General Framework for Classification at the Top

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Motivation

Binary classification

- Two group of samples:
  - negative samples with label $y = 0$,
  - positive samples with label $y = 1$.

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- Classifier usually has two parts:
  - model f maps a sample $\boldsymbol{x}$ to its classification score $s \in \mathbb{R}$,
  - decision threshold $t \in \mathbb{R}$ decides whether a sample is classified as positive or not

$$\hat{y} = \begin{cases} 1 & \text{if } s \geq t, \\ 0 & \text{otherwise.} \end{cases}$$

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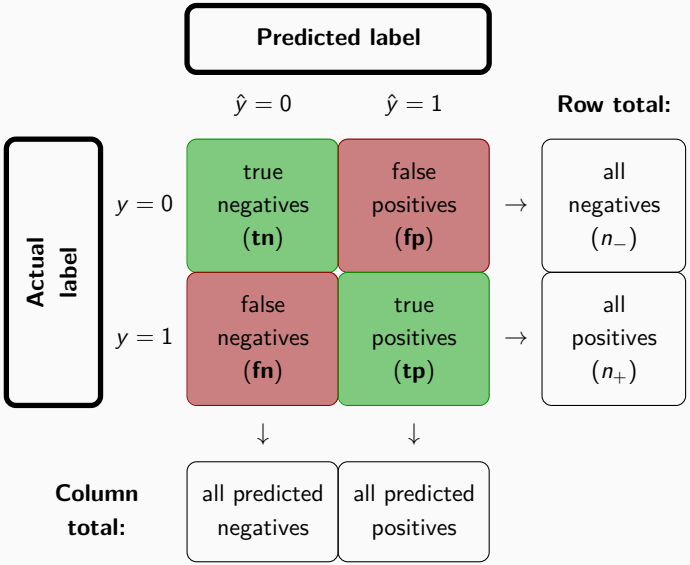
- Usually, the model returns the probability that the sample is from the positive class and the threshold is 0.5.
- **Goal:** find classifier which predicts labels for unknown samples with the lowest possible error.

Confusion matrix



Binary Classification

- General form of binary classification

$$\begin{aligned} \underset{\boldsymbol{w},\, t}{\text{minimize}} \quad & \frac{1}{n_-} \sum_{i \in \mathcal{I}_-} \mathbb{1}_{[s_i \geq t]} + \frac{1}{n_+} \sum_{i \in \mathcal{I}_+} \mathbb{1}_{[s_i < t]} \\ \text{subject to} \quad & s_i = f(\boldsymbol{x}_i; \boldsymbol{w}), \quad i \in \mathcal{I}, \end{aligned}$$

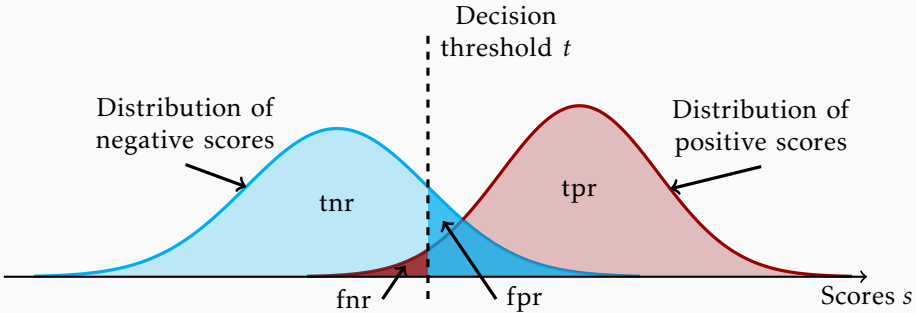
- $\mathcal{I} = \mathcal{I}_- \cup \mathcal{I}_+$ is a set of indices of all sample where

$$\begin{aligned} \mathcal{I}_- &= \{ i \mid i \in \{1, 2, \ldots, n\} \ \wedge \ y_i = 0 \}, \\ \mathcal{I}_+ &= \{ i \mid i \in \{1, 2, \ldots, n\} \ \wedge \ y_i = 1 \}, \end{aligned}$$

