A Structural SVM Based Approach for Optimizing the Partial AUC

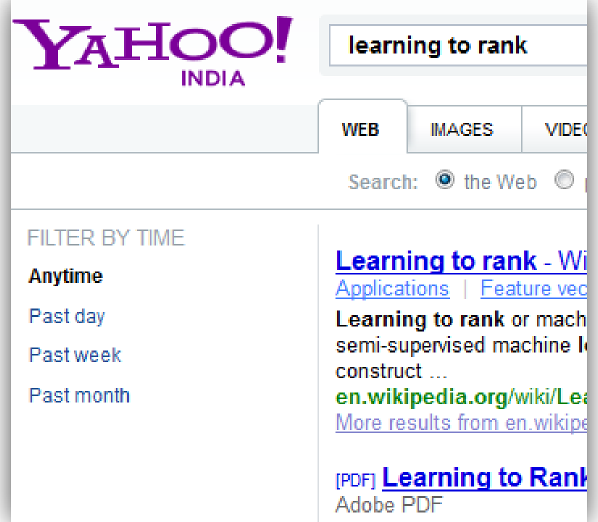
Harikrishna Narasimhan

(Joint work with Shivani Agarwal)

A paper on this work has been accepted in ICML 2013

Learning with Binary Supervision

Learning with Binary Supervision



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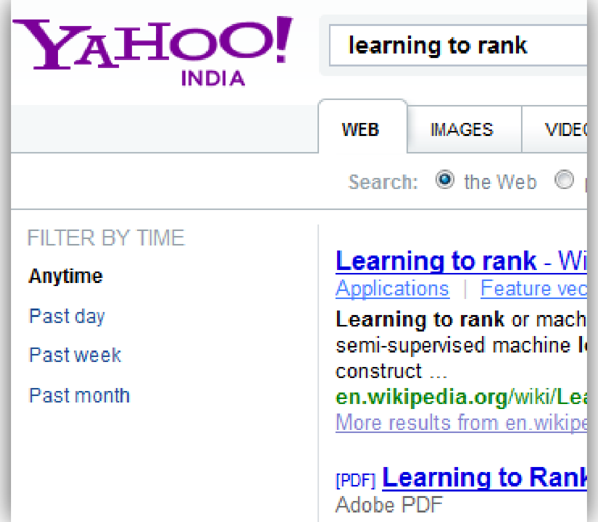

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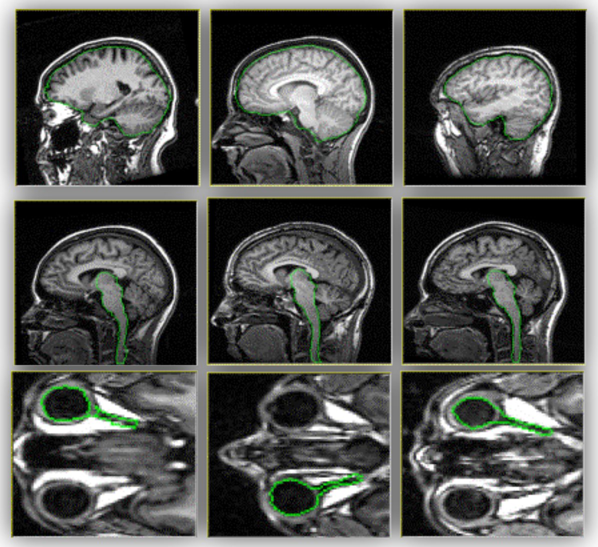

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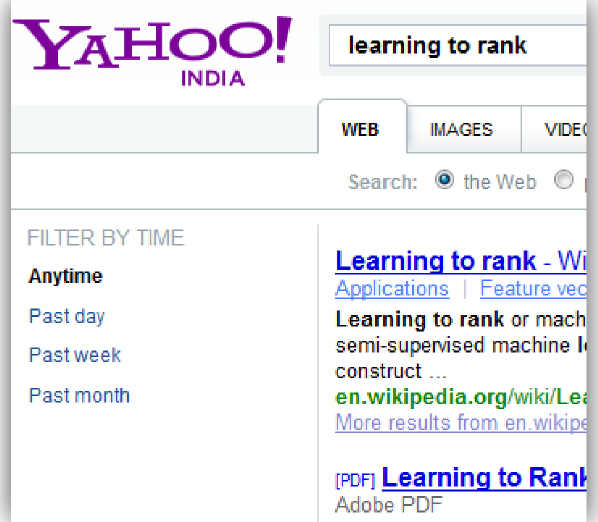

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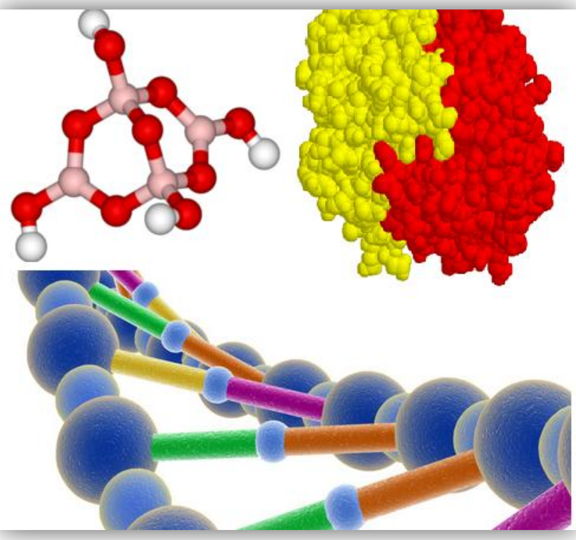

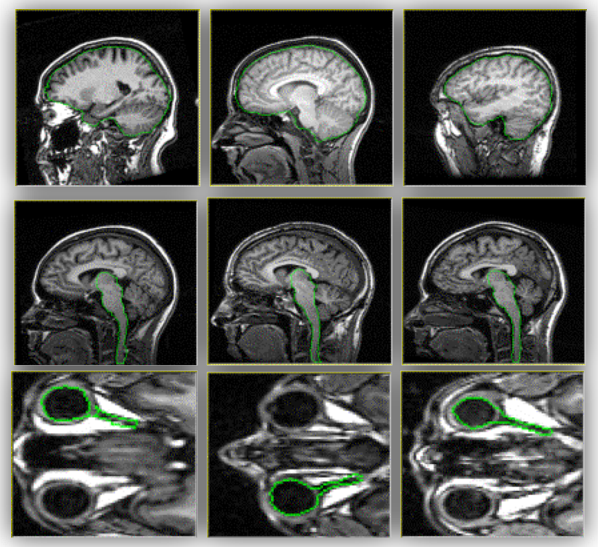

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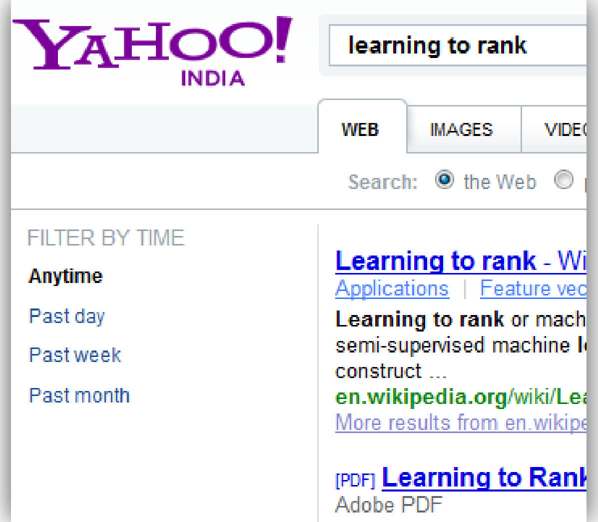

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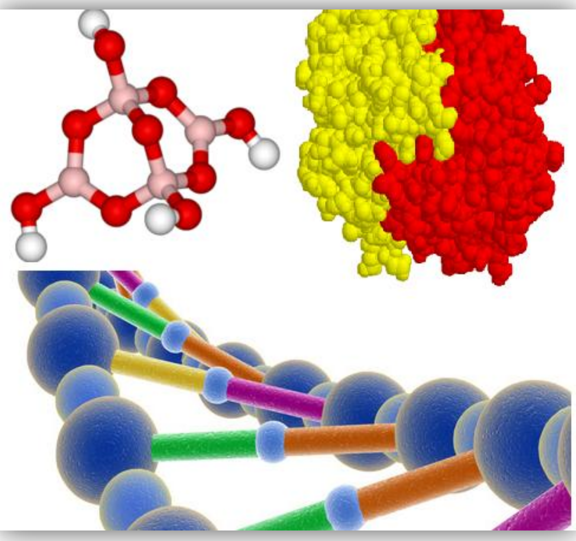

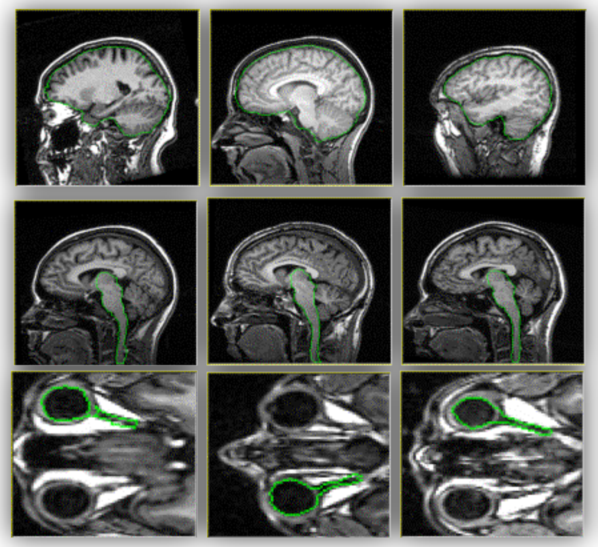

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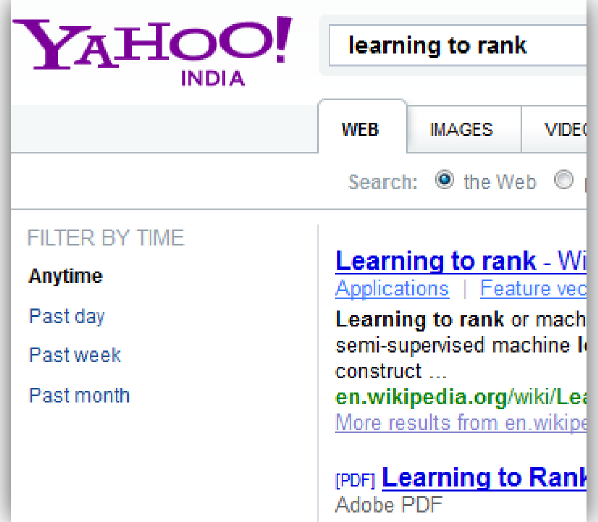

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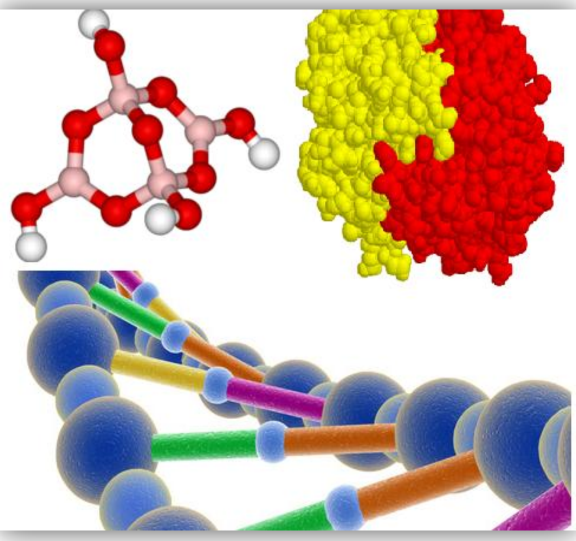

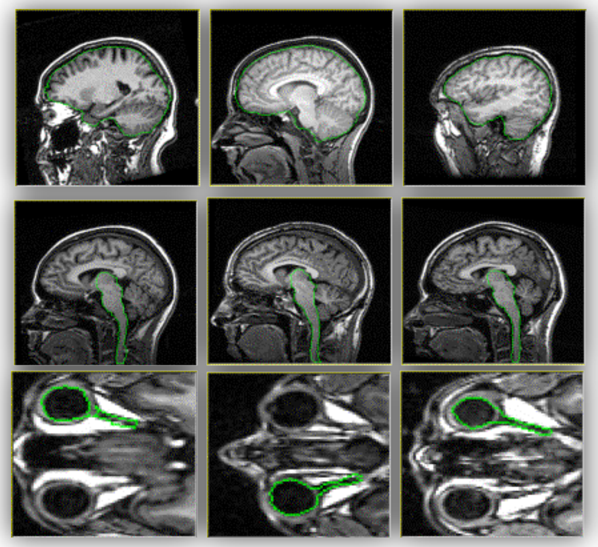

Good evaluation metric?

