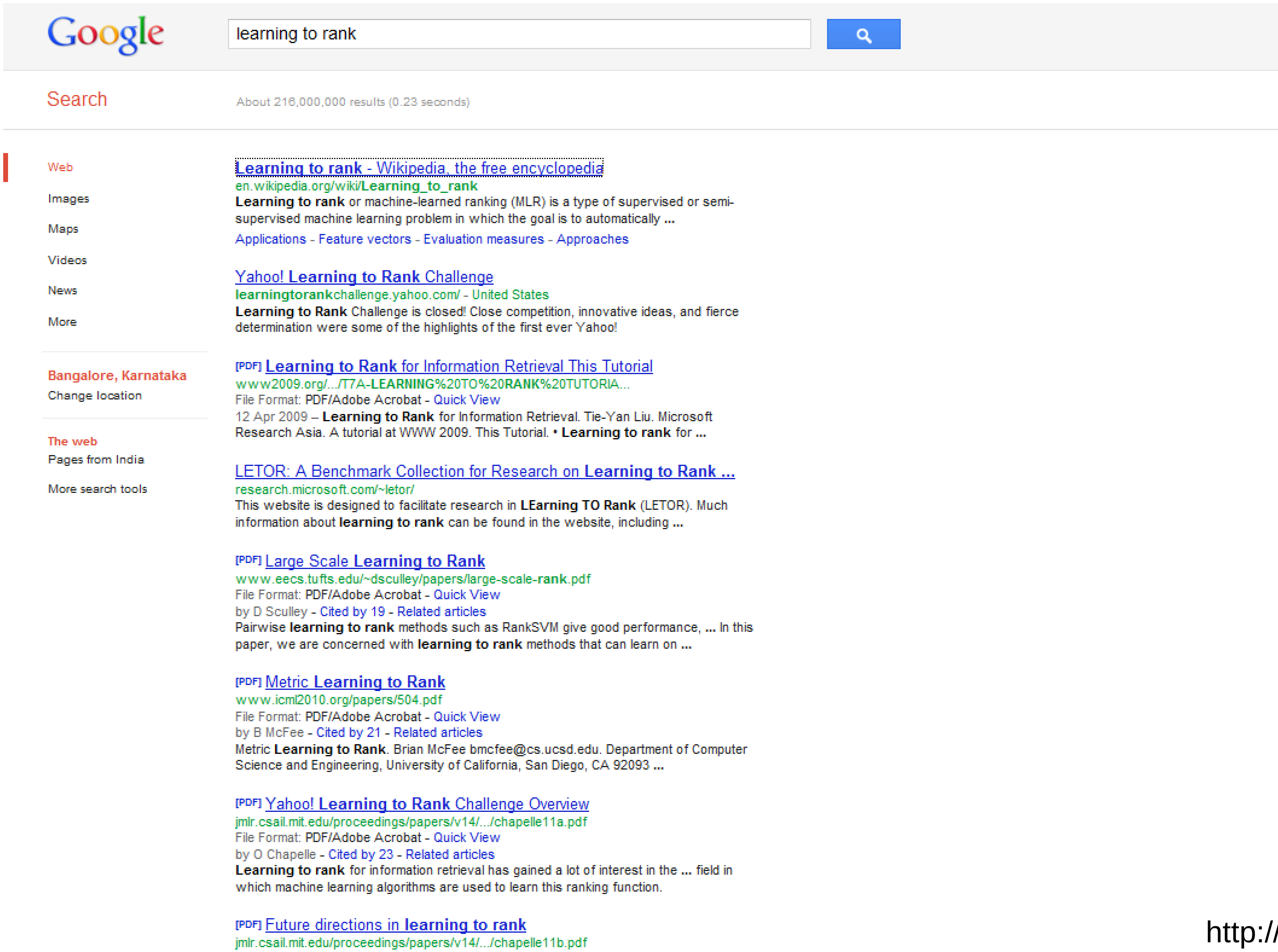
Full AUC

Vs



Partial AUC

Ranking



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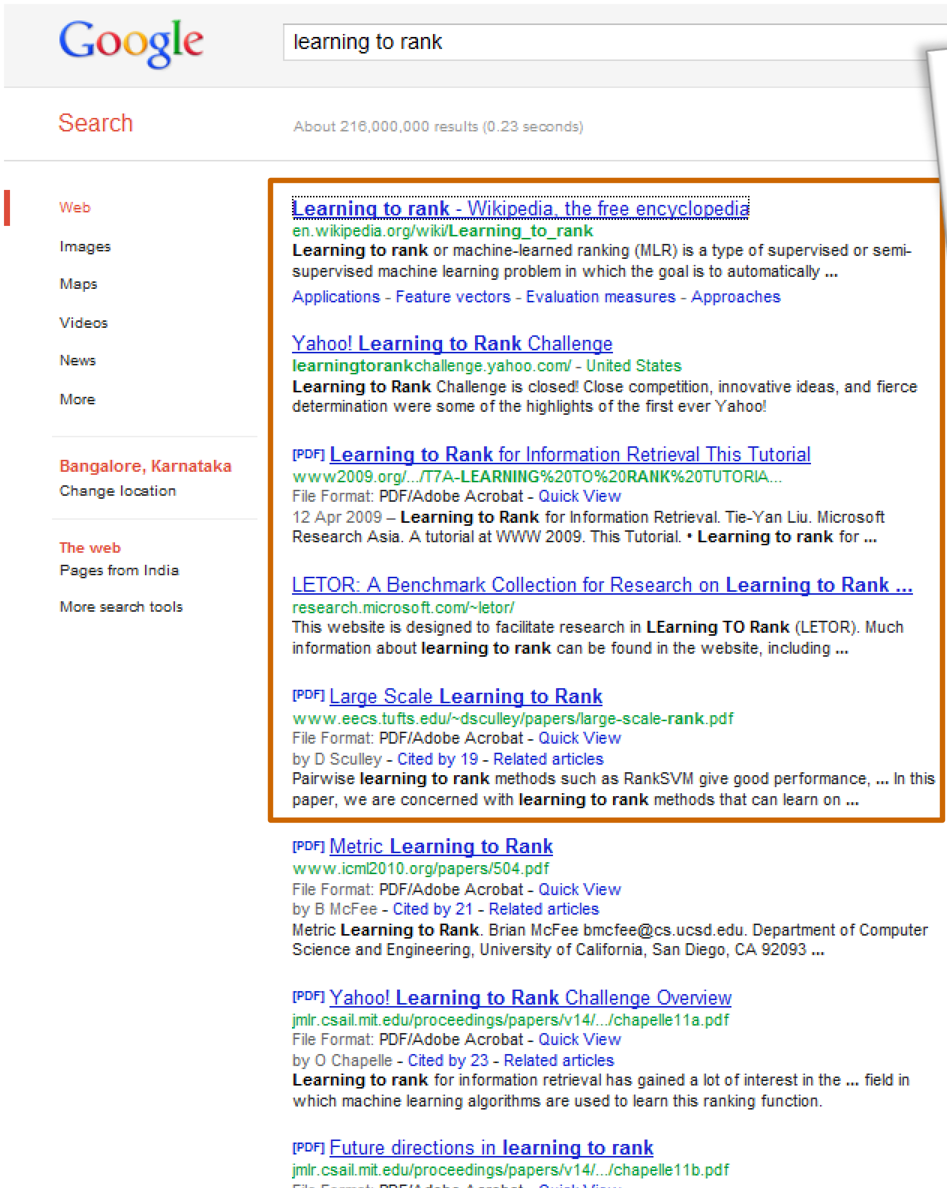
Ranking



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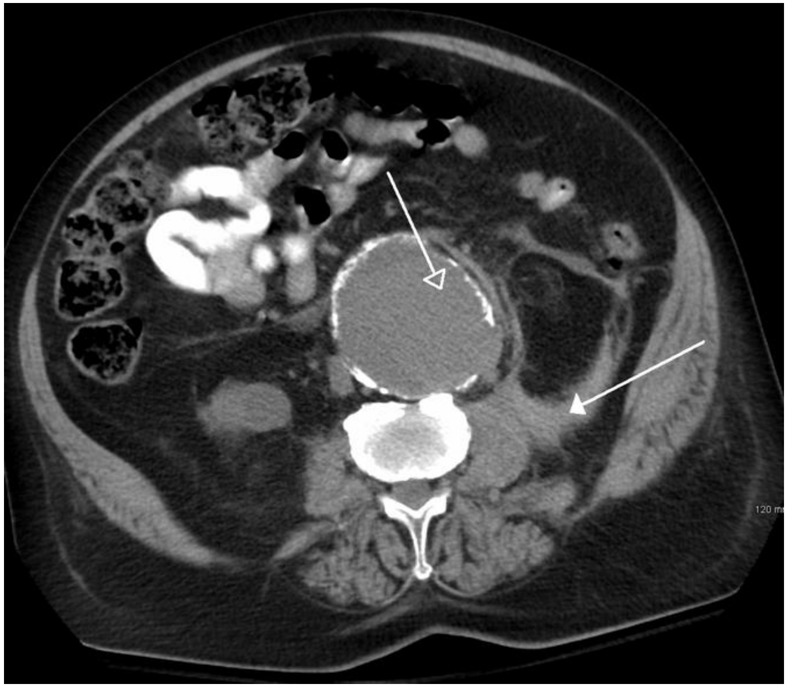
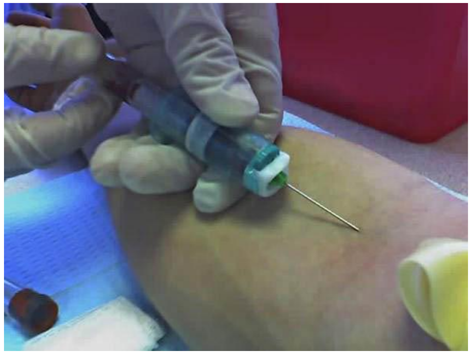
Medical Diagnosis