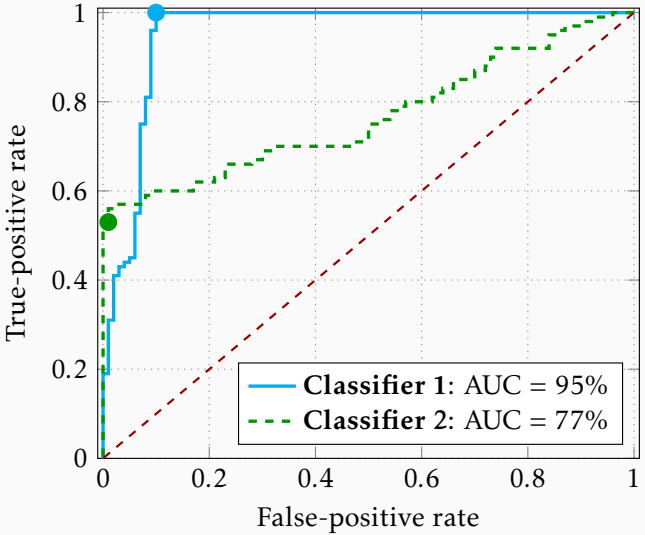
- $\mathbb{1}_{[\cdot]}$ is Iverson function defined by

$$\mathbb{1}_{[x]} = \begin{cases} 0 & \text{if } x \text{ is false,} \\ 1 & \text{if } x \text{ is true.} \end{cases}$$

ROC curves


Decision
threshold t
Distribution of
negative scores
Distribution of
positive scores
tnr
tpr
fnr
fpr
Scores s

ROC curves


True-positive rate
False-positive rate
0
0.2
0.4
0.6
0.8
1
Classifier 1: AUC = 95%
Classifier 2: AUC = 77%

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  - Malware detection: false-alarms are disruptive to the user.
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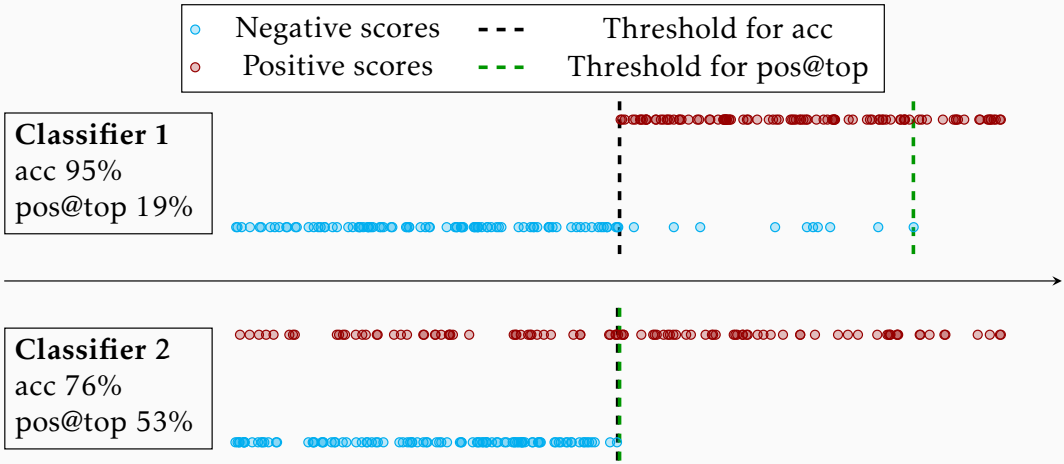
- In such cases, **Classifier 2** may be better.
- **Classifier 1** maximizes accuracy

$$\text{acc}(\boldsymbol{s}) = \frac{1}{n} \sum_{i \in \mathcal{I}} \mathbb{1}_{[y_i = \hat{y}_i]}.$$

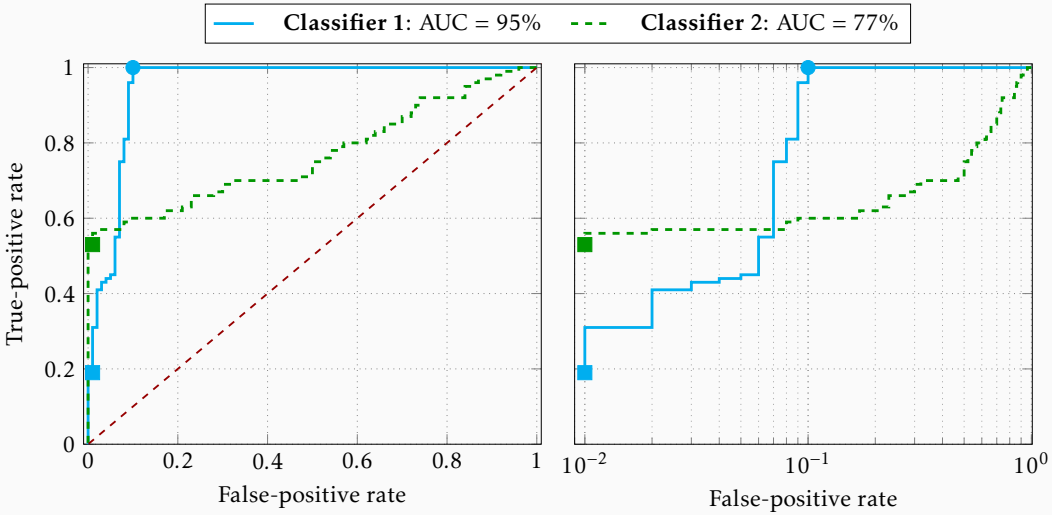
- **Classifier 2** maximizes the number of positive samples at the top