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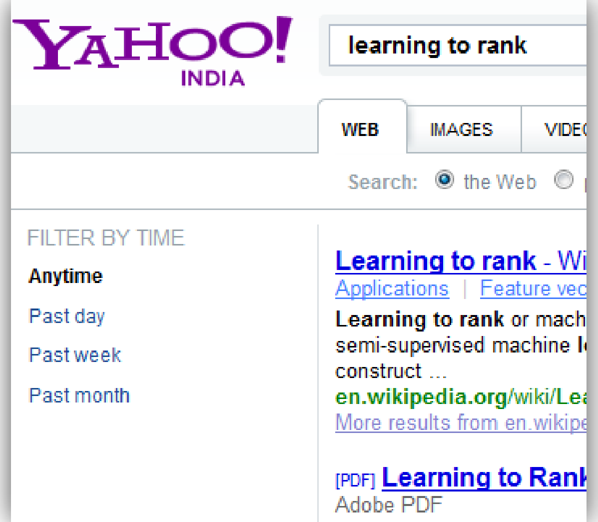

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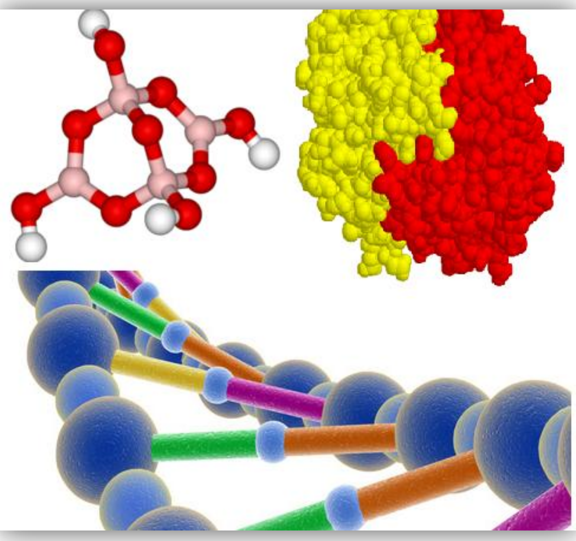

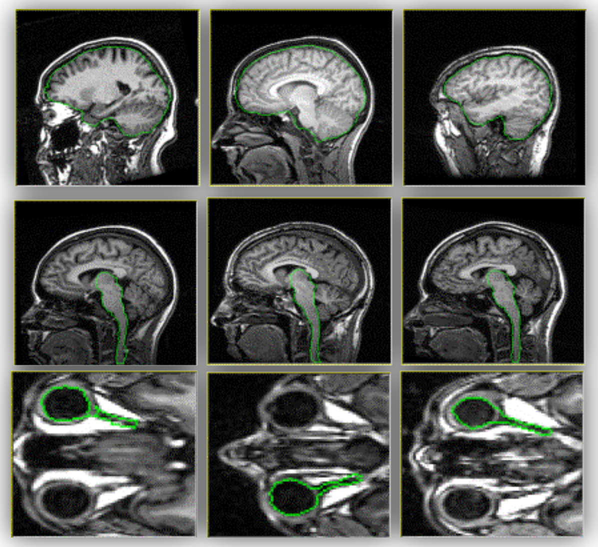

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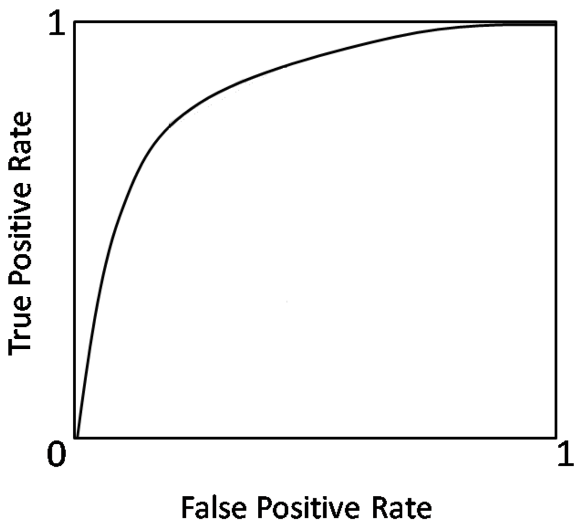

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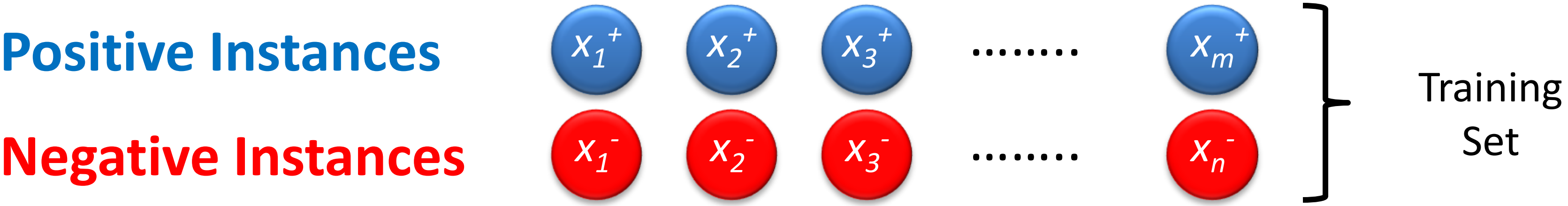
Learning with Binary Supervision



Positive Instances x_1^+ x_2^+ x_3^+ …….. x_m^+

Negative Instances x_1^- x_2^- x_3^- …….. x_n^-

Training Set

Learning with Binary Supervision

Positive Instances x_1^+ x_2^+ x_3^+ …….. x_m^+

Negative Instances x_1^- x_2^- x_3^- …….. x_n^-

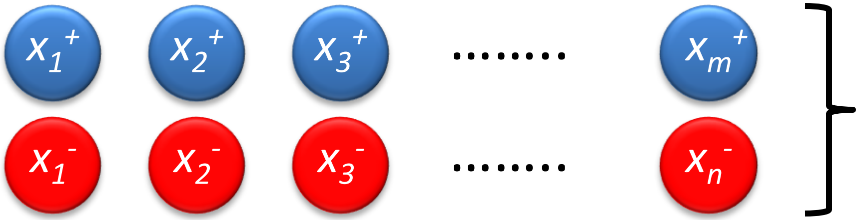
Training Set

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

Learning with Binary Supervision

Positive Instances

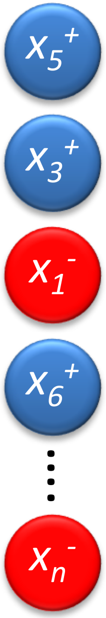
Negative Instances



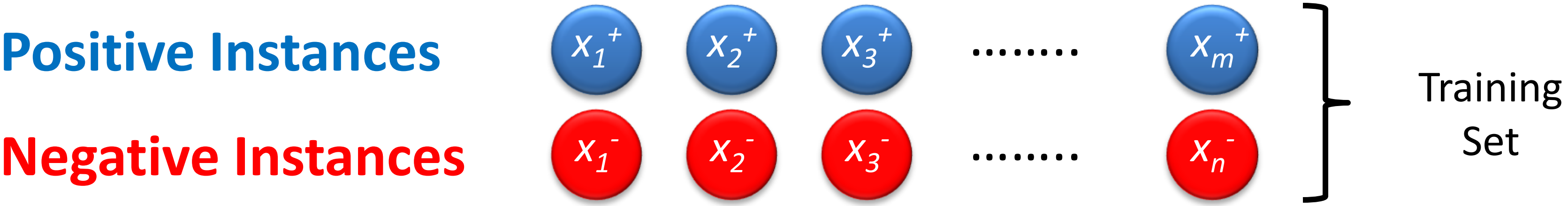
Training
Set

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

Rank objects



Learning with Binary Supervision



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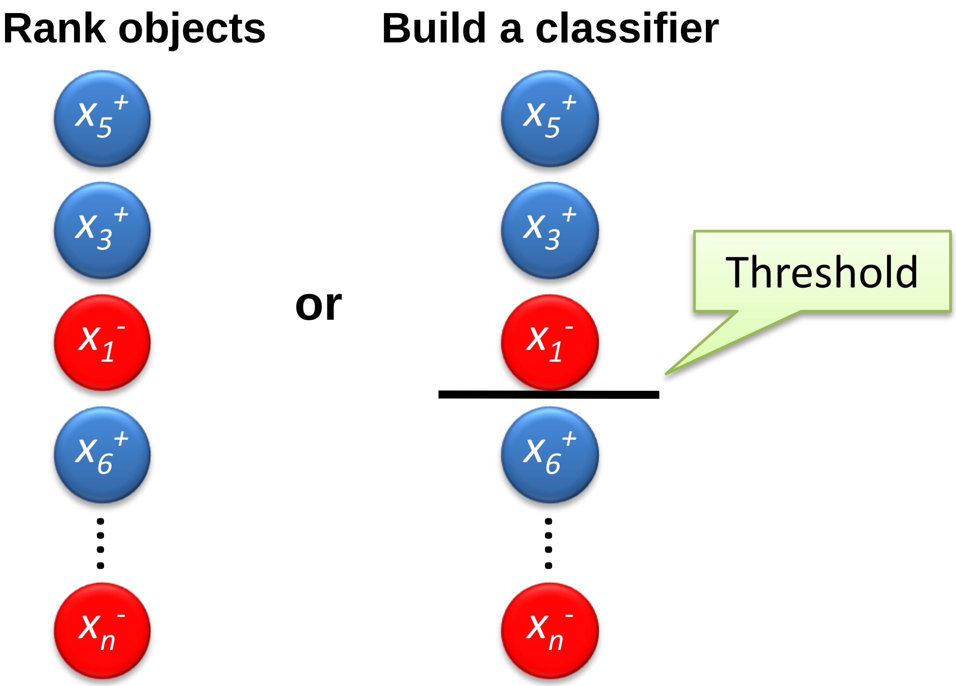


Rank objects

x_5^+

x_3^+

x_1^-

x_6^+

⋮

x_n^-

or

Build a classifier

x_5^+

x_3^+

x_1^-

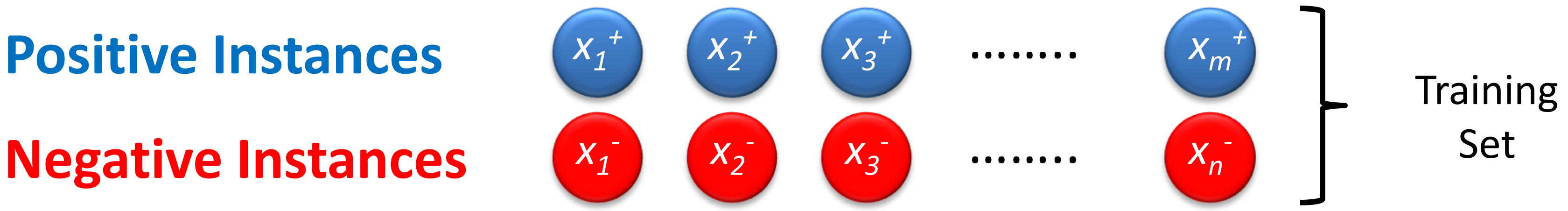
Threshold

x_6^+

⋮

x_n^-

Learning with Binary Supervision



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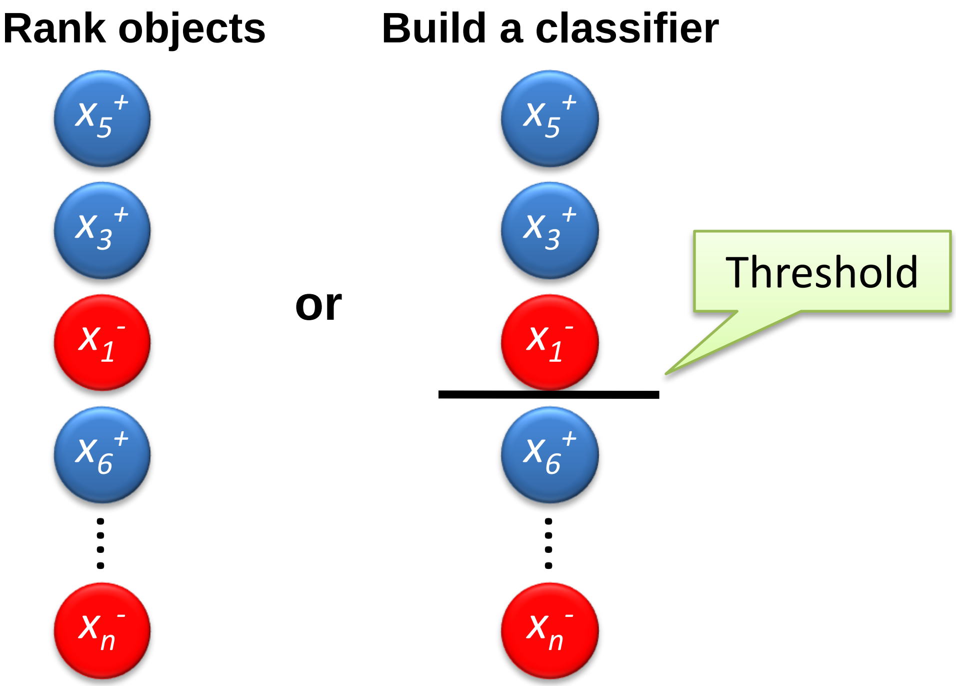
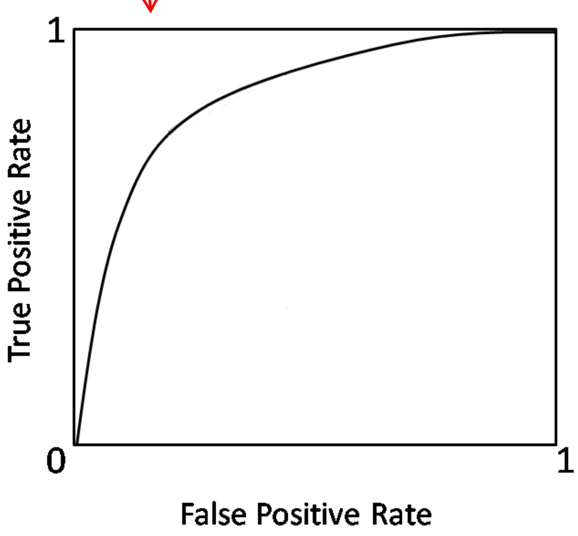


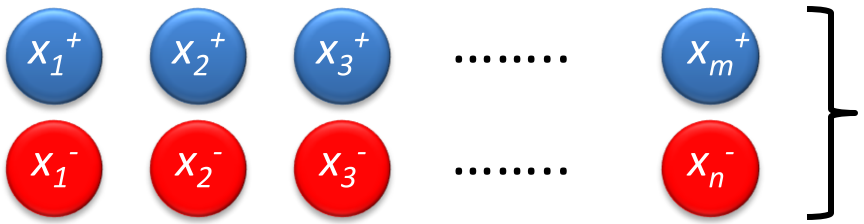
Quality of score function?