http://en.wikipedia.org/

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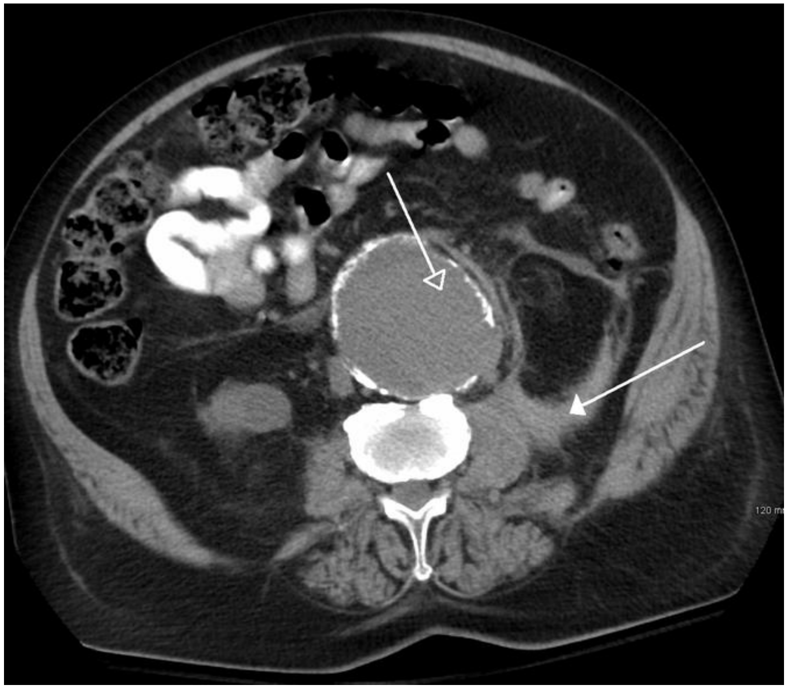

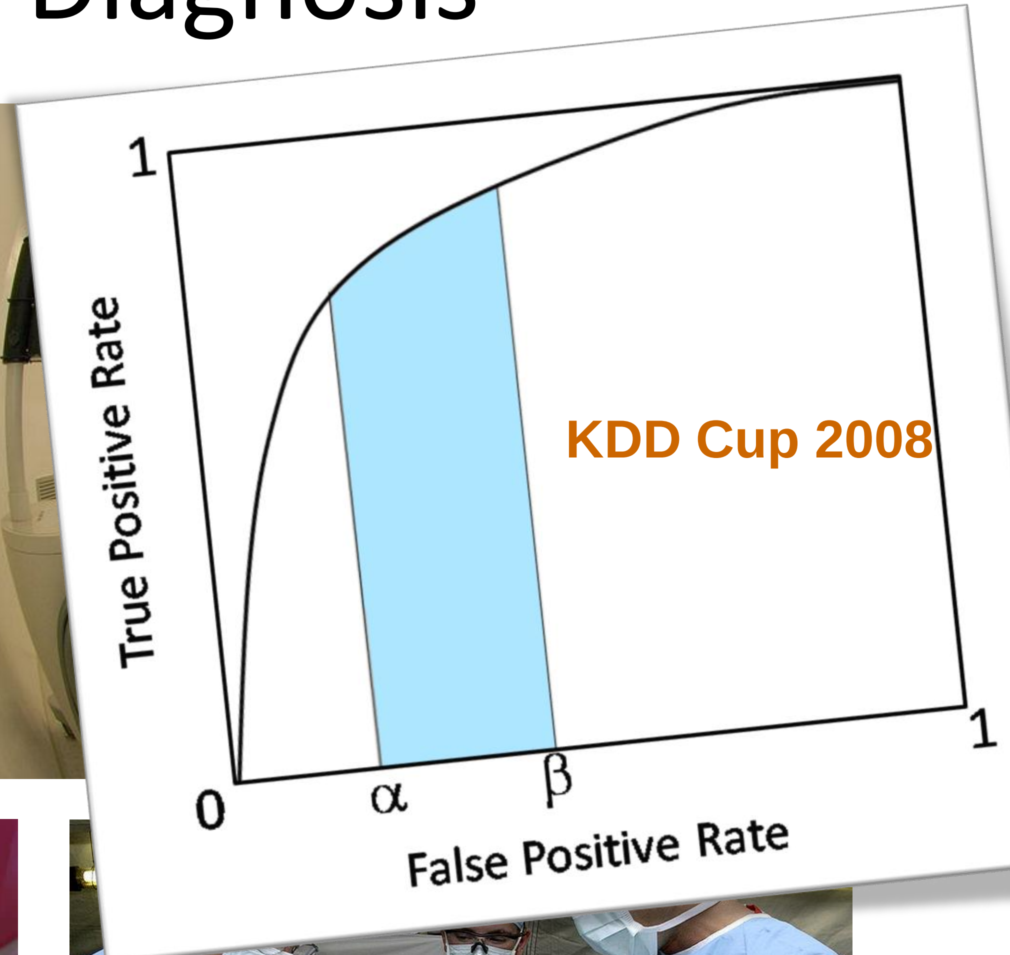

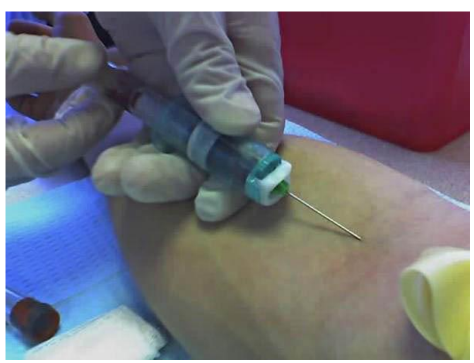

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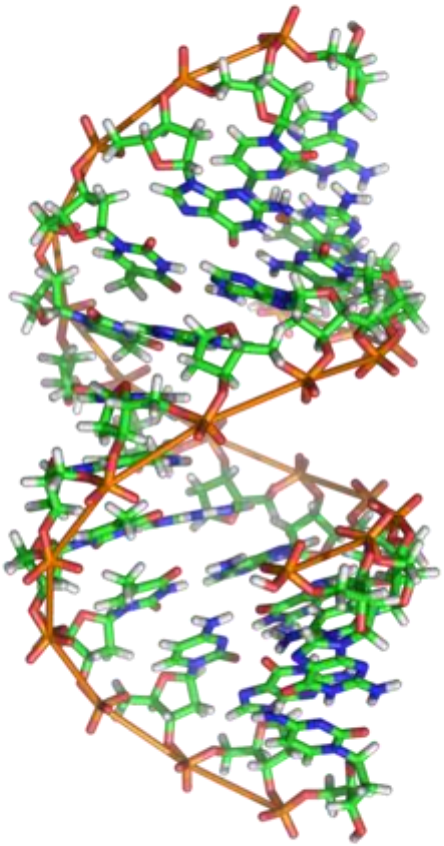
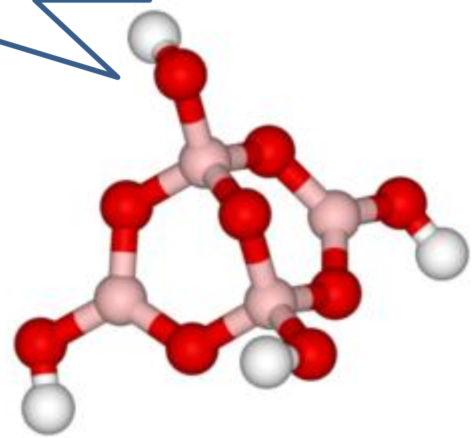
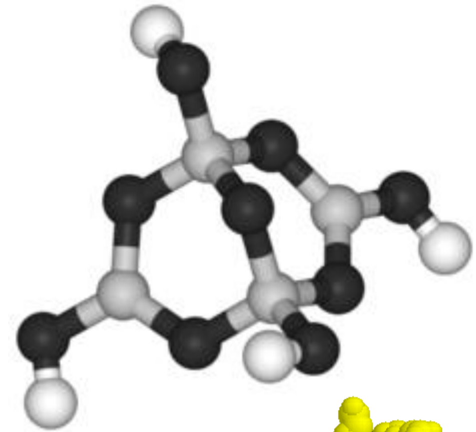
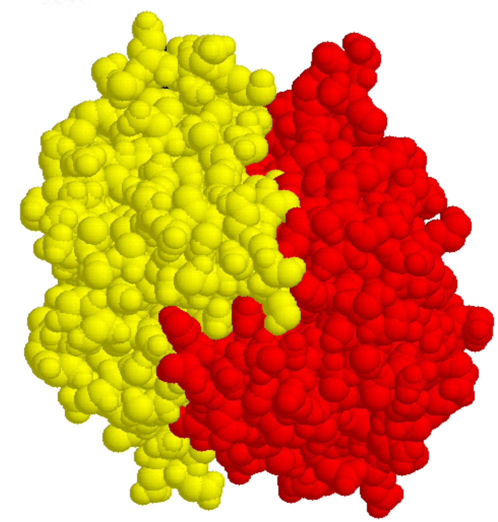
Bioinformatics