$$\text{pos@top}(\boldsymbol{s}) = \frac{1}{n_+} \sum_{i \in \mathcal{I}_+} \mathbb{1}_{\left[s_i \geq \max_{j \in \mathcal{I}_-} s_j\right]}.$$

ROC curves


Negative scores
Positive scores
Threshold for acc
Threshold for pos@top
Classifier 1
acc 95%
pos@top 19%
Classifier 2
acc 76%
pos@top 53%

ROC curves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10^{-2}
10^{-1}
10^{0}

Classification at the Top

Problem formulation

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- General formulation

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  where threshold t is a function of all scores.
- Difficult problem: constrained, discontinuous, non-convex, and non-decomposable.

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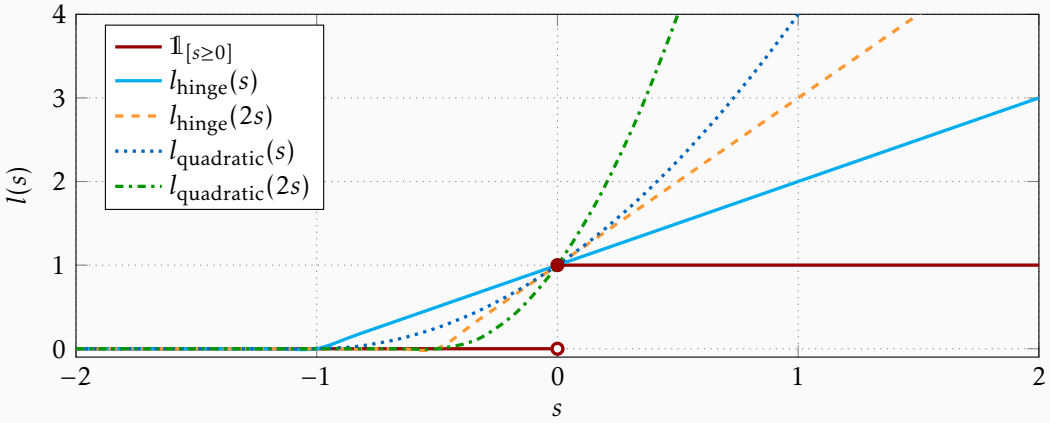
$\mathbb{1}_{[s\geq 0]}$
$l_{\text{hinge}}(s)$
$l_{\text{hinge}}(2s)$
$l_{\text{quadratic}}(s)$
$l_{\text{quadratic}}(2s)$
$l(s)$
s
4
3
2
1
0
−2
−1
0
1
2

Surrogate approximation

- General surrogate formulation

$$\begin{aligned} \underset{\boldsymbol{w}}{\text{minimize}} \quad & \frac{1}{2}\|\boldsymbol{w}\|^2 + \frac{1}{n_+}\sum_{i\in\mathcal{I}_+} l(t - s_i) \\ \text{subject to} \quad & s_i = f(\boldsymbol{x}_i; \boldsymbol{w}), \quad i \in \mathcal{I}, \\ & t = G(\boldsymbol{s}, \boldsymbol{y}). \end{aligned}$$

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- *TopPush* maximizes the number of positive samples at the top

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- *TopPush* maximizes the number of positive samples at the top

$$t = \max_{j\in\mathcal{I}_-} s_j.$$

- *Pat&Mat-NP* maximizes true-positive rate with fixed false-positive rate

$$t \text{ solves } \frac{1}{n_-}\sum_{i\in\mathcal{I}_-} l\left(\vartheta(s_i - t)\right) = \tau.$$

Classification at the Top: Linear Model

- Linear model $f(\boldsymbol{x}; \boldsymbol{w}) = \boldsymbol{w}^\top \boldsymbol{x}$.
- General surrogate formulation with linear model

$$\begin{aligned} \underset{\boldsymbol{w}}{\text{minimize}} \quad & \frac{1}{2} \|\boldsymbol{w}\|^2 + \frac{1}{n_+} \sum_{i \in \mathcal{I}_+} l(t - s_i) \\ \text{subject to} \quad & s_i = \boldsymbol{w}^\top \boldsymbol{x}_i, \quad i \in \mathcal{I}, \\ & t = G(\boldsymbol{s}, \boldsymbol{y}). \end{aligned}$$

- Properties that we are interested in:
  - Convexity of the objective function.
  - Robustness to outliers.