Learning with Binary Supervision

Positive Instances

Negative Instances



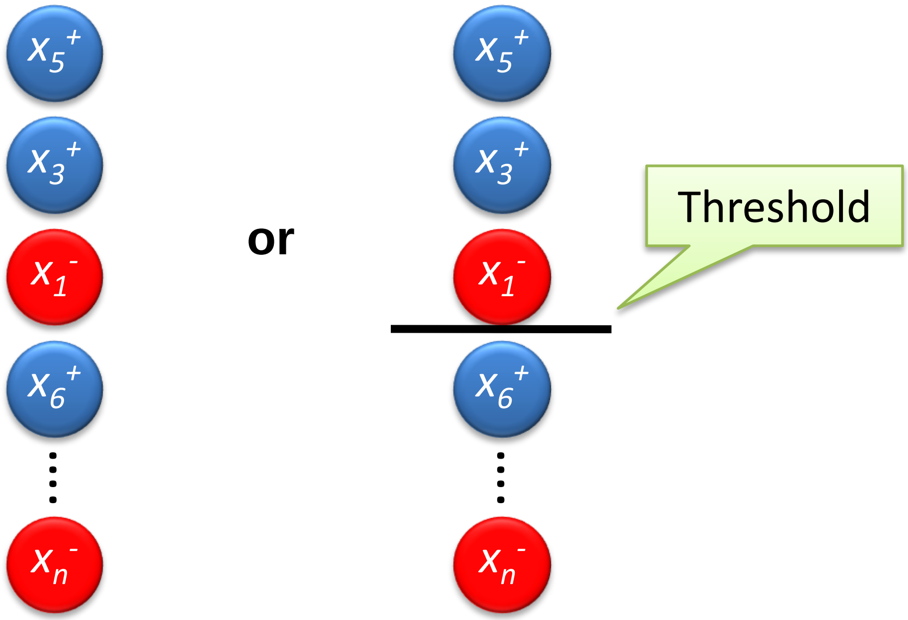
Training Set

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

Rank objects

or

Build a classifier



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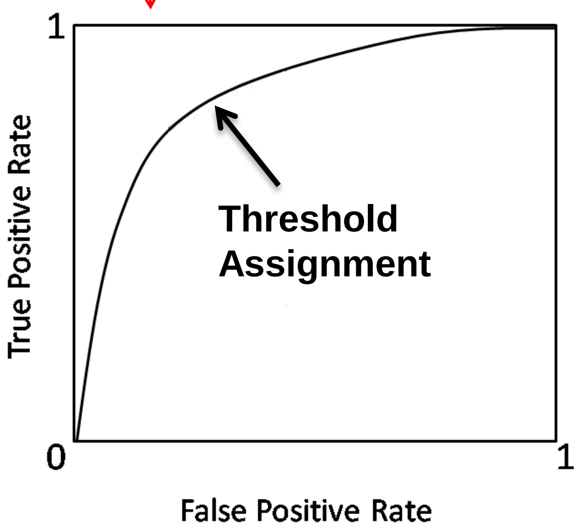
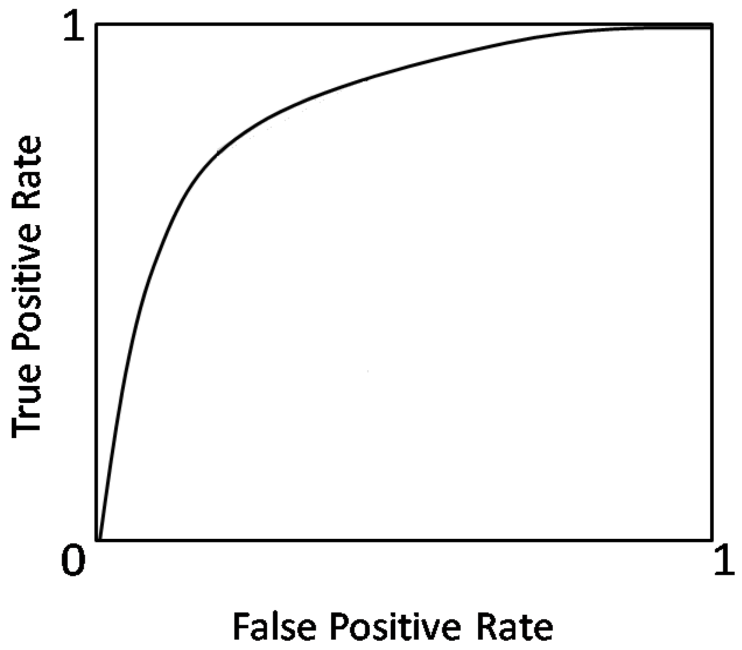


Receiver Operating Characteristic Curve

Captures how well a prediction model discriminates between positive and negative examples



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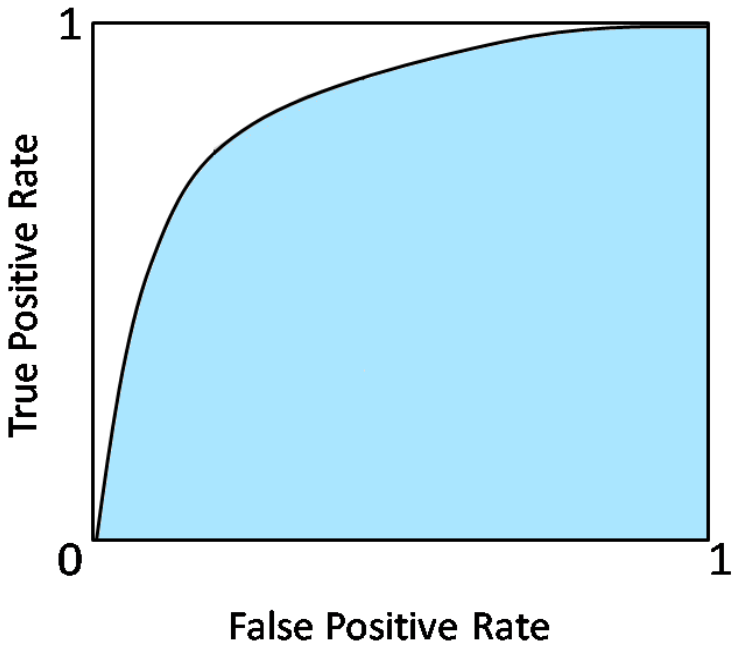
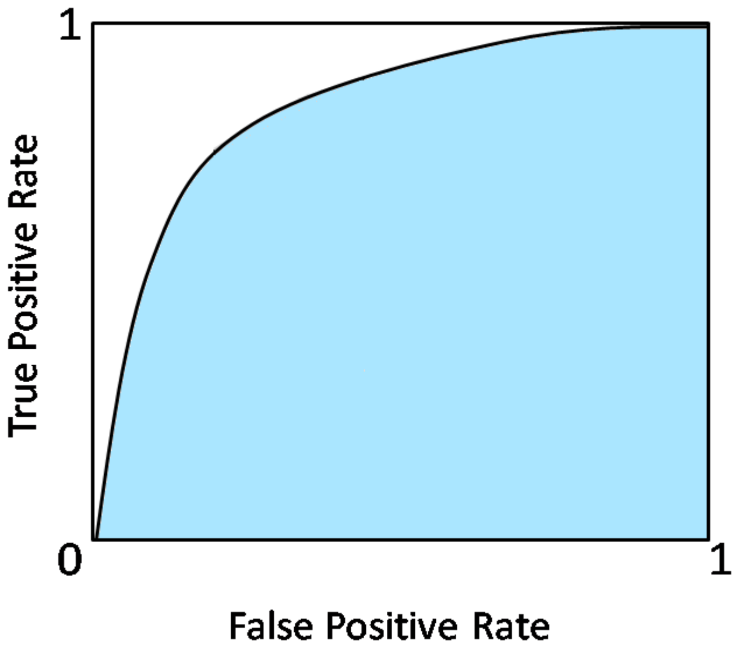


Full AUC

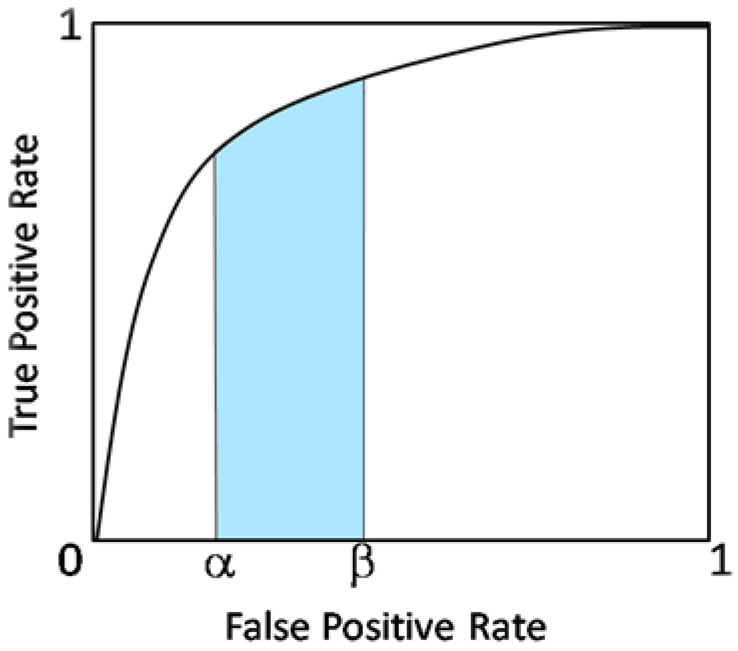
Receiver Operating Characteristic Curve

Captures how well a prediction model discriminates between positive and negative examples



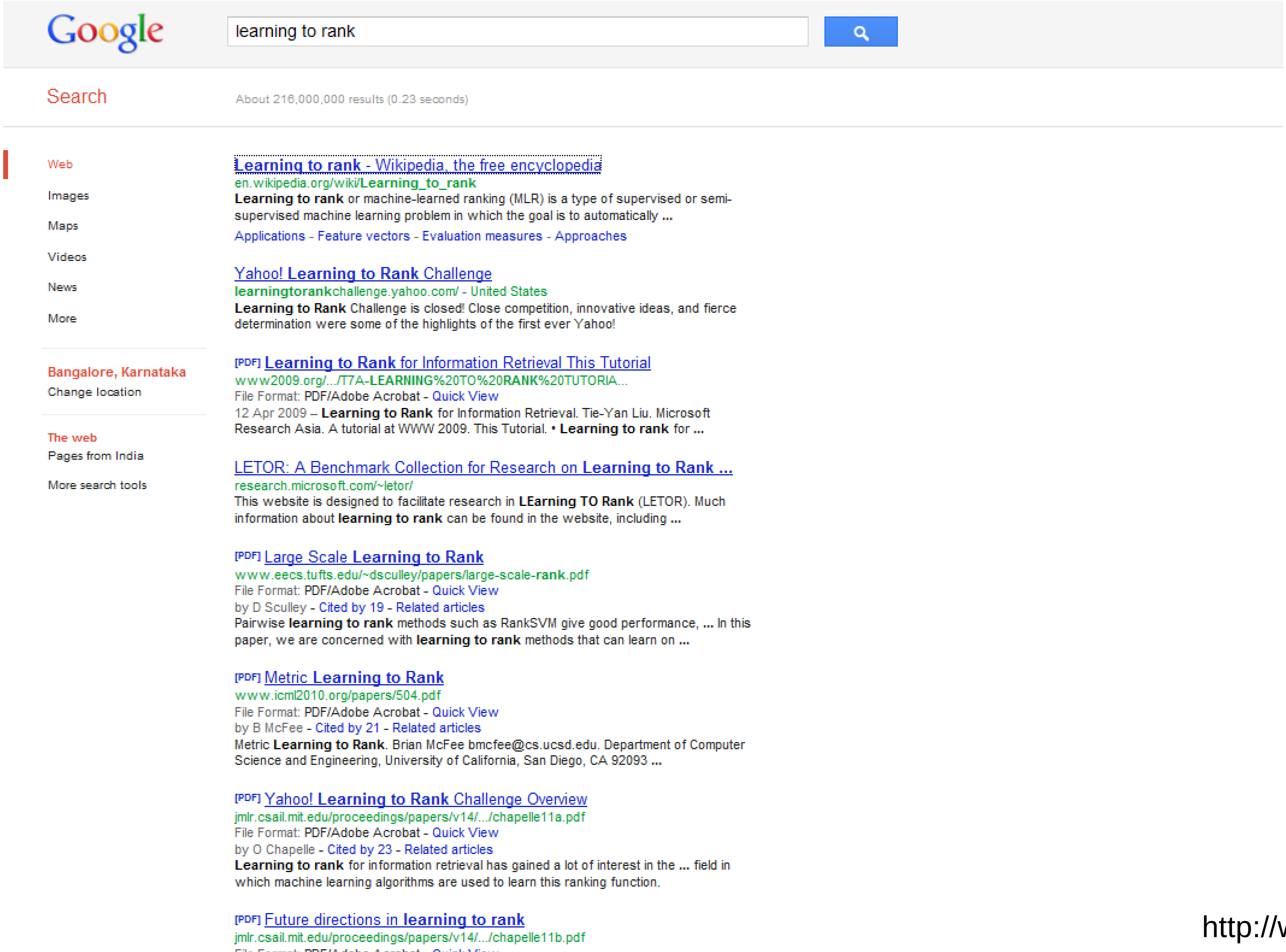
Full AUC

Vs



Partial AUC

Ranking



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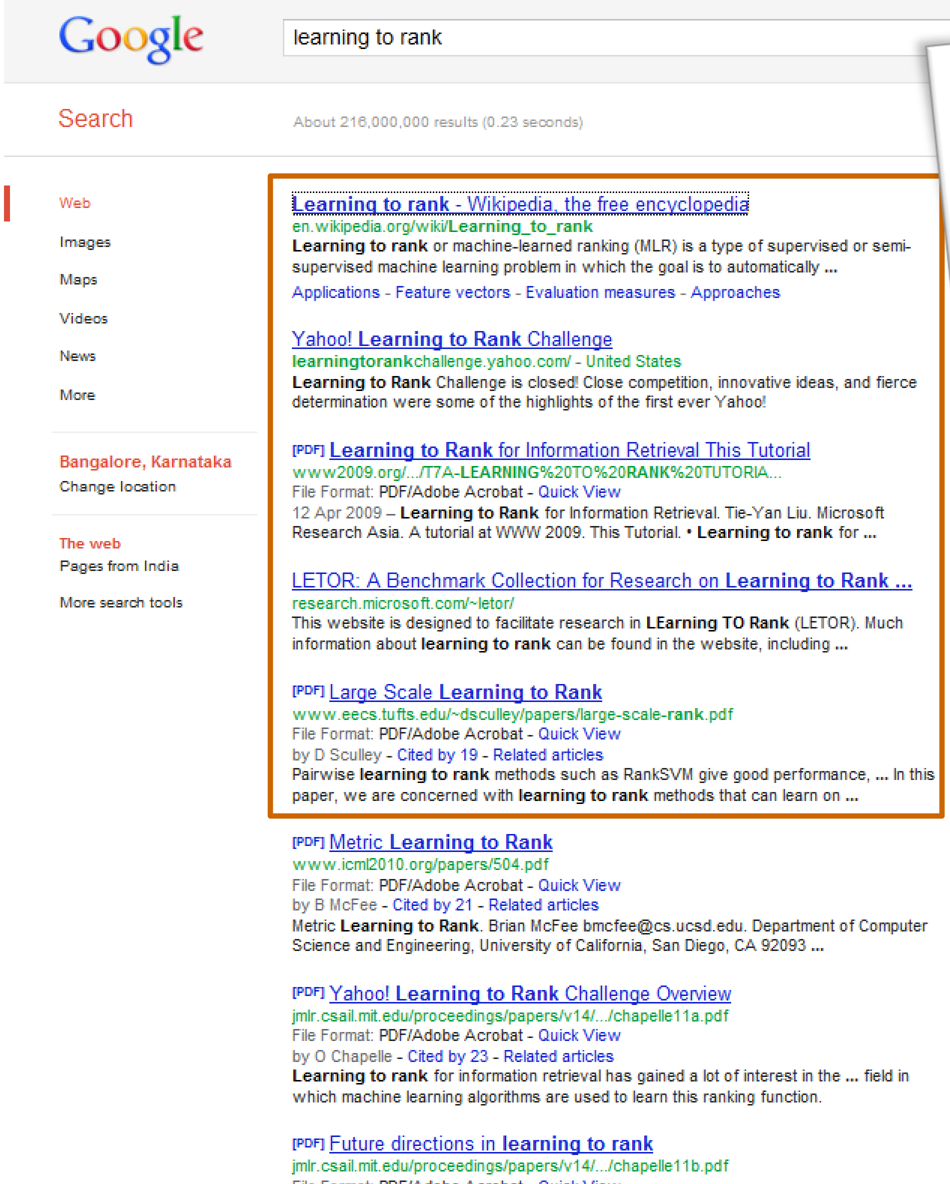
Ranking