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









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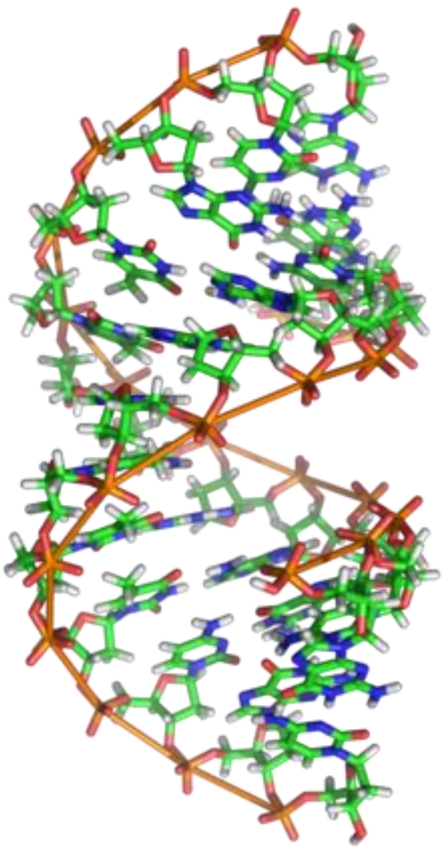

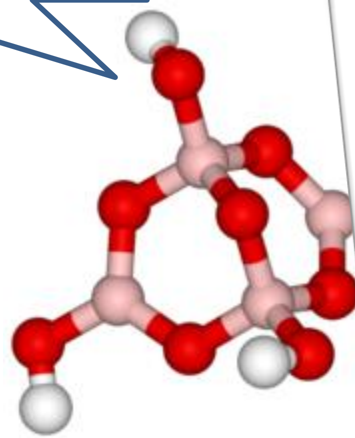

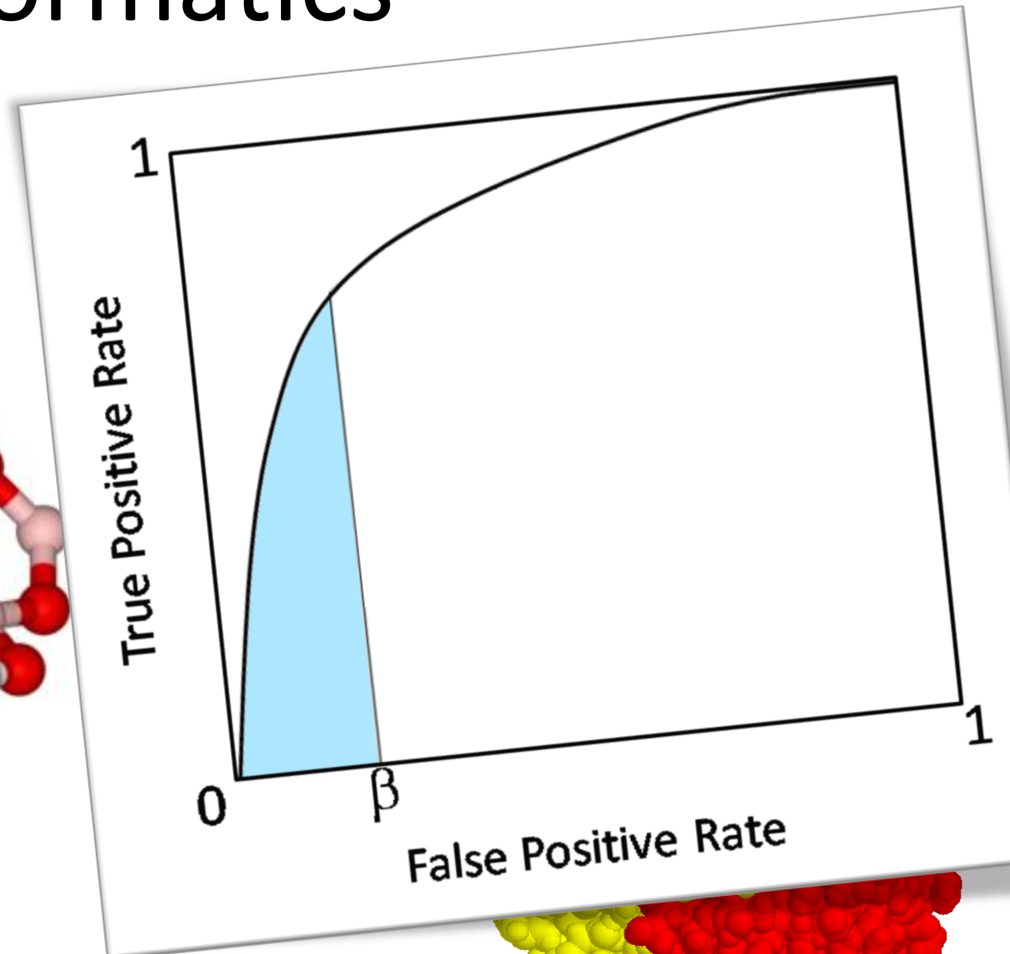

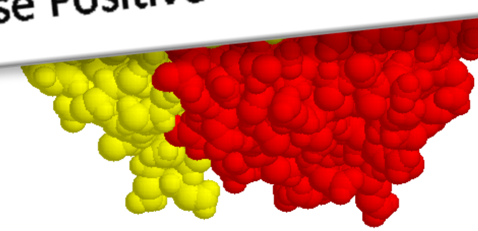

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http://commons.wikimedia.org/
http://www.google.com/imghp

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.

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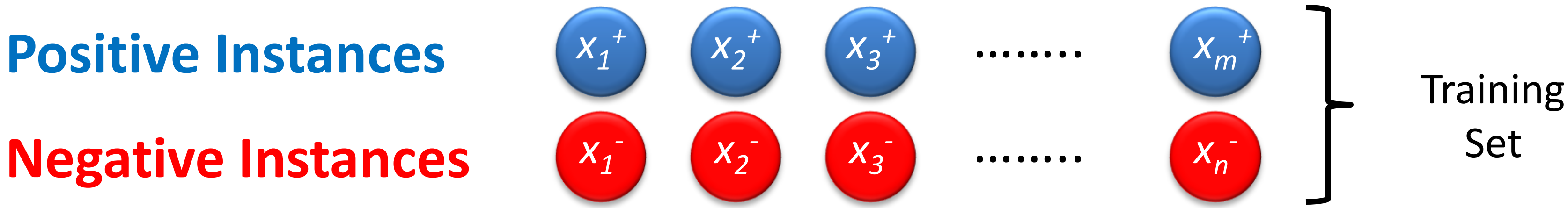
- Improvements over baselines on several real-world applications

Outline

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

Receiver Operating Characteristic Curve



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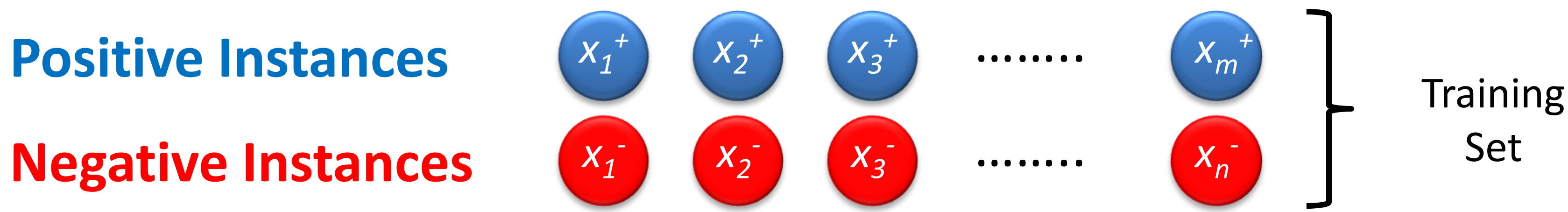
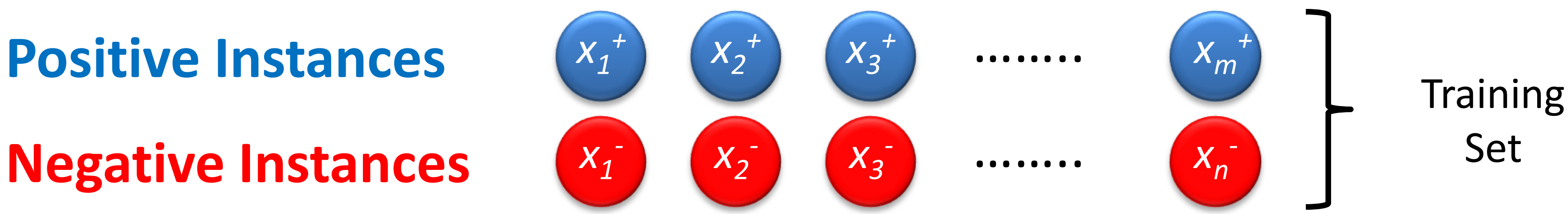


GOAL? Learn a scoring function $f : X \rightarrow \mathbb{R}$

Receiver Operating Characteristic Curve



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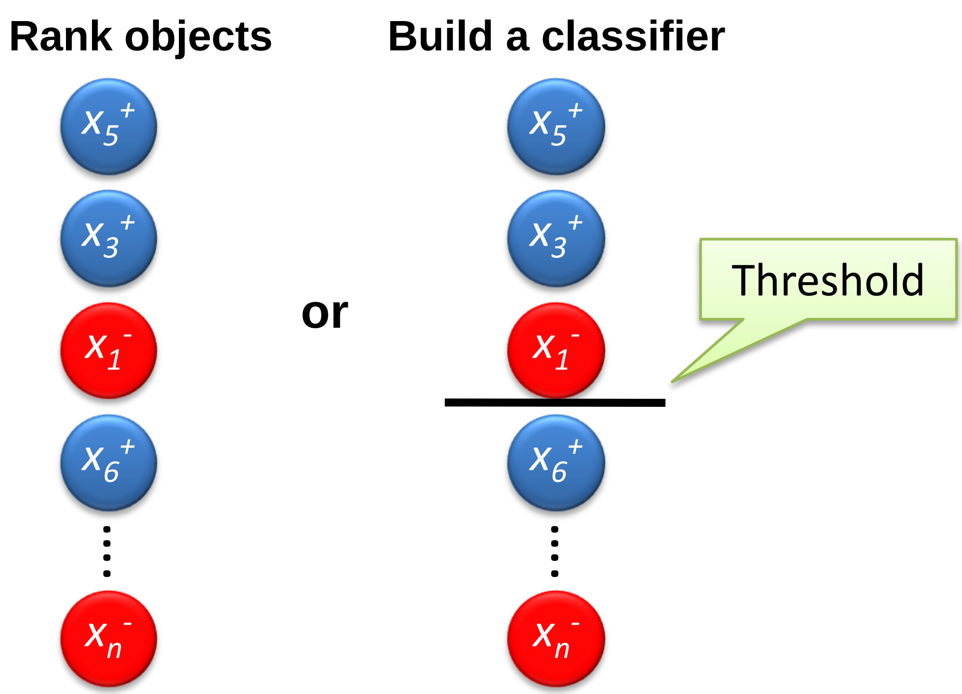