Convexity of the objective function

Theorem

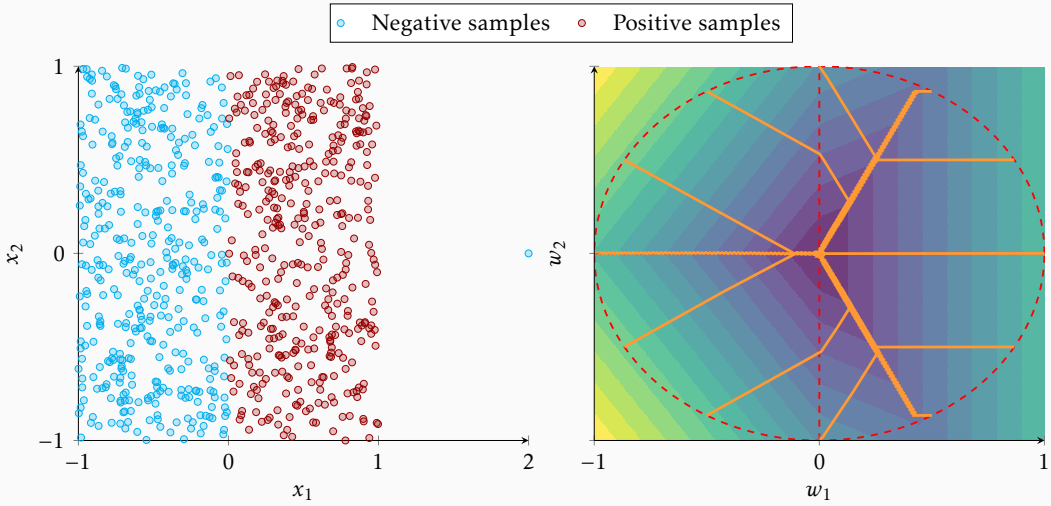
If the threshold t is a convex function of the weights $\boldsymbol{w}$, then function

$$L(\boldsymbol{w}) = \frac{1}{2}\|\boldsymbol{w}\|^2 + \frac{1}{n_+}\sum_{i\in\mathcal{I}_+} l(t - s_i)$$

is convex.

- Both formulations *TopPush* and *Pat&Mat-NP* have convex thresholds.
- Both formulations are convex and continuous.

When convexity is not enough...



How to solve it?

- Using gradient descent

$$\boldsymbol{w}^{k+1} \leftarrow \boldsymbol{w}^k - \alpha^k \cdot \nabla L(\boldsymbol{w}^k),$$

where $\alpha^k > 0$ is a learning rate, and $\nabla L(\boldsymbol{w}^k)$ is a gradient of the objective function

$$\nabla L(\boldsymbol{w}) = \boldsymbol{w} + \frac{1}{n_+} \sum_{i \in \mathcal{I}_+} l' \left(t(\boldsymbol{w}) - f(\boldsymbol{x}_i; \boldsymbol{w}) \right) \left(\nabla t(\boldsymbol{w}) - \nabla f(\boldsymbol{x}_i; \boldsymbol{w}) \right).$$

Classification at the Top: Non-linear Model

???

- General surrogate formulation with non-linear model

$$
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- Disadvantages:
  - Objective function is not convex.
  - Non-linear models are usually large and expensive to train.

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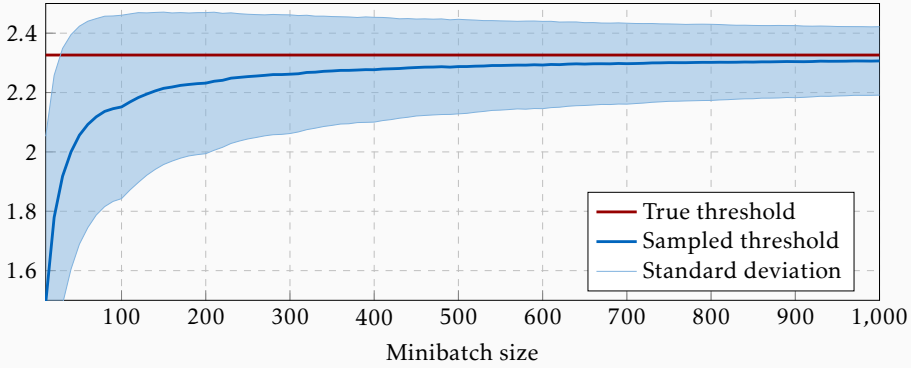
- Disadvantages:
  - Objective function is not convex.
  - Non-linear models are usually large and expensive to train.
- What to do if the dataset is too large to fit in memory?
- Stochastic gradient descent: the gradient is computed only on a small subset of all data called minibatch.