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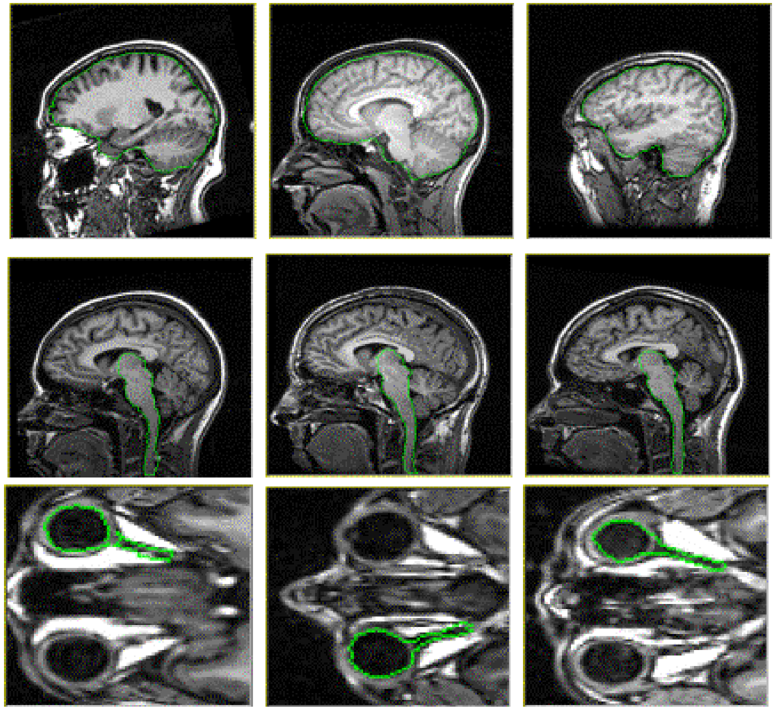

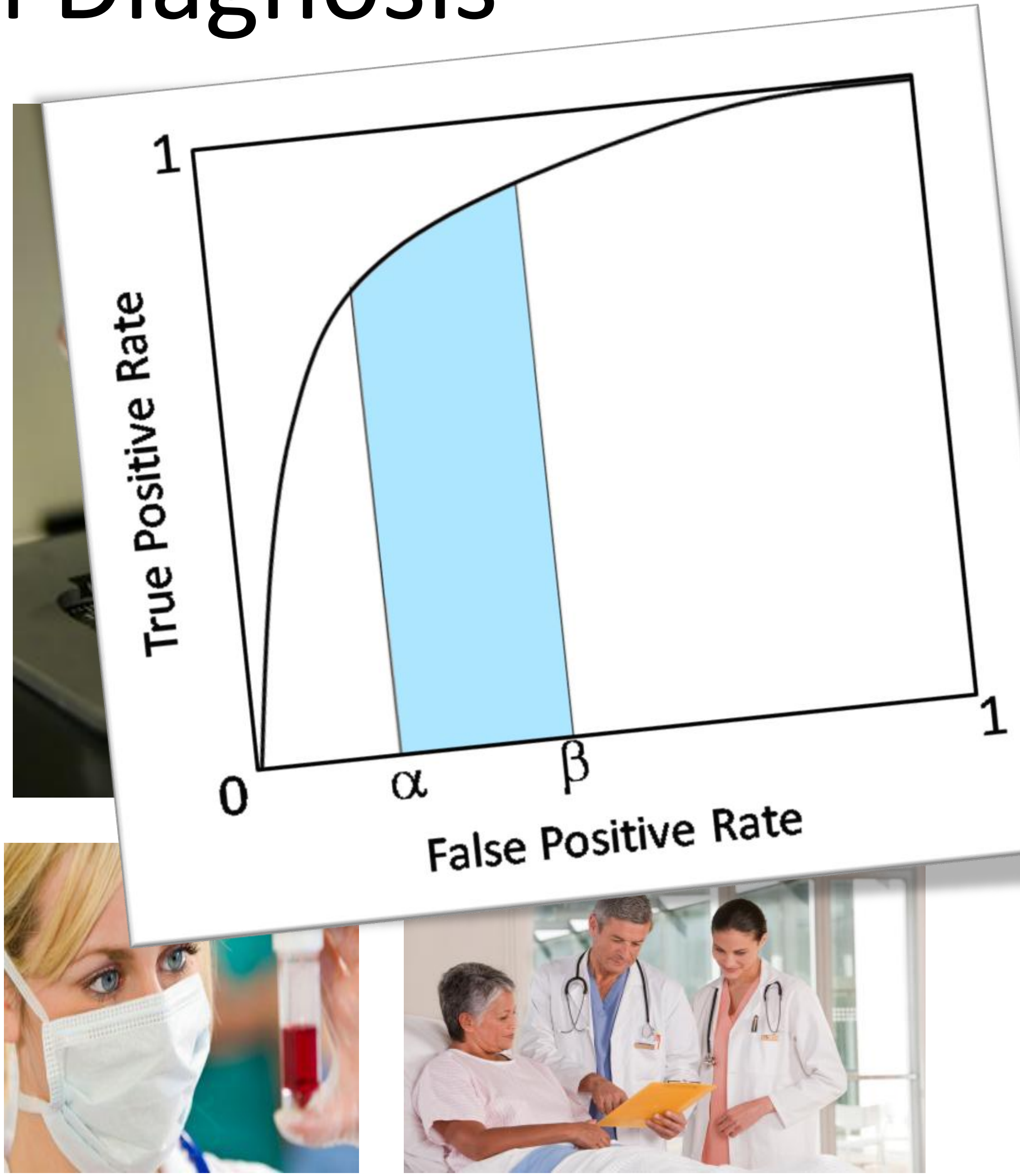

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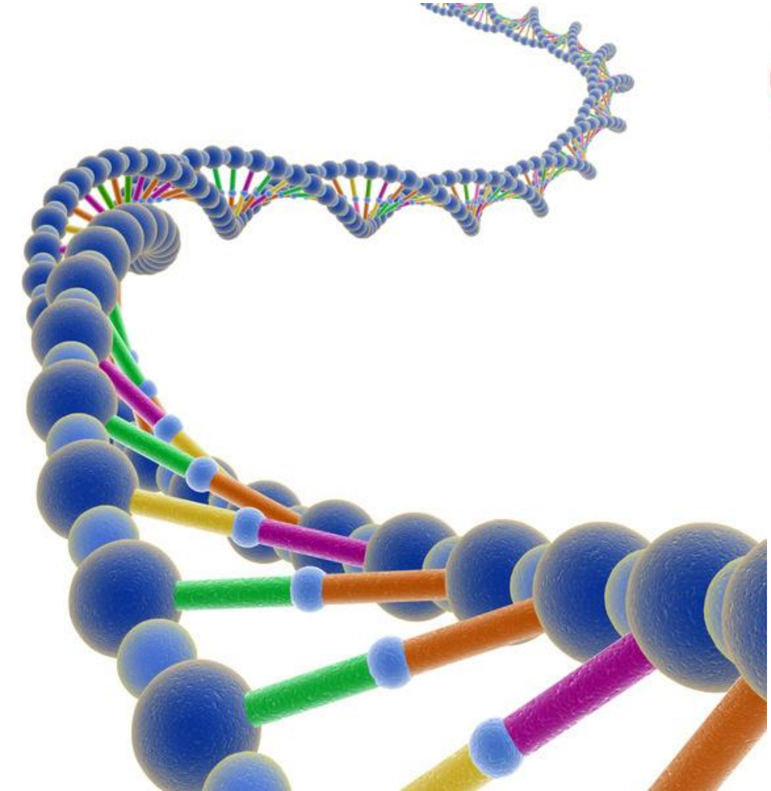
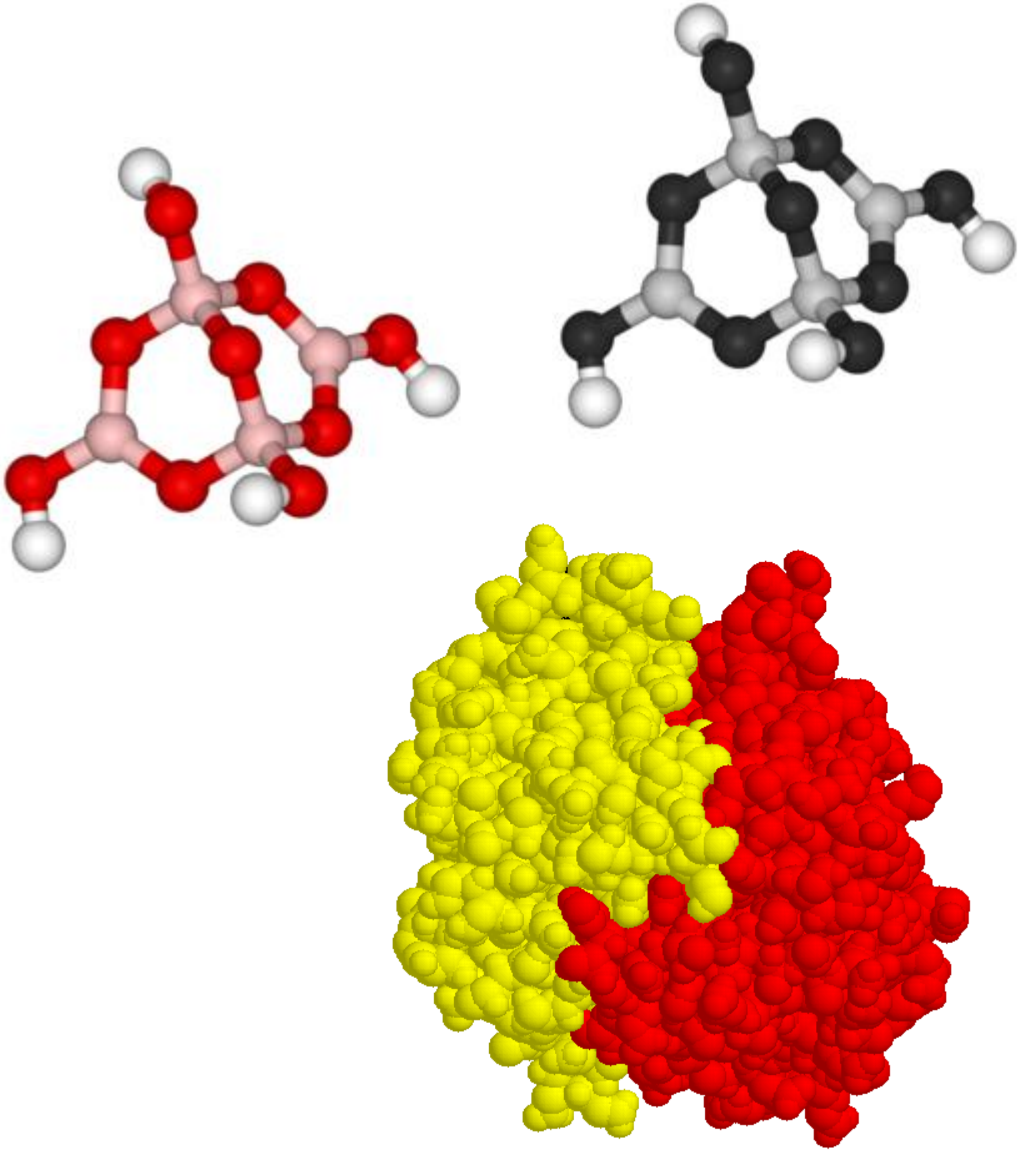
- Drug Discovery
- Gene Prioritization
- Protein Interaction Prediction
- ……





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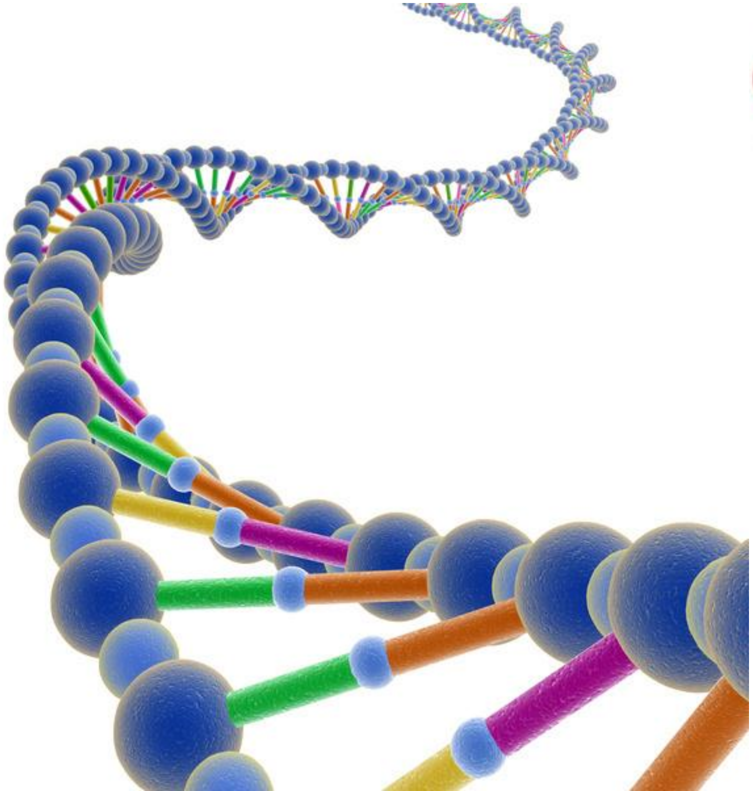