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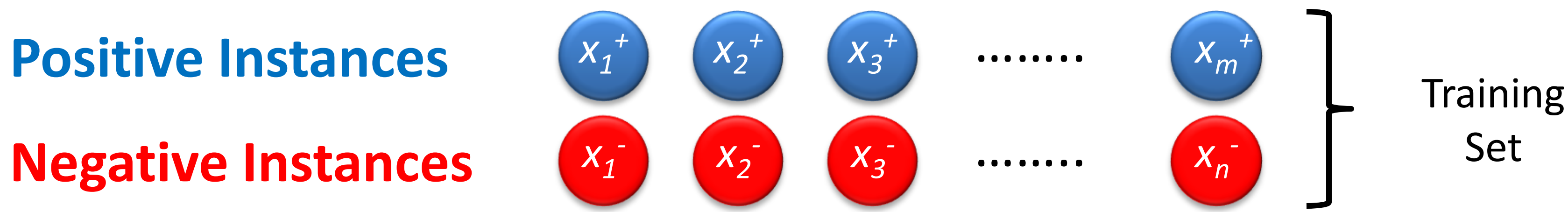

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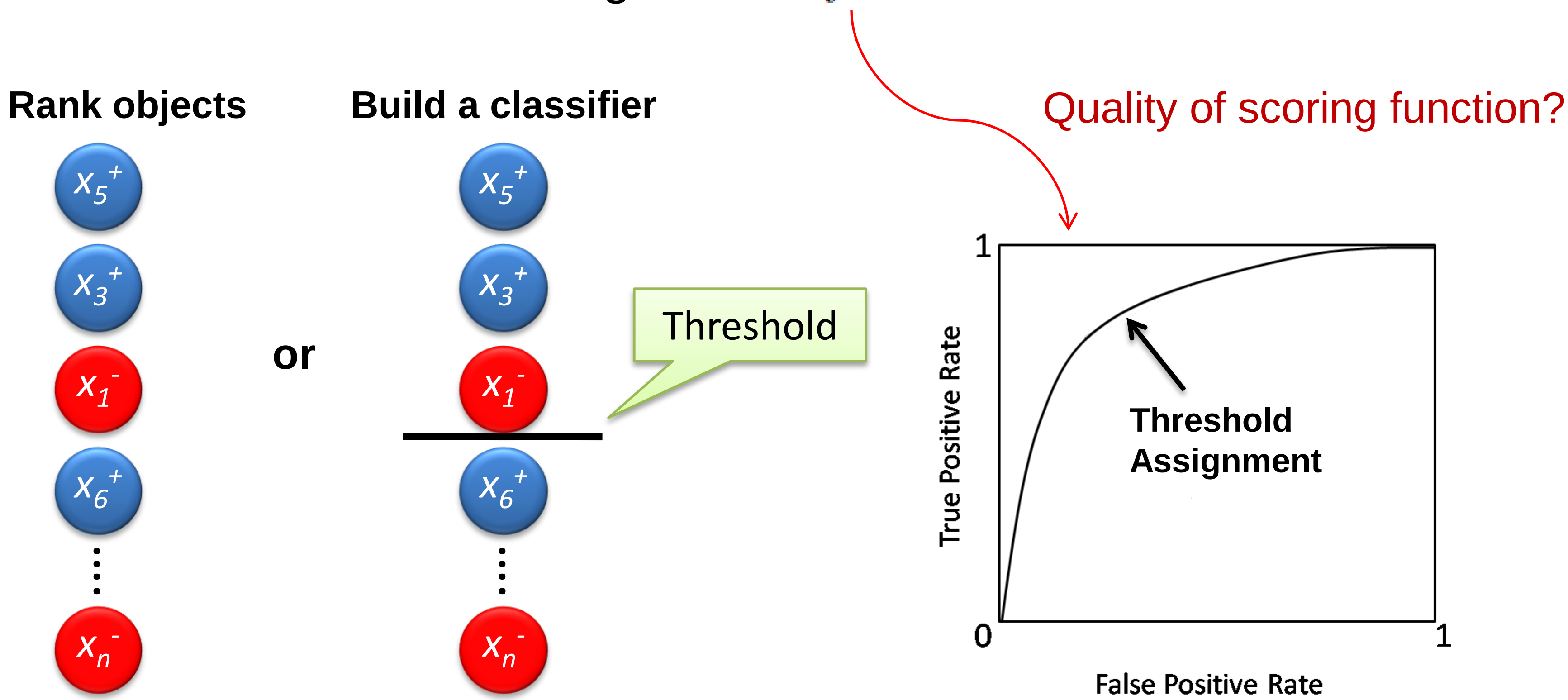
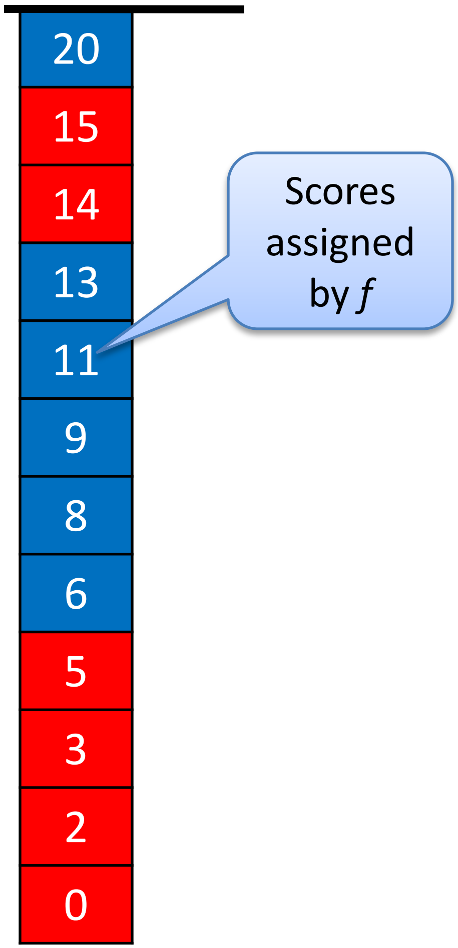
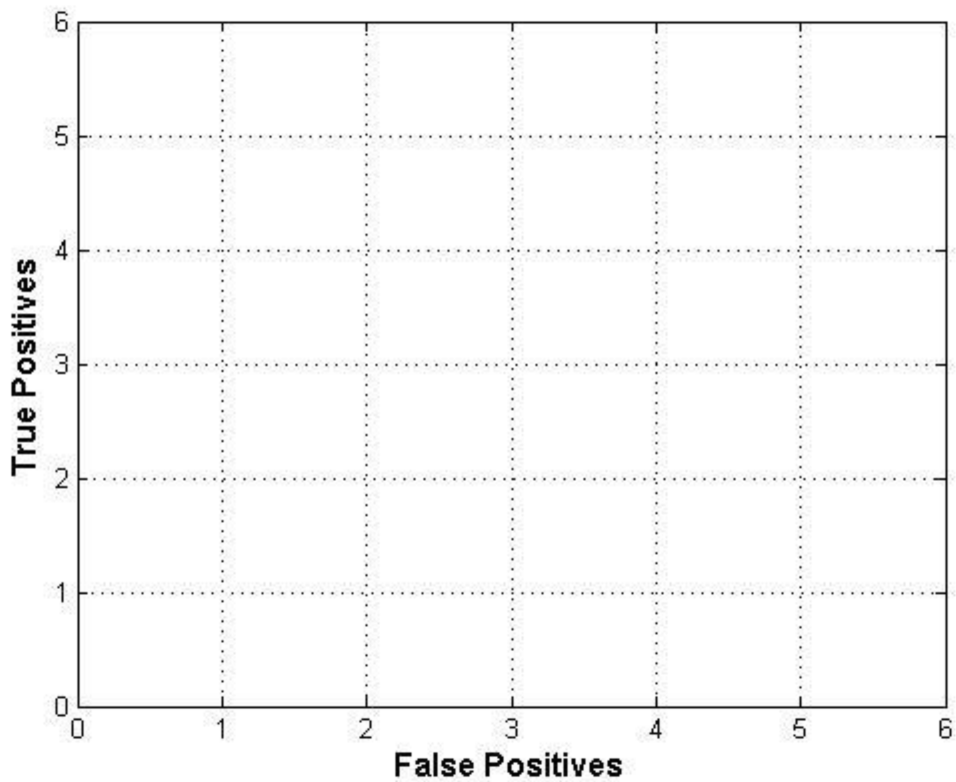