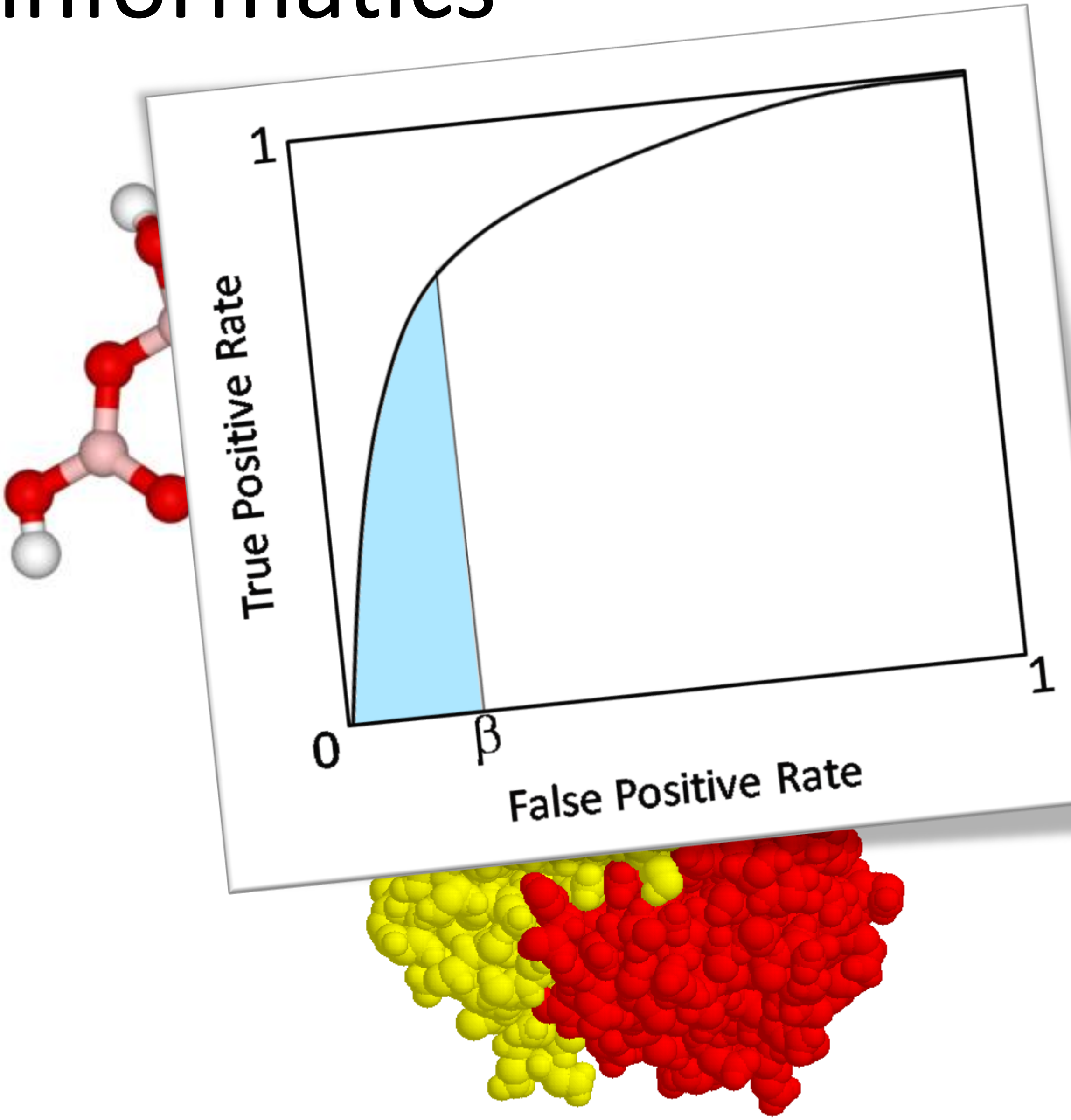

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Partial Area Under the ROC Curve is critical to many applications

Partial AUC Optimization

- Many existing approaches are either heuristic or solve special cases of the problem.

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- Improvements over baselines on several real-world applications

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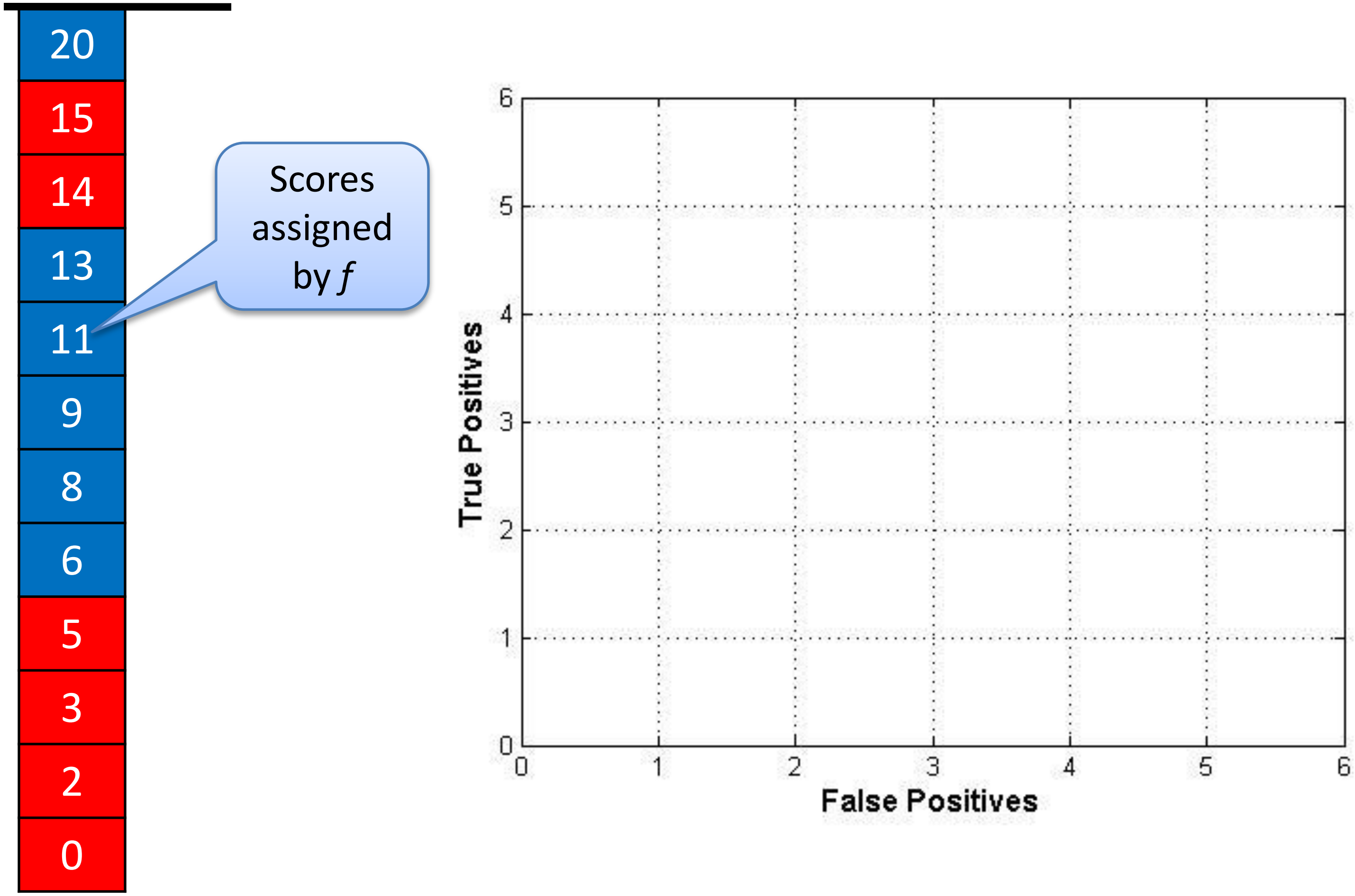
ROC Curve