ROC Curve

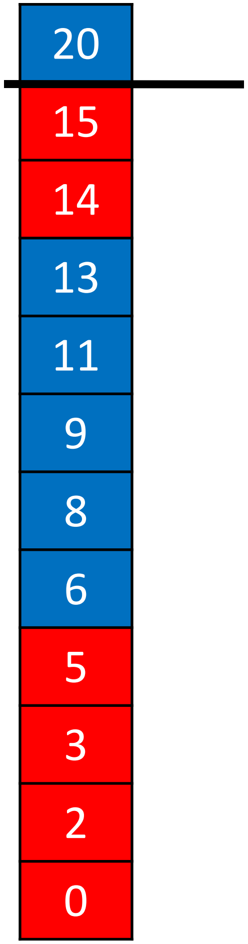
Receiver Operating Characteristic Curve

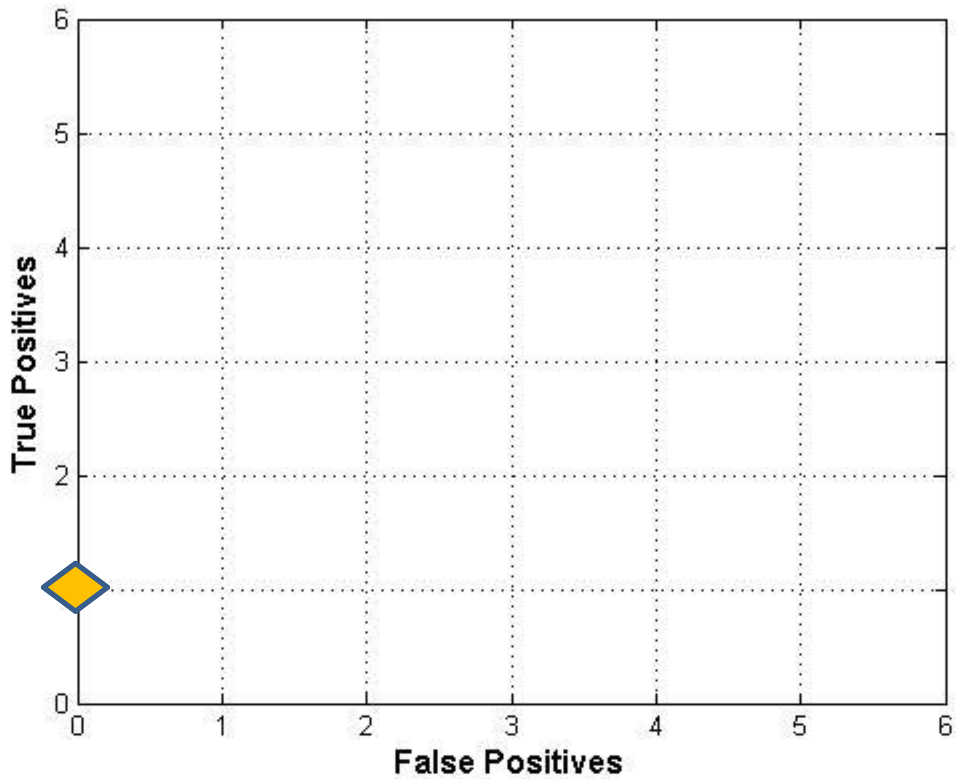




ROC Curve

Receiver Operating Characteristic Curve





ROC Curve

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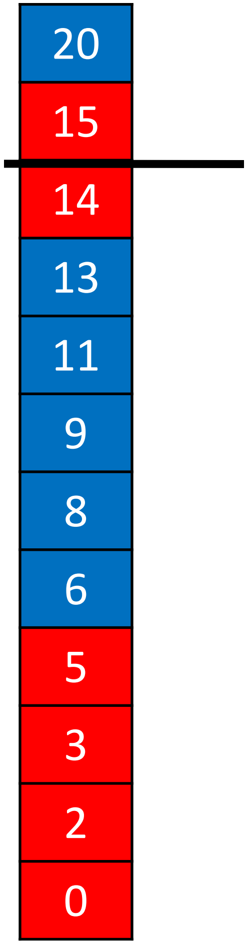

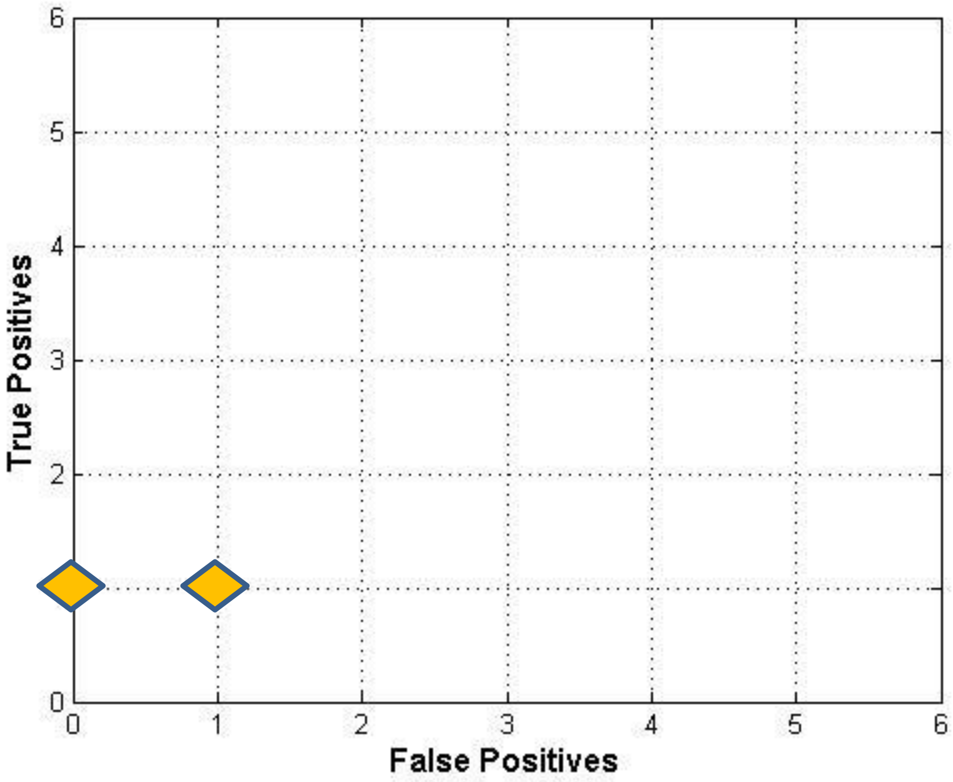

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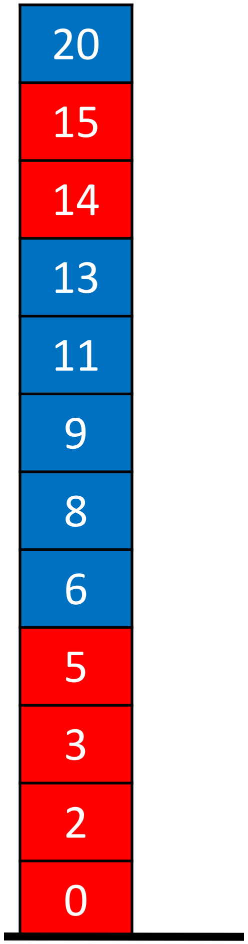
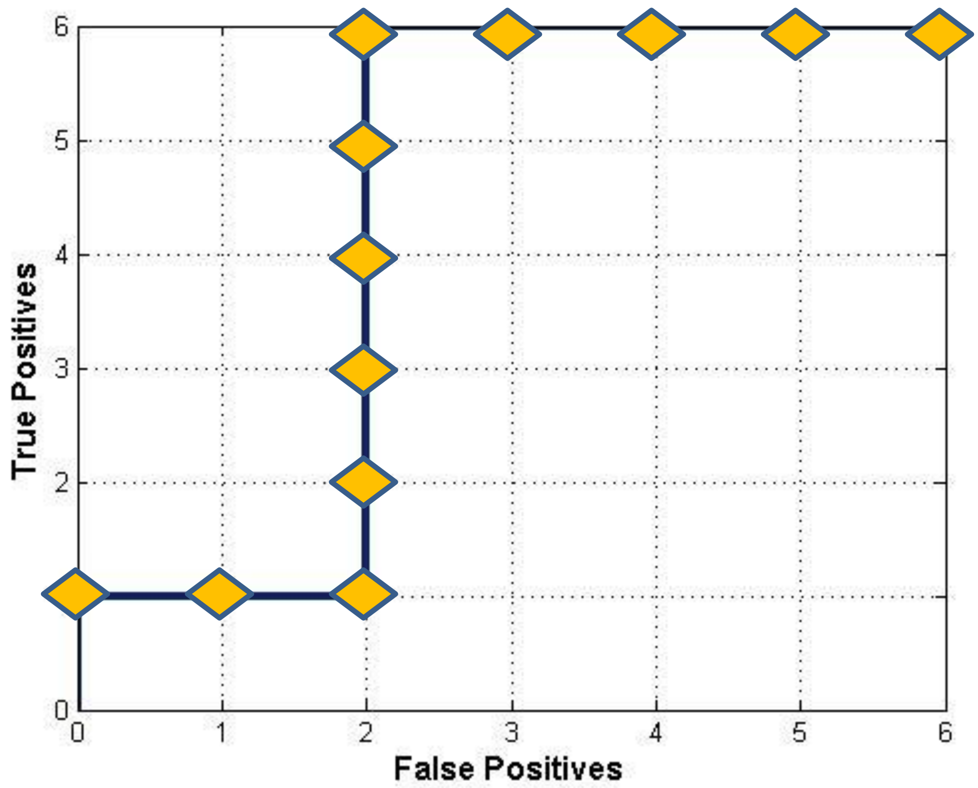
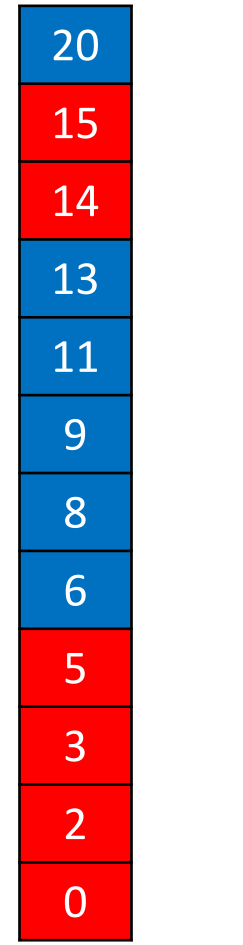
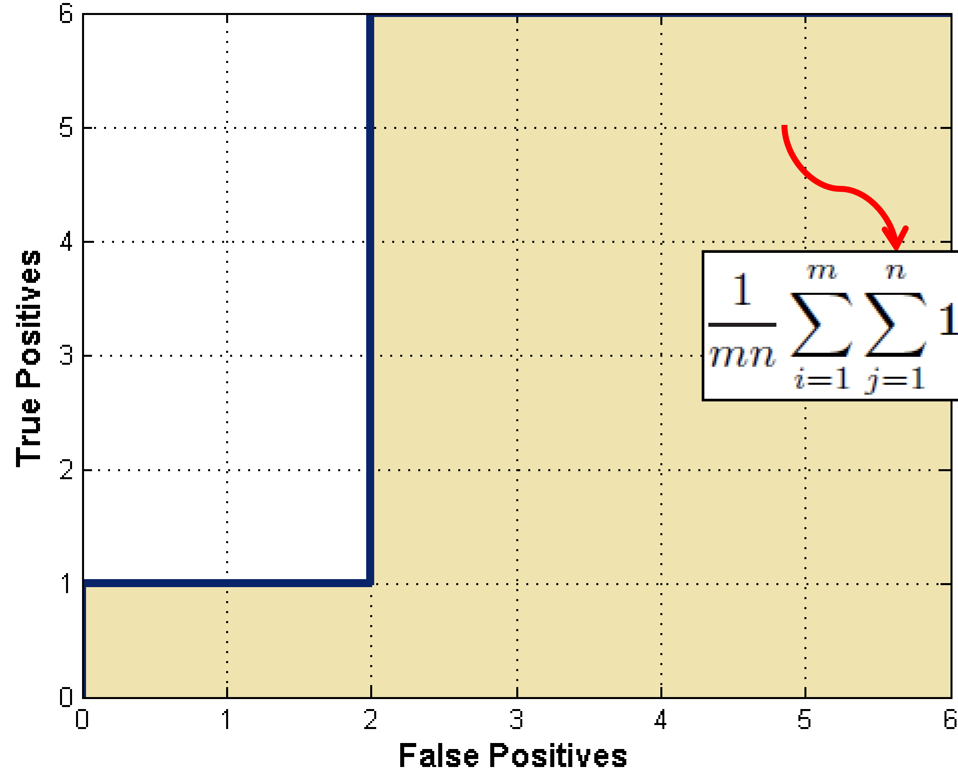