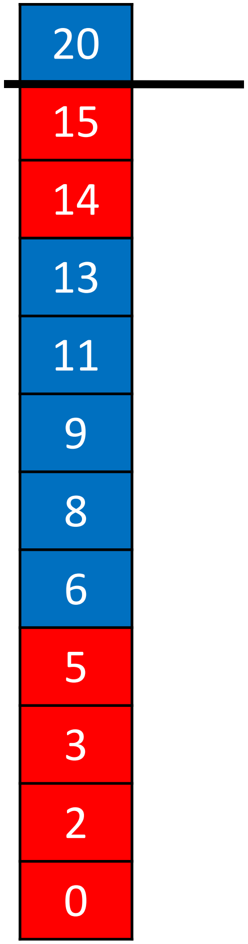
Receiver Operating Characteristic Curve

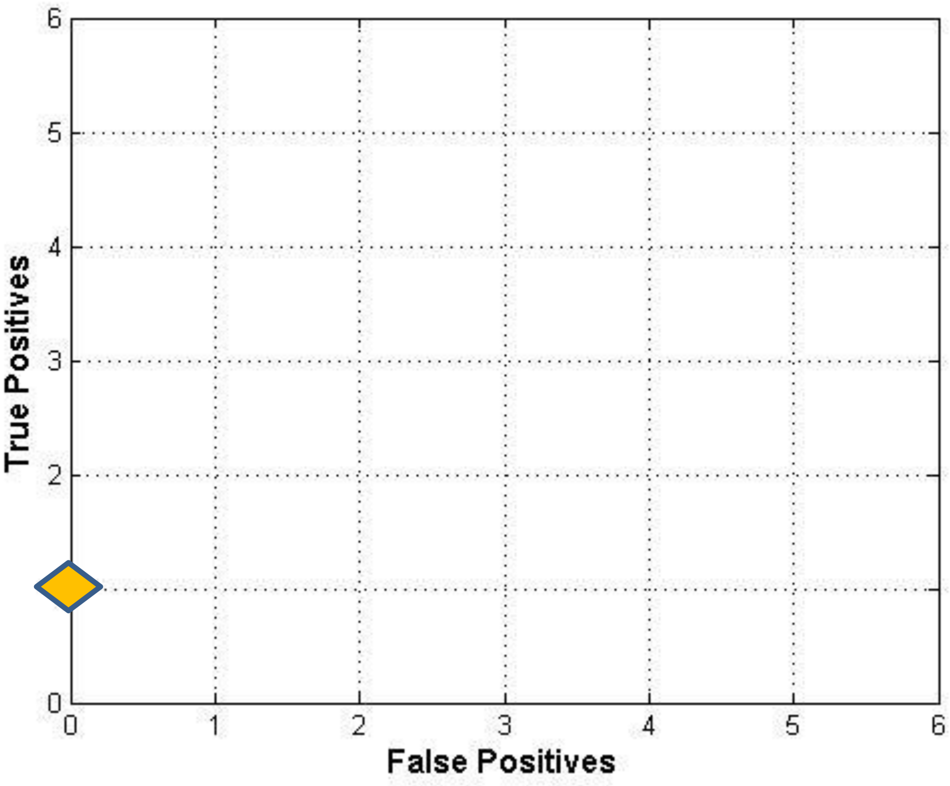


Scores assigned by *f*

ROC Curve

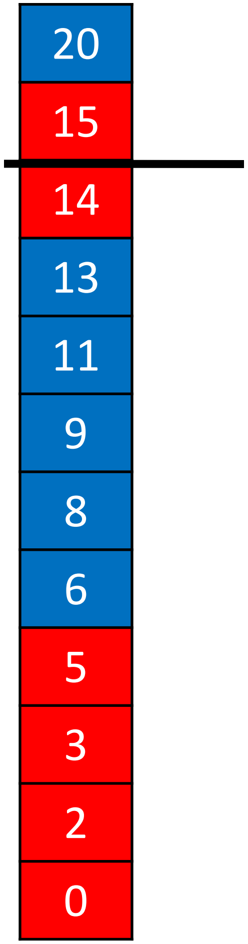
Receiver Operating Characteristic Curve

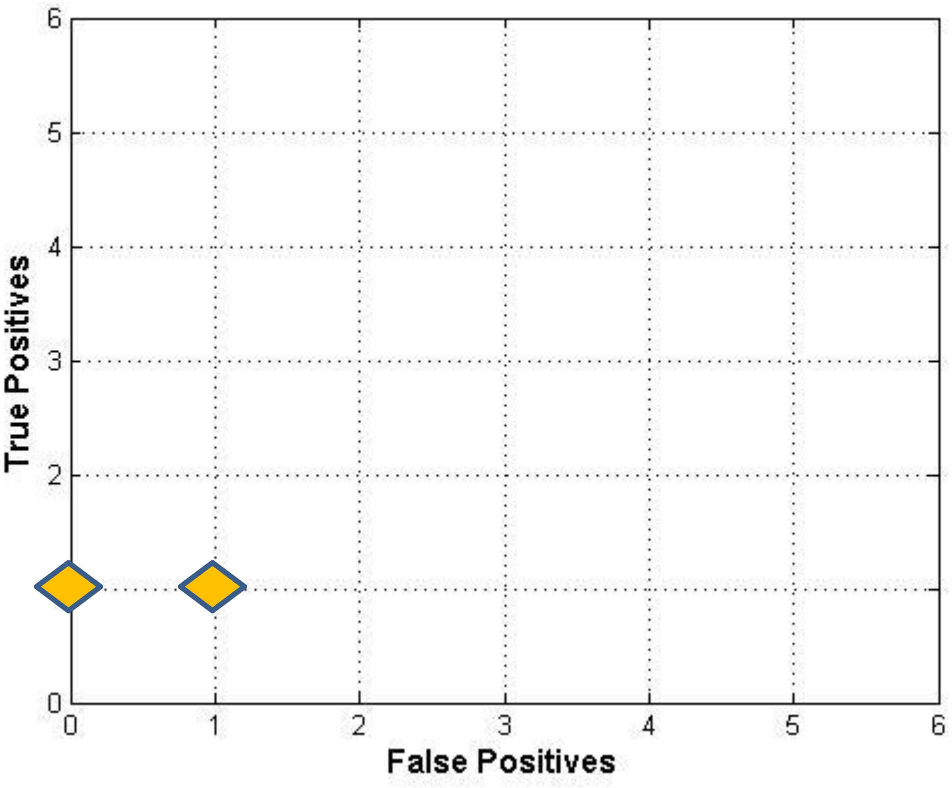




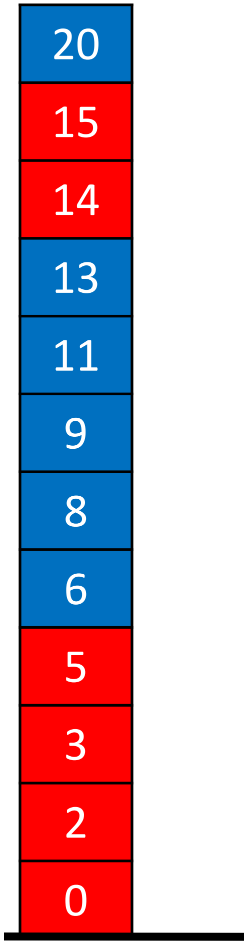
ROC Curve

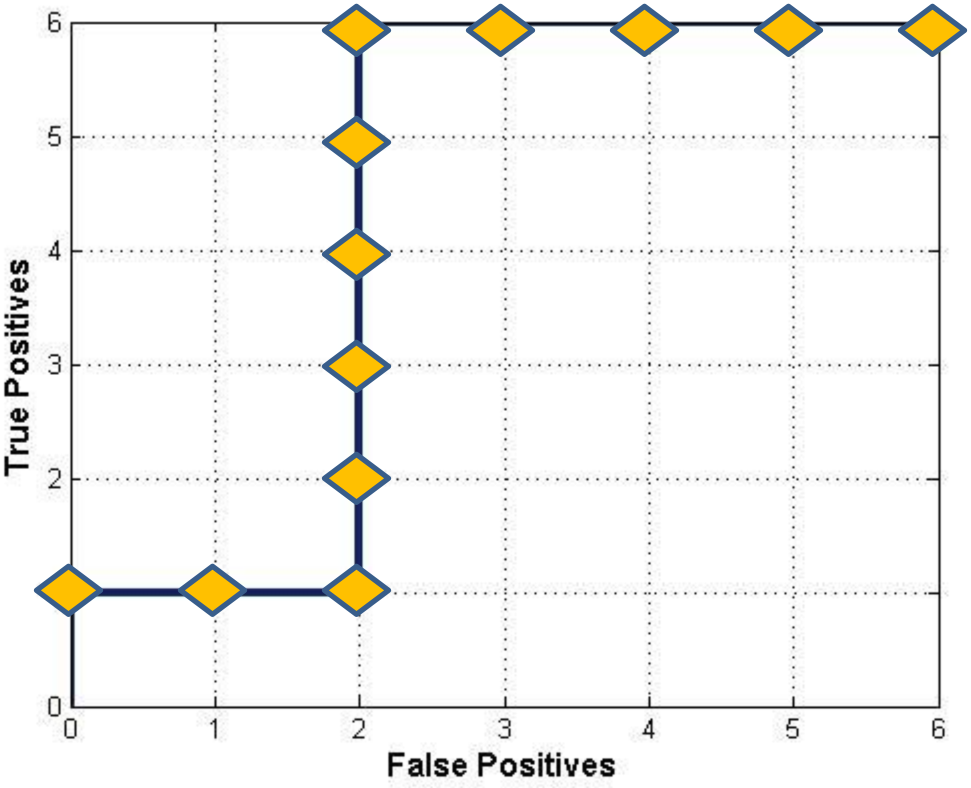
Receiver Operating Characteristic Curve





ROC Curve
Receiver Operating Characteristic Curve





Partial AUC Optimization

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

Partial AUC Optimization

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

Discrete and
Non-differentiable

Partial AUC Optimization

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

Discrete and
Non-differentiable

$\Downarrow$

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

Partial AUC Optimization

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

Discrete and
Non-differentiable

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

Partial AUC Optimization

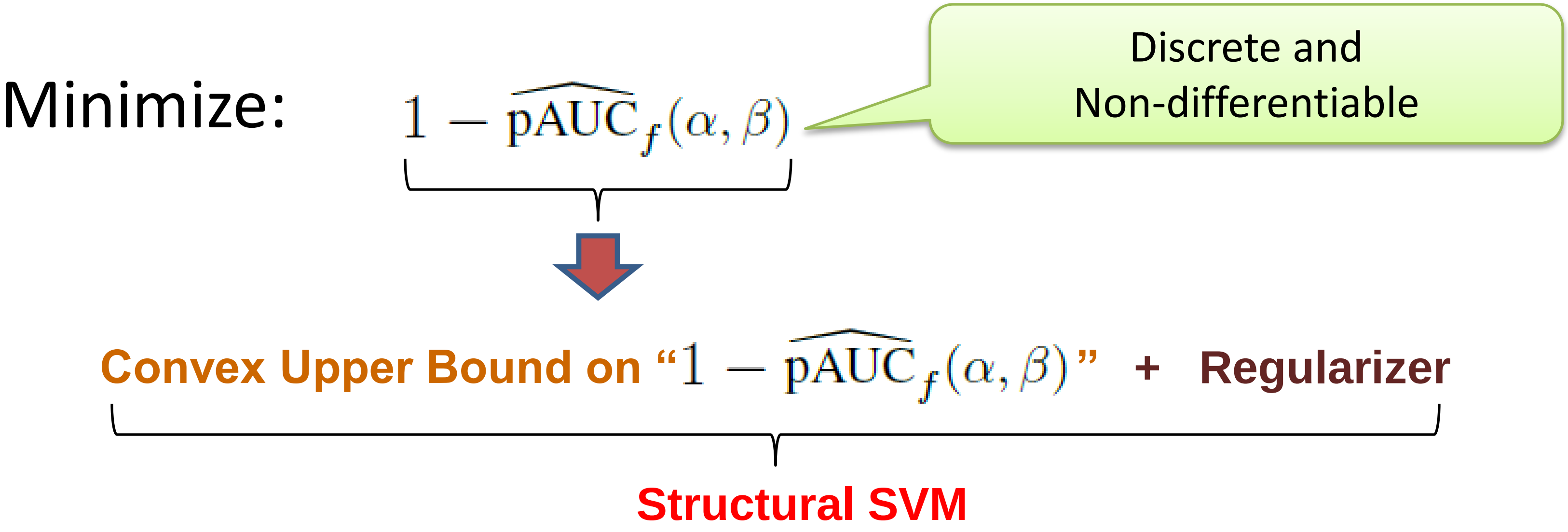
Minimize: $\underbrace{1 - \widehat{\text{pAUC}}_f(\alpha, \beta)}$

Discrete and
Non-differentiable

$$\Downarrow$$

$$\underbrace{\textbf{Convex Upper Bound on } \text{“}1 - \widehat{\text{pAUC}}_f(\alpha, \beta)\text{”} \; + \; \textbf{Regularizer}}_{\textbf{Structural SVM}}$$

Partial AUC Optimization



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

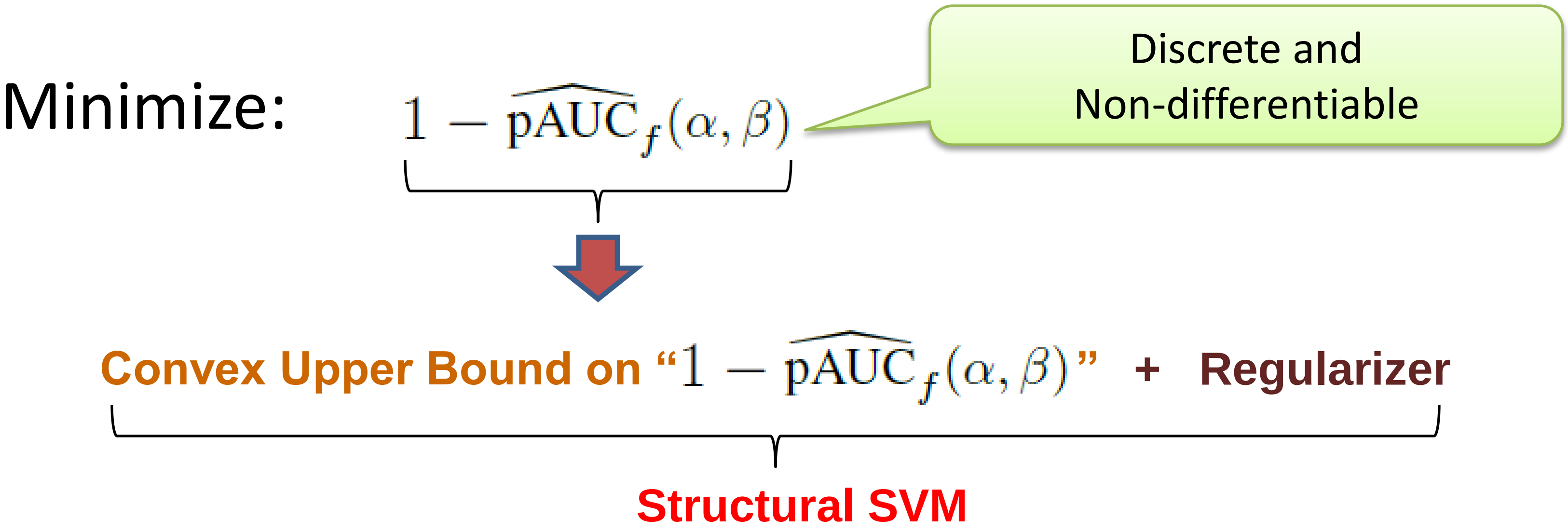
Discrete and
Non-differentiable

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

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

T. Joachims, *“A Support Vector Method for Multivariate Performance Measures”,* ICML 2005.

Partial AUC Optimization



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

Discrete and
Non-differentiable

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

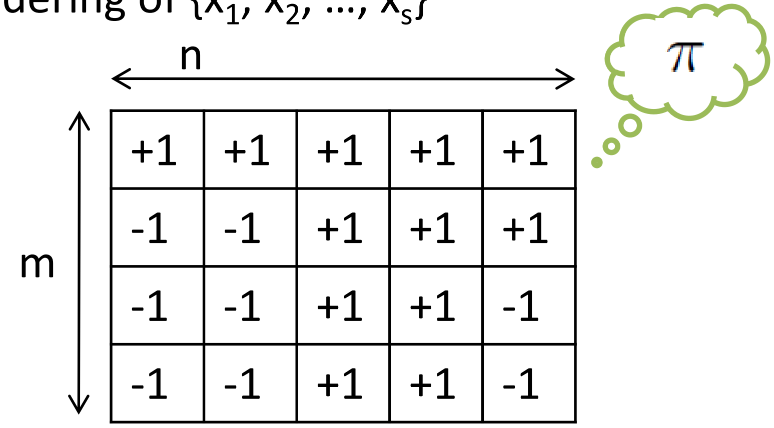
- Extends Joachims' approach for full AUC optimization, but leads to a trickier combinatorial optimization step.
- Efficient solver with the same time complexity as that for full AUC.

T. Joachims, *"A Support Vector Method for Multivariate Performance Measures"*, ICML 2005.

Structural SVM Based Approach

Structural SVM Based Approach

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



+1	+1	+1	+1	+1
-1	-1	+1	+1	+1
-1	-1	+1	+1	-1
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Structural SVM Based Approach

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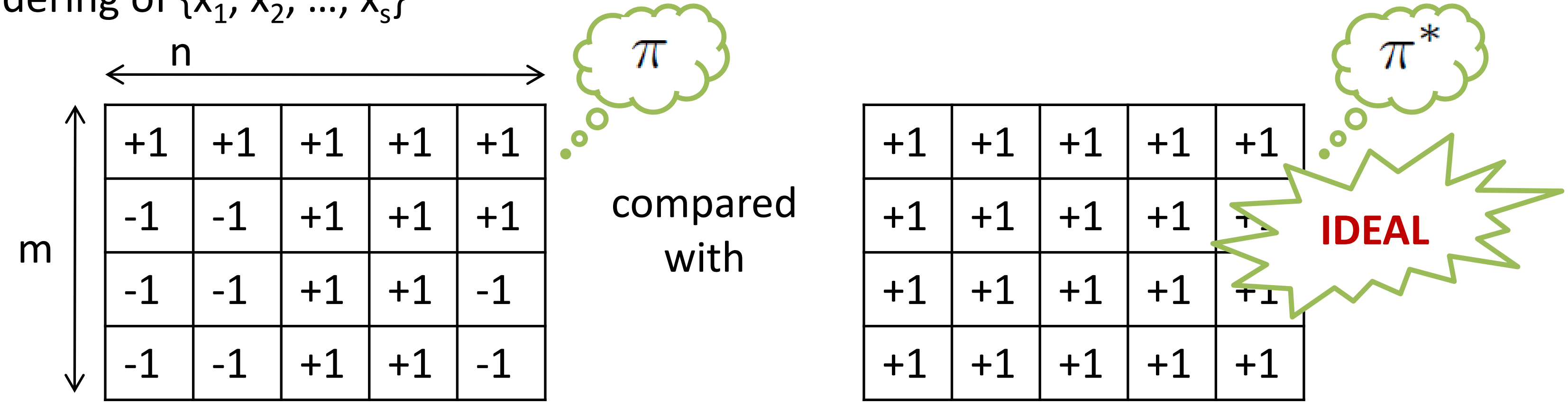
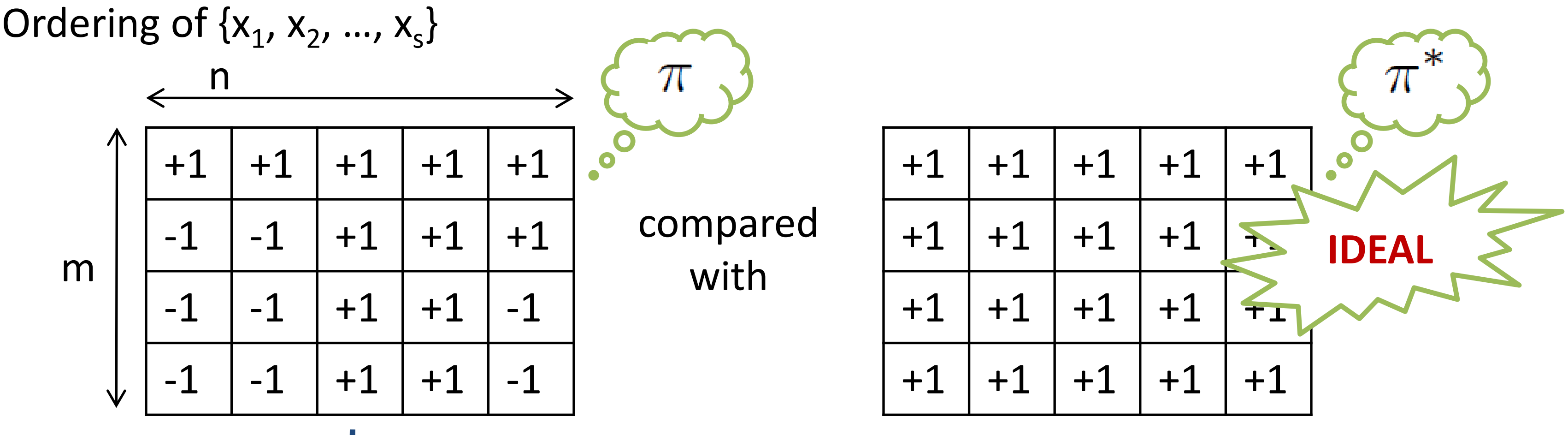