ROC Curve
Receiver Operating Characteristic Curve





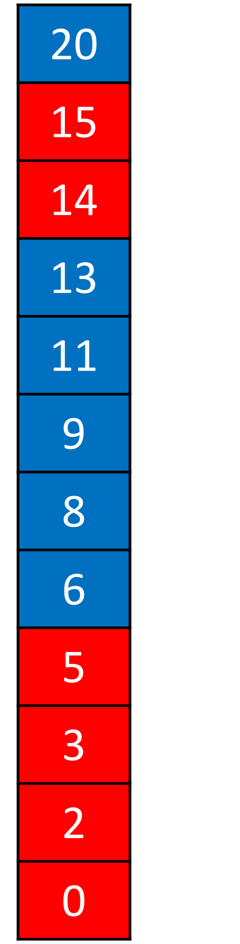
Area Under the Curve (AUC)

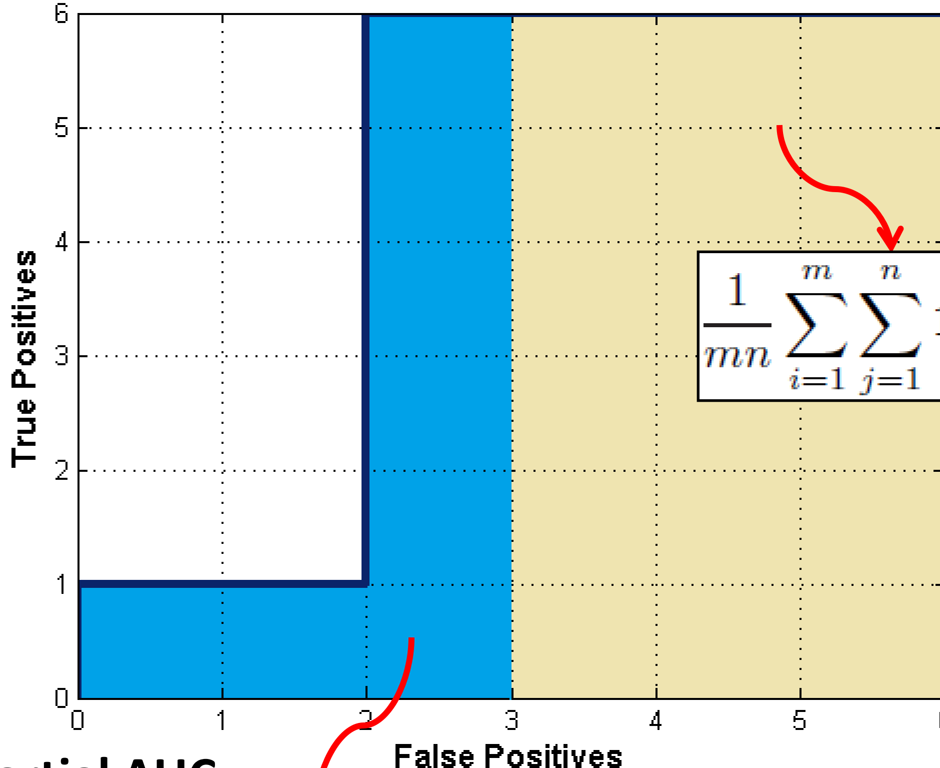
$$\frac{1}{mn}\sum_{i=1}^{m}\sum_{j=1}^{n}\mathbf{1}\left(f(x_i^+) > f(x_j^-)\right)$$

Pair-wise accuracy

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

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

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Structural SVM

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

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

Partial AUC Optimization

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

Discrete and
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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.
- Efficient solver with the same time complexity as that for full AUC.

Outline

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

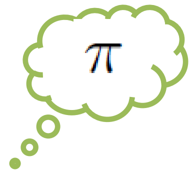
Structural SVM Based Approach

Structural SVM Based Approach

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

n (columns) × m (rows):

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

n × m (n columns, m rows)

π

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

compared with

π^*

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

IDEAL

Structural SVM Based Approach

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

π

n (columns) × m (rows)

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

compared with

π^* **IDEAL**

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

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

s.t.

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

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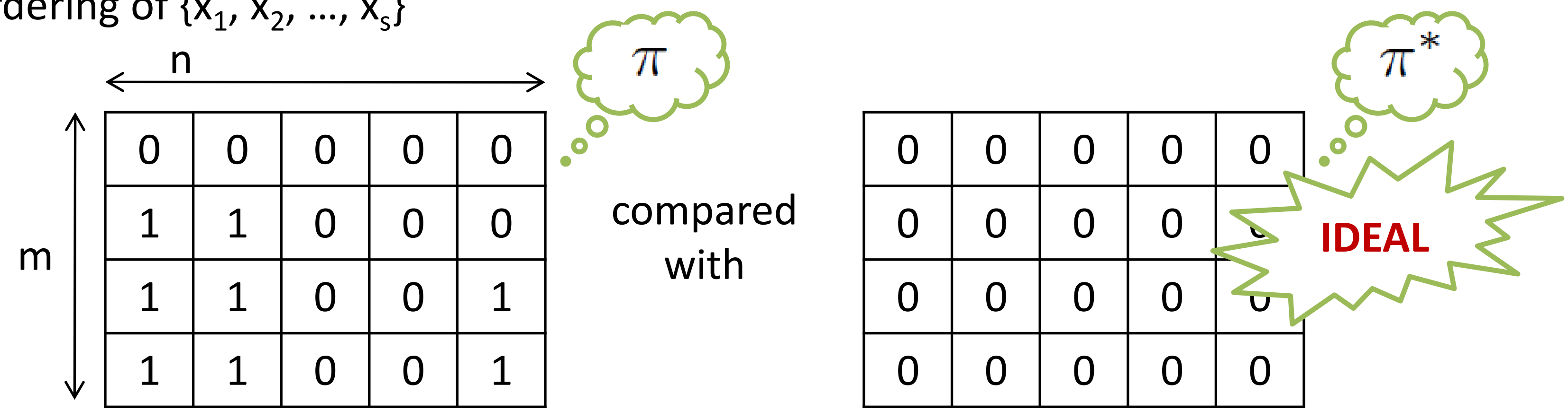

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pAUC Loss

Structural SVM Based Approach

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

π (n columns × m rows)

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

compared with

π^* — **IDEAL**

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

Upper Bound on (1 – pAUC)

Regularizer

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π (n × m)

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compared with

π^* — IDEAL

0	0	0	0	0
0	0	0	0	0
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Exponential Number of Output Matrices!!

Cutting-plane Solver

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

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

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

Repeat:

1. Solve OP for a subset of constraints.

Cutting-plane Solver

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

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Repeat:

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

Cutting-plane Solver

Converges in constant number of iterations

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

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

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

Break down!

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

Cutting-plane Solver

Converges in constant number of iterations

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

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

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

Repeat:

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

Break down!