+1	+1	+1	+1	+1
-1	-1	+1	+1	+1
-1	-1	+1	+1	-1
-1	-1	+1	+1	-1

compared with

+1	+1	+1	+1	+1
+1	+1	+1	+1	+1
+1	+1	+1	+1	+1
+1	+1	+1	+1	+1

Structural SVM Based Approach



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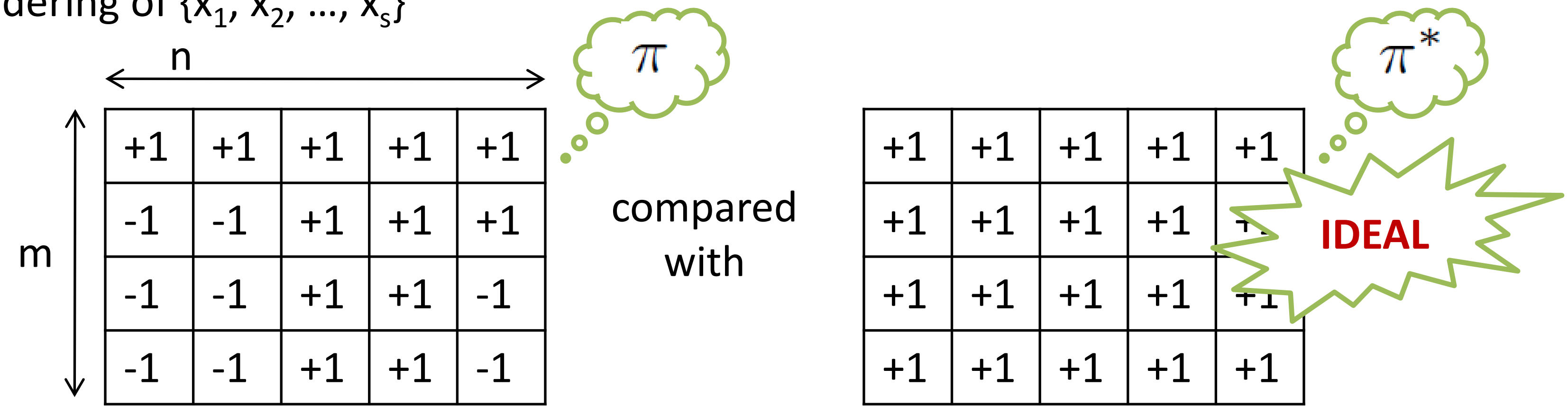
+1	+1	+1	+1	+1
+1	+1	+1	+1	+
+1	+1	+1	+1	+1
+1	+1	+1	+1	+1

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

s.t.

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

Structural SVM Based Approach



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compared with

+1	+1	+1	+1	+1
+1	+1	+1	+1	+
+1	+1	+1	+1	+1
+1	+1	+1	+1	+1

Upper Bound on (1 – pAUC)

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

s.t.

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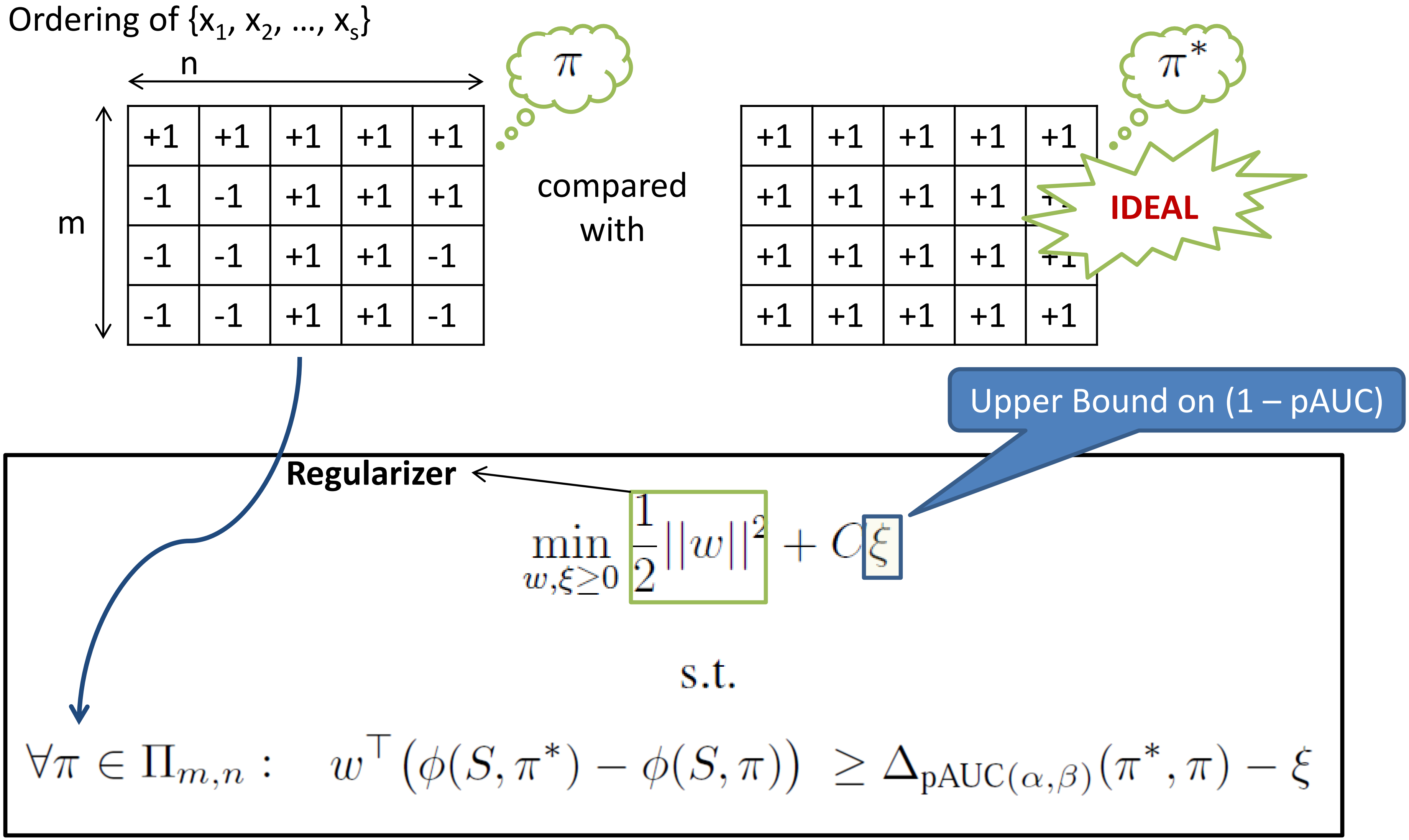

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+1	+1	+1	+1	+1
+1	+1	+1	+1	+1

Upper Bound on (1 – pAUC)

Regularizer

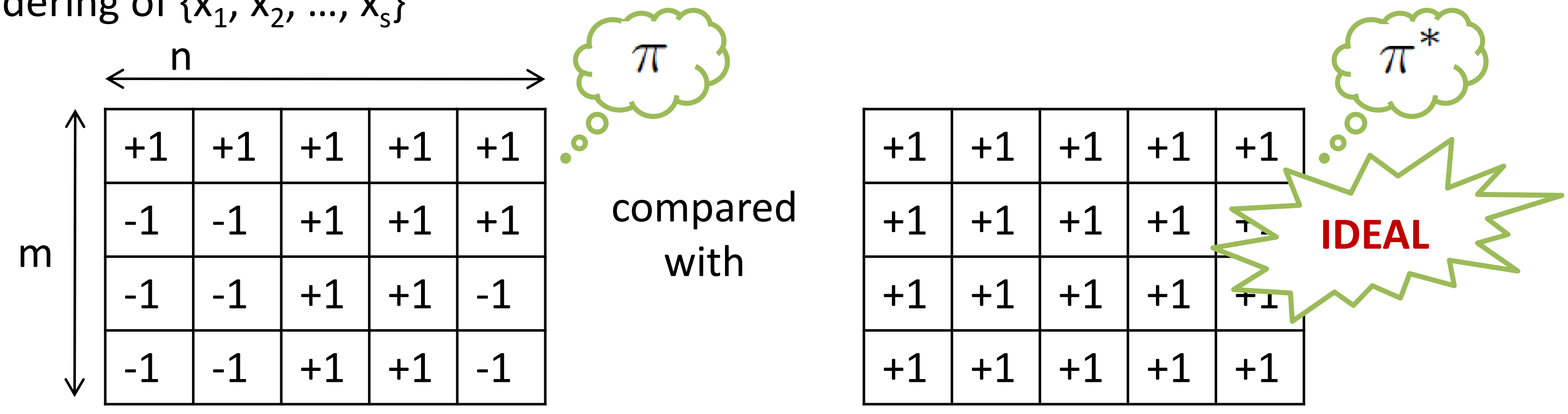
$$\min_{w,\xi\geq 0} \boxed{\frac{1}{2}||w||^2} + C\boxed{\xi}$$

s.t.

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

Structural SVM Based Approach

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



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+1	+1	+1	+1	+1
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+1	+1	+1	+1	+1

Upper Bound on (1 – pAUC)

Regularizer

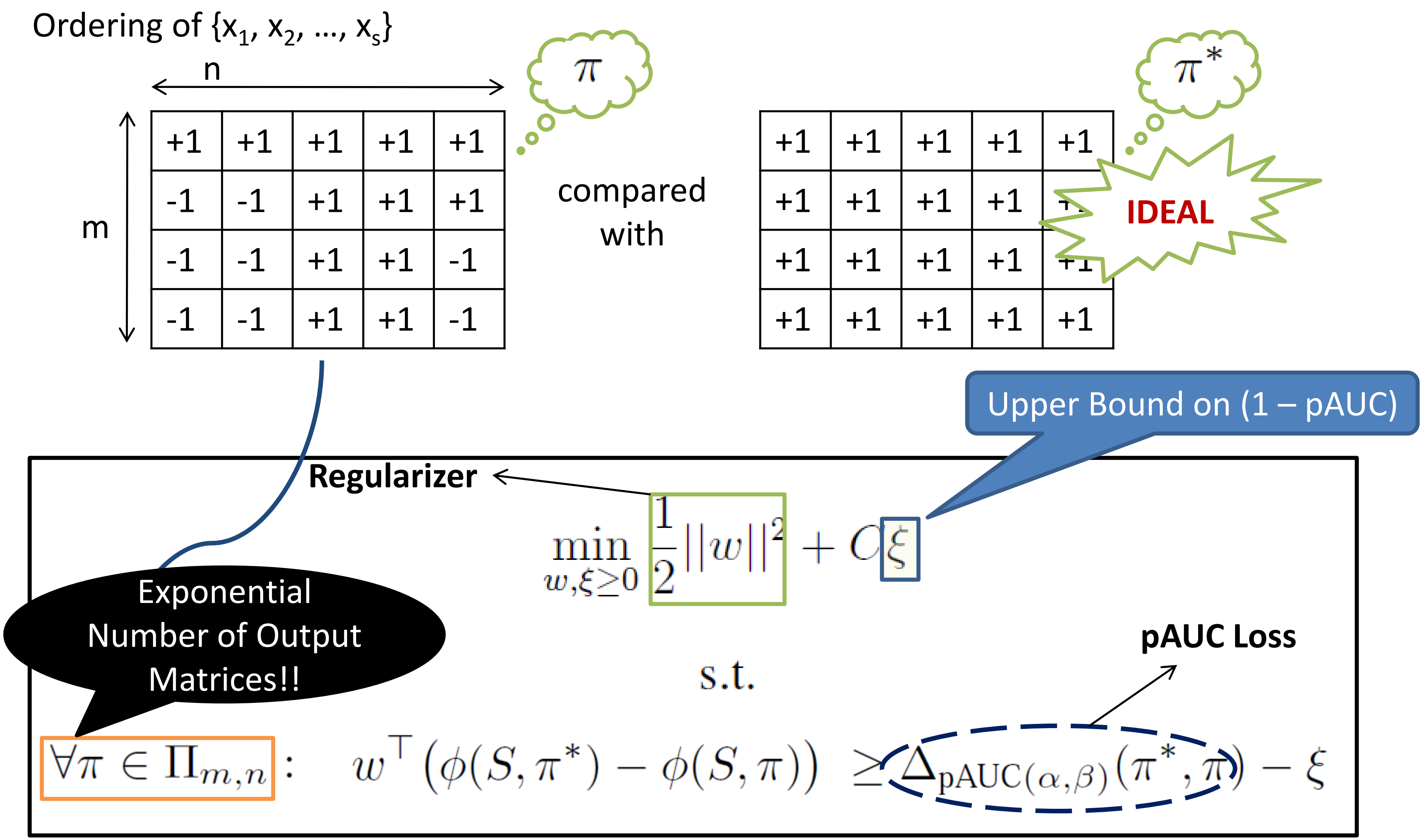
$$\min_{w,\xi \geq 0} \boxed{\frac{1}{2}||w||^2} + C\boxed{\xi}$$

pAUC Loss

s.t.

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

Structural SVM Based Approach



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pAUC Loss

s.t.

Exponential Number of Output Matrices!!

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

Optimization Solver

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

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

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

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Repeat:

1. Solve OP for a subset of constraints.

Optimization Solver

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

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

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

Repeat:

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

Optimization Solver

Converges in constant number of iterations

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

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

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

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Break down!

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

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Break down!

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

Full AUC

+1	+1	+1	+1	+1
-1	-1	+1	+1	+1
-1	-1	+1	+1	-1
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Optimization Solver

Converges in constant number of iterations

Repeat:

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

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Break down!