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

Full AUC

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

Partial AUC

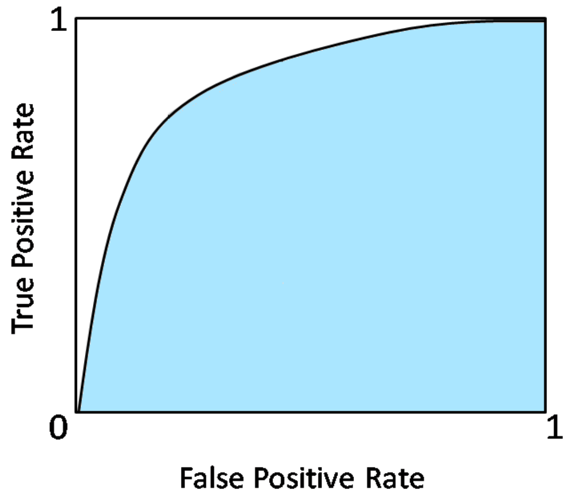
0	1	0	1	0
1	1	0	0	0
1	1	0	0	1
1	1	0	0	1

?

Trickier Optimization Problem

Full AUC

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

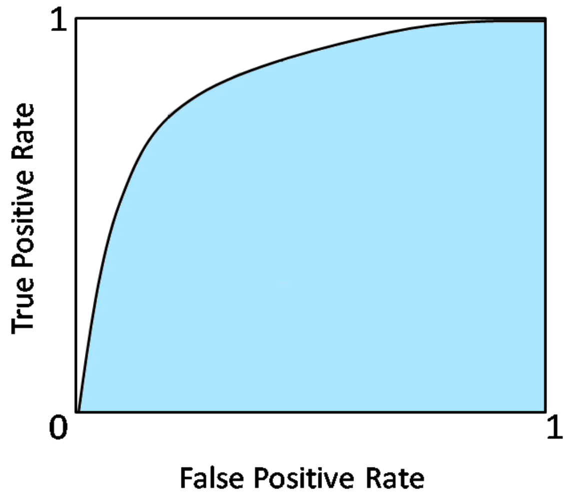


Trickier Optimization Problem

All Pairs

Full AUC

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



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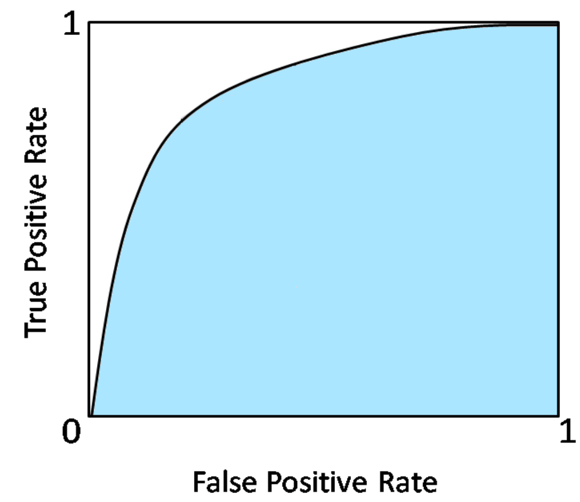

Partial AUC

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

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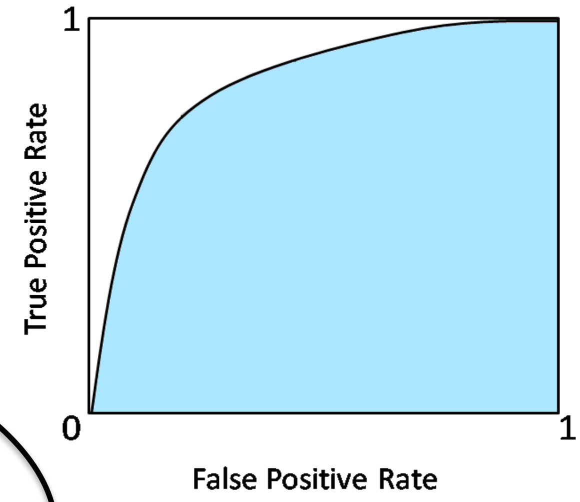

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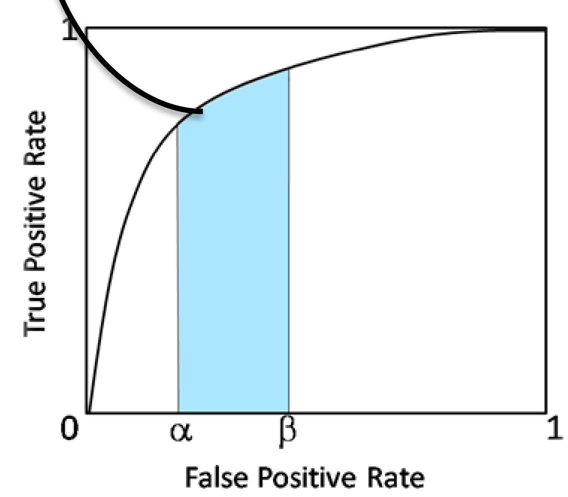

Subset of negative instances in the specified FPR range [α, β]

Find Most Violated Constraint

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

Partial AUC

0	1	0	1	0
1	1	0	0	0
1	1	0	0	1
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Equivalent easy-to-solve optimization problem

$$\operatorname*{argmax}_{\pi \in \Pi_{m,n}} Q_w(\pi) \iff \operatorname*{argmax}_{\pi \in \Pi^w_{m,n}} \widetilde{Q}_w(\pi) \iff \operatorname*{argmax}_{\pi \in R^w_1 \times \ldots \times R^w_m} \widetilde{Q}_w(\pi)$$

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

Partial AUC

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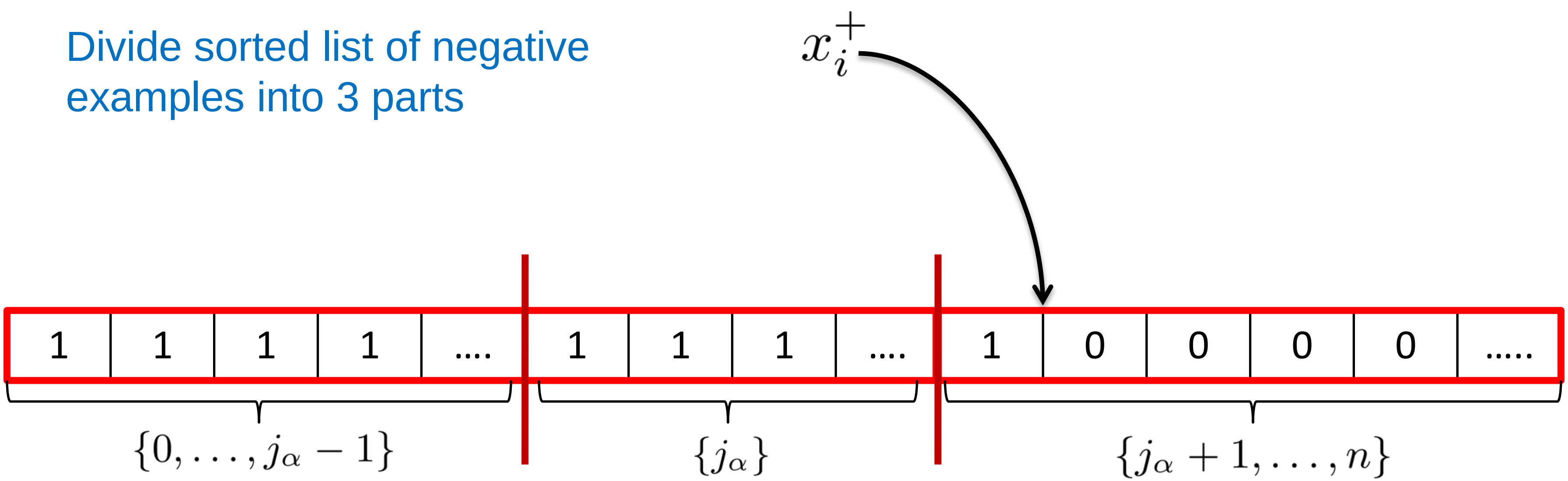
Divide sorted list of negative examples into 3 parts



Find Most Violated Constraint

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

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Divide sorted list of negative examples into 3 parts

x_i^+

Closed-form solution

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

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

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

1	1	1	1	....	1	1	1	....	1	0	0	0	0	.....

$\{0, \ldots, j_\alpha - 1\}$ $\{j_\alpha\}$ $\{j_\alpha + 1, \ldots, n\}$

Find Most Violated Constraint

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

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

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

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

End For

Output: $\bar{\pi}$

y-to-solve optimization problem

$\operatorname{argmax}_{\pi \in \Pi^w_{m,n}} \widetilde{Q}_w(\pi)$ ⟺ $\operatorname{argmax}_{\pi \in R^w_1 \times \ldots \times R^w_m} \widetilde{Q}_w(\pi)$

Closed-form

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

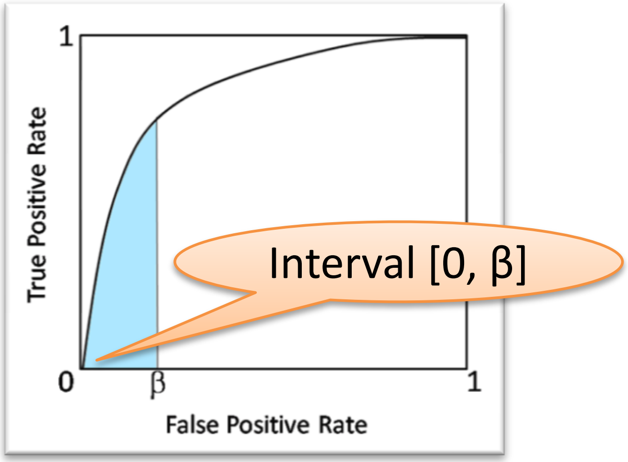
1	0	0	0	0	.....

$\{0, \ldots, j_\alpha - 1\}$ $\{j_\alpha\}$ $\{j_\alpha + 1, \ldots, n\}$

Outline

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

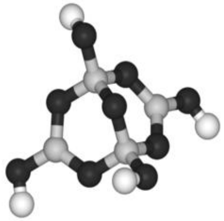
Experimental Results



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-Heuristic[0,0.1]	8.33 *



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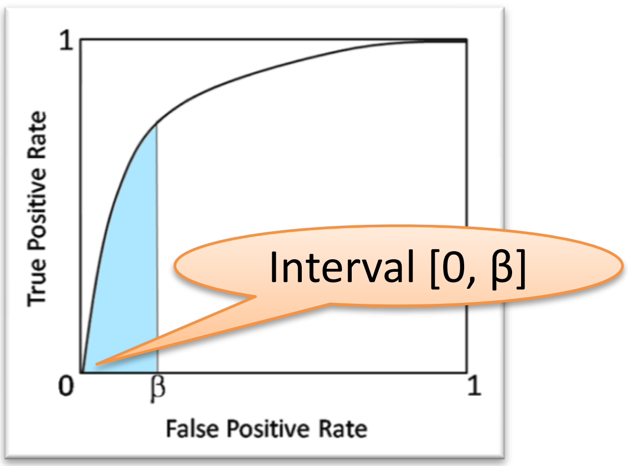

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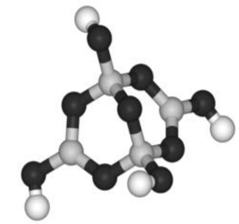
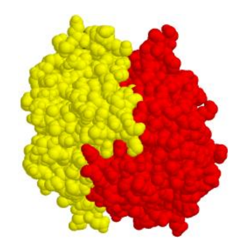


Protein-Protein Interaction Prediction

~$3x10^3$ 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 *



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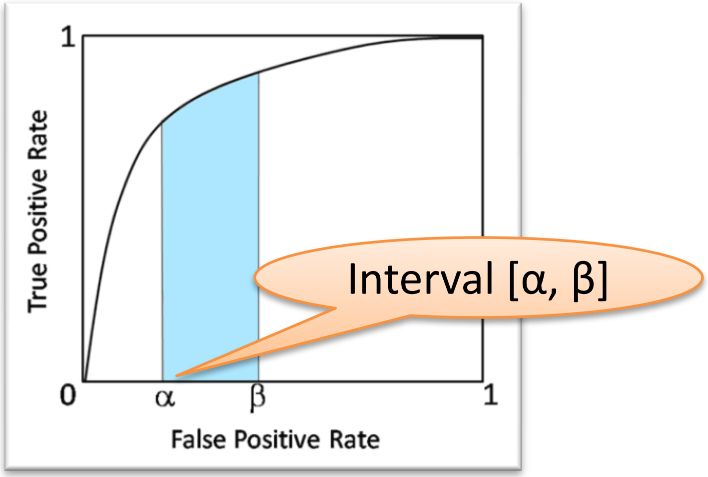
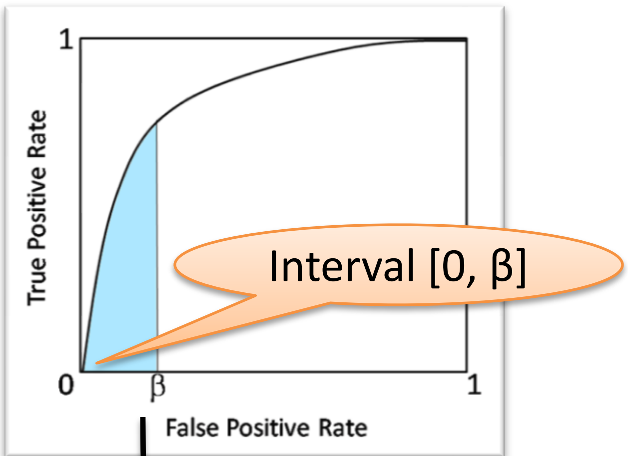


KDD Cup 2008
Breast Cancer Detection
~600 malignant ROIs / ~10^5 benign ROIs

	pAUC($0.2s, 0.3s$)
$\text{SVM}_{\text{pAUC}}[0.2s, 0.3s]$	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.
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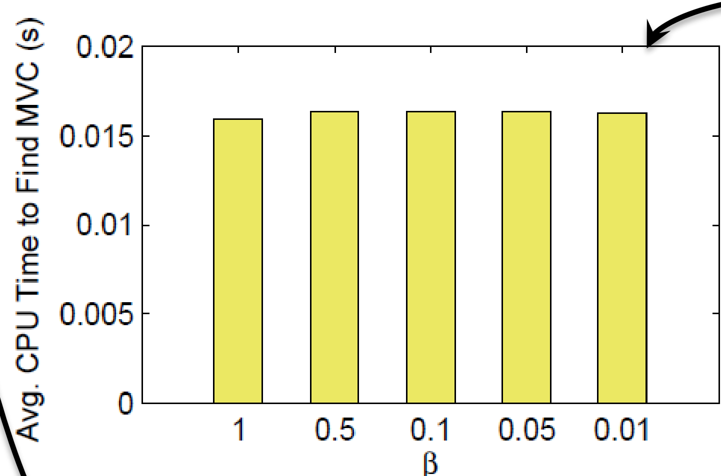

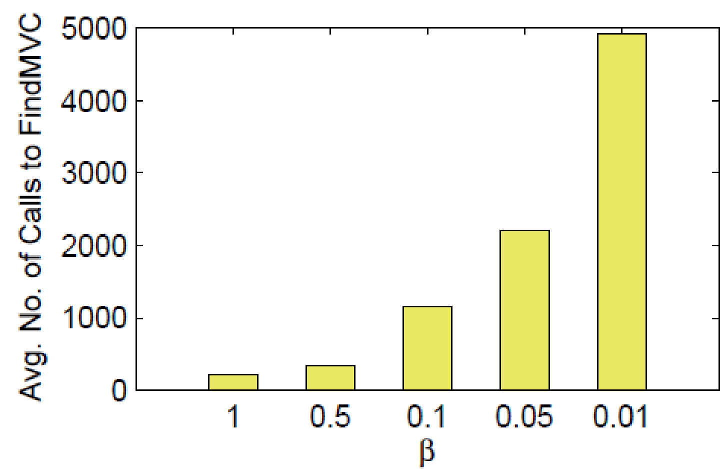

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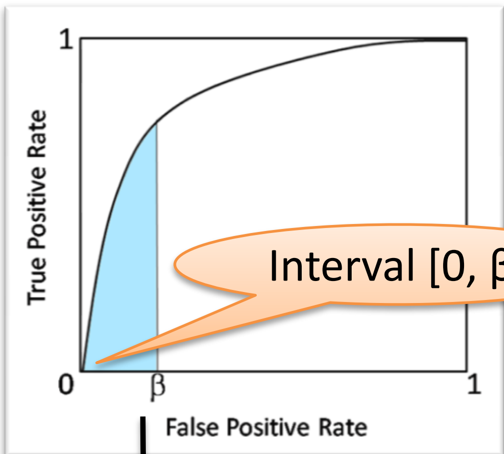

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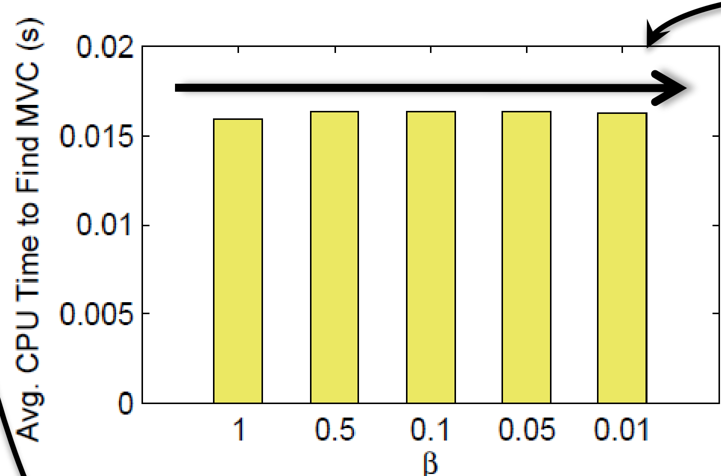

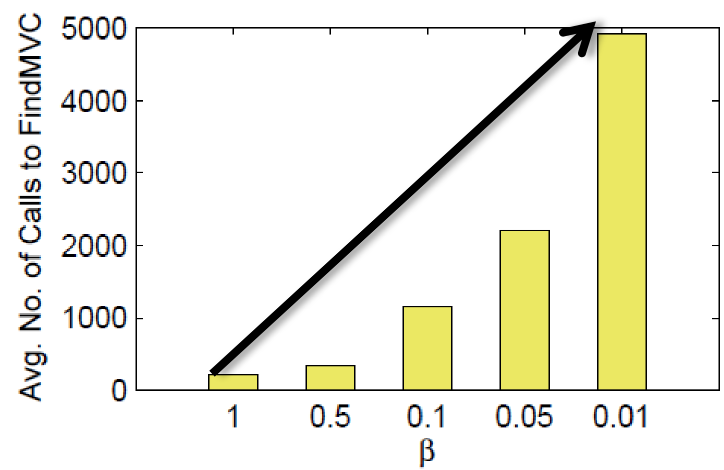

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- Follow up: Improved algorithm that optimizes a tighter upper bound on the partial AUC loss

Narasimhan, H. and Agarwal, S. $\mathrm{SVM}_{\mathrm{pAUC}}^{\mathrm{tight}}$: **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?