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

Full AUC

+1	+1	+1	+1	+1
-1	-1	+1	+1	+1
-1	-1	+1	+1	-1
-1	-1	+1	+1	-1

Partial AUC

+1	+1	+1	+1	+1
-1	-1	+1	+1	+1
-1	-1	+1	+1	-1
-1	-1	+1	+1	-1

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Optimization Solver

Converges in constant number of iterations

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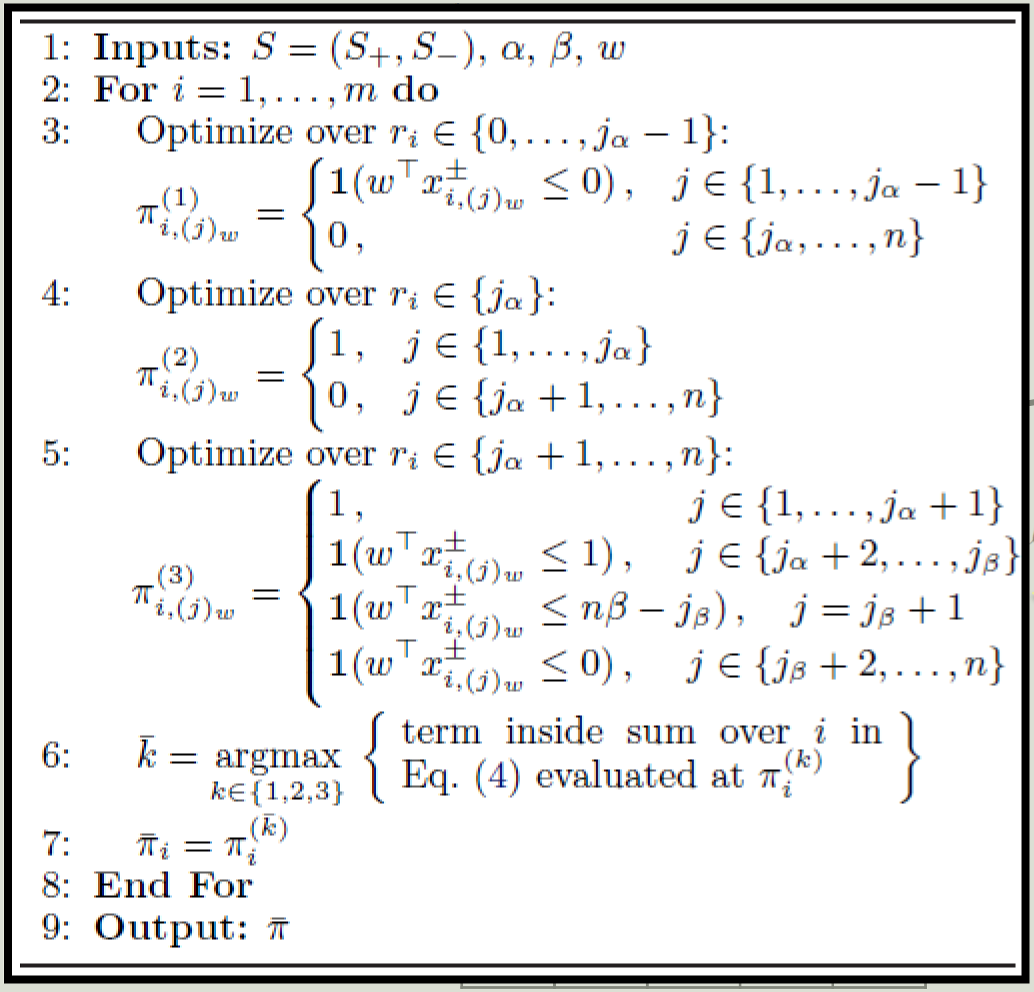

```
Inputs: $S = (S_+, S_-)$, $\alpha$, $\beta$, $w$
For $i = 1, \dots, m$ do
    Optimize over $r_i \in \{0, \dots, j_\alpha - 1\}$:
    $\pi^{(1)}_{i,(j)_w} = \begin{cases} \mathbf{1}(w^\top x^{\pm}_{i,(j)_w} \le 0)\,, & j \in \{1, \dots, j_\alpha - 1\} \\ 0\,, & j \in \{j_\alpha, \dots, n\} \end{cases}$
    Optimize over $r_i \in \{j_\alpha\}$:
    $\pi^{(2)}_{i,(j)_w} = \begin{cases} 1\,, & j \in \{1, \dots, j_\alpha\} \\ 0\,, & j \in \{j_\alpha + 1, \dots, n\} \end{cases}$
    Optimize over $r_i \in \{j_\alpha + 1, \dots, n\}$:
    $\pi^{(3)}_{i,(j)_w} = \begin{cases} 1\,, & j \in \{1, \dots, j_\alpha + 1\} \\ \mathbf{1}(w^\top x^{\pm}_{i,(j)_w} \le 1)\,, & j \in \{j_\alpha + 2, \dots, j_\beta\} \\ \mathbf{1}(w^\top x^{\pm}_{i,(j)_w} \le n\beta - j_\beta)\,, & j = j_\beta + 1 \\ \mathbf{1}(w^\top x^{\pm}_{i,(j)_w} \le 0)\,, & j \in \{j_\beta + 2, \dots, n\} \end{cases}$
    $\bar{k} = \operatorname*{argmax}_{k \in \{1,2,3\}} \left\{ \begin{array}{l} \text{term inside sum over } i \text{ in} \\ \text{Eq. (4) evaluated at } \pi^{(k)}_i \end{array} \right\}$
    $\bar{\pi}_i = \pi^{(\bar{k})}_i$
End For
Output: $\bar{\pi}$
```

Break down!

$$^{\top}\left(\phi(S,\pi^*) - \phi(S,\pi)\right)$$

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

+1	+			
-1	-1	+1	+1	+1
-1	-1	+1	+1	-1
-1	-1	+1	+1	-1

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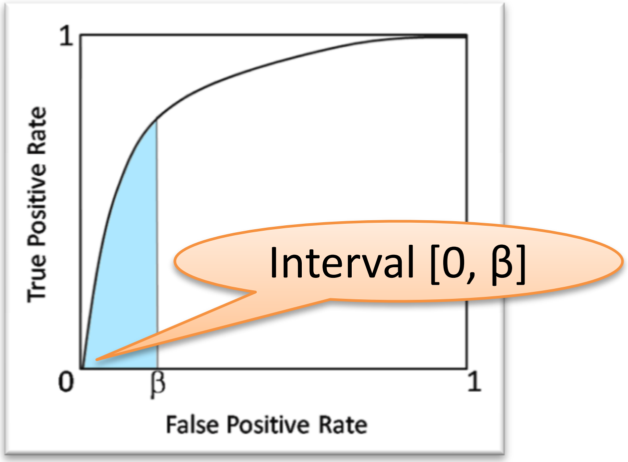
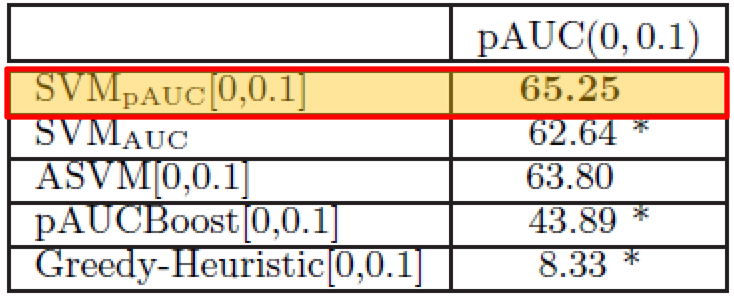
Experimental Results

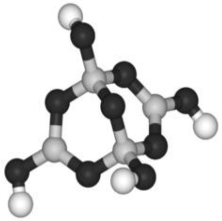
Experimental Results



Drug Discovery



	pAUC(0, 0.1)
SVM$_{\text{pAUC}}$[0,0.1]	**65.25**
SVM$_{\text{AUC}}$	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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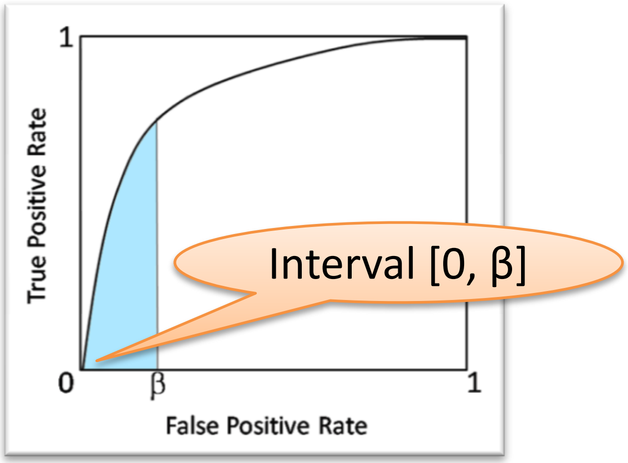

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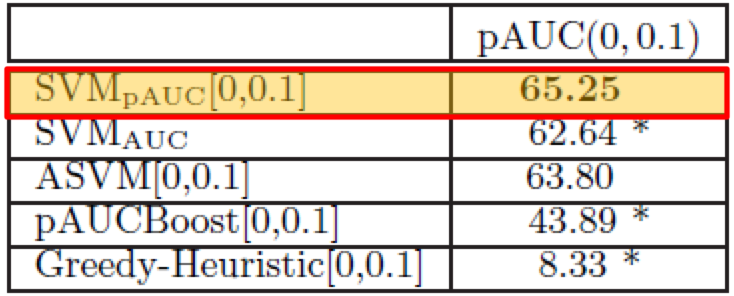

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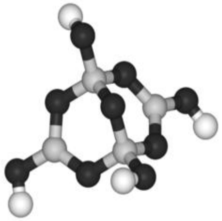
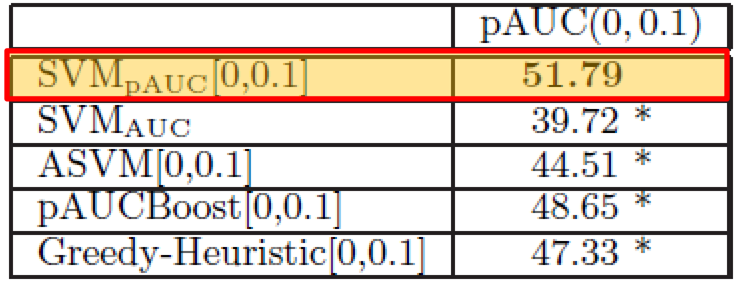


Protein Interaction Prediction



	pAUC(0, 0.1)
$\text{SVM}_{\text{pAUC}}[0,0.1]$	**51.79**
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ASVM[0,0.1]	44.51 *
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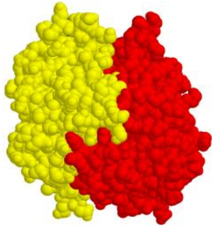

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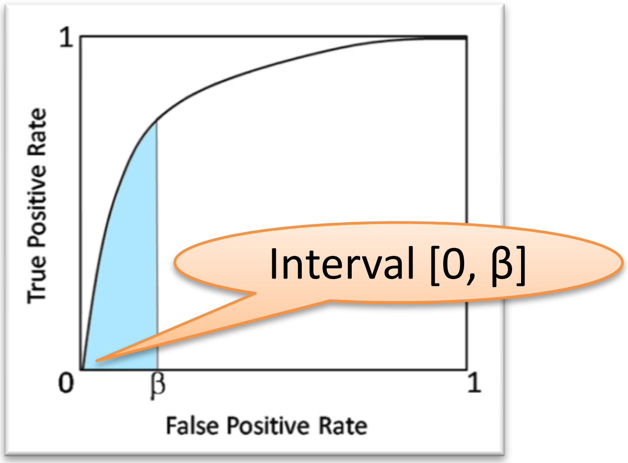

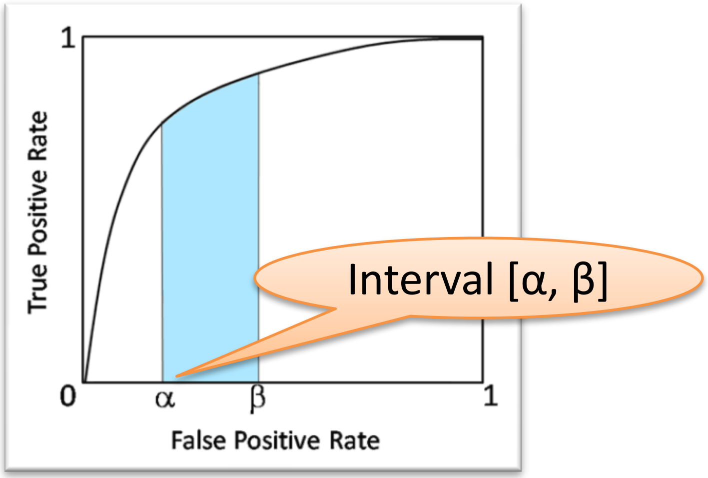

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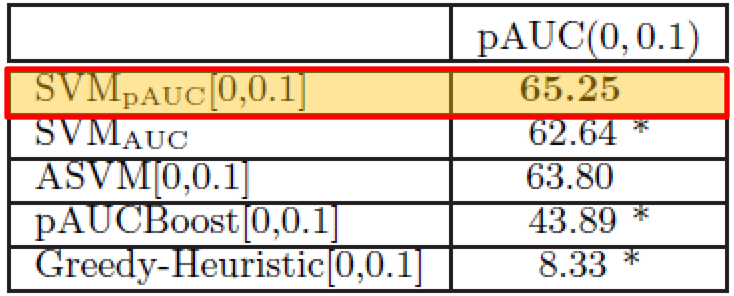

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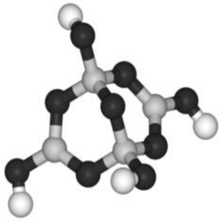

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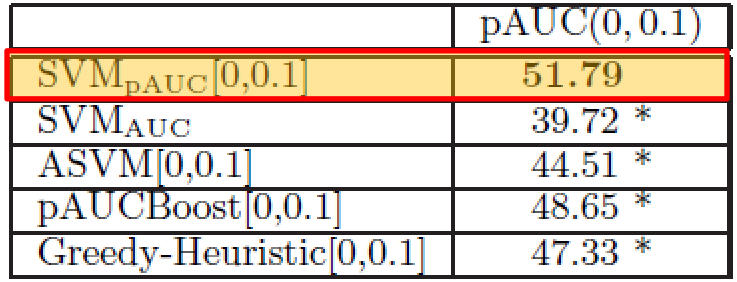

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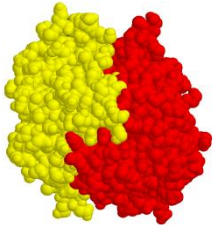
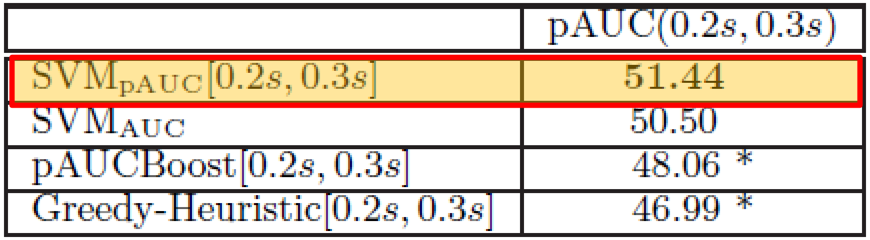
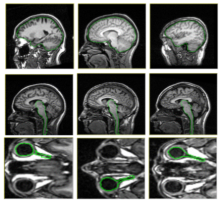


KDD Cup 2008 Breast Cancer Detection



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



Conclusions

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- Efficient algorithm for solving the inner combinatorial optimization step
- Experimental results confirm the efficacy of the algorithm

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- Efficient algorithm for solving the inner combinatorial optimization step
- Experimental results confirm the efficacy of the algorithm
- Future work:
  - Characterize upper bound on partial AUC?
  - Tighter upper bound on partial AUC?
  - Statistical consistency?