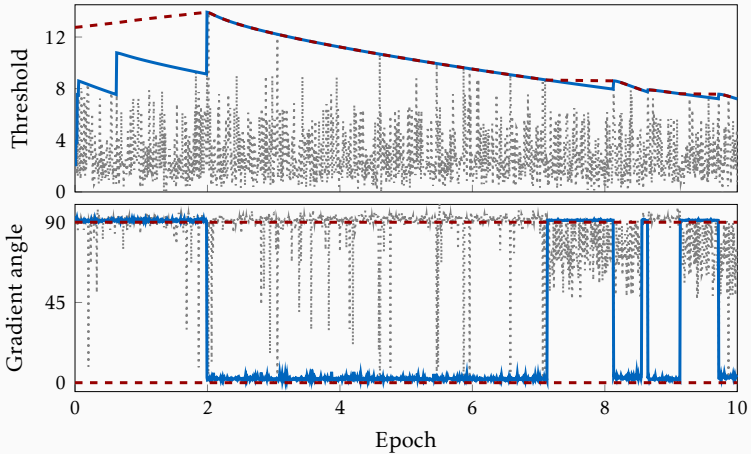
Issues when passing to mini-batches

- Problems:
  - The threshold is a function of all scores $\rightarrow$ the loss function is non-decomposable.
  - As a result, stochastic gradient descent provides a biased gradient estimate.



How to reduce bias?

- Increase size of minibatch $\rightarrow$ *Pat&Mat-NP*.
- Add threshold from last minibatch $\rightarrow$ *DeepTopPush*.

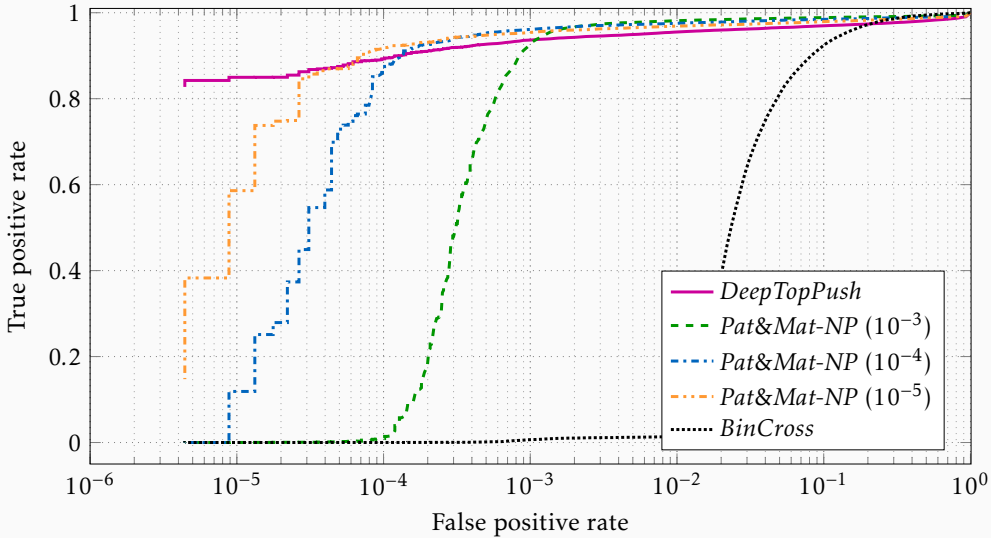


How does it work?

Steganography

- Dataset: 205 579 samples, 9% of samples are positive.
- Each sample consists of 22 510 features.
- Only linear model.
- **Goals:**
  - Maximize the true-positive rate at extremely low levels of the false-positive rate.

Steganography



AVAST: Malware detection

- Dataset: 6 580 166 samples, 87% of samples are positive.
- Hierarchical data structure:
  - Each sample is a JSON file, which may consist of other JSON files.
  - Each sample is of a different size (from 1 KB to 2.5 MB).
  - *DeepTopPush* and *Pat&Mat-NP* used as an extension for hierarchical multi-instance learning (HMIL).
- **Goals:**
  - Maximize the true-positive rate at extremely low levels of the false-positive rate.
  - The false-positive rate must be as low as possible to avoid disruptive false alarms for the end-user.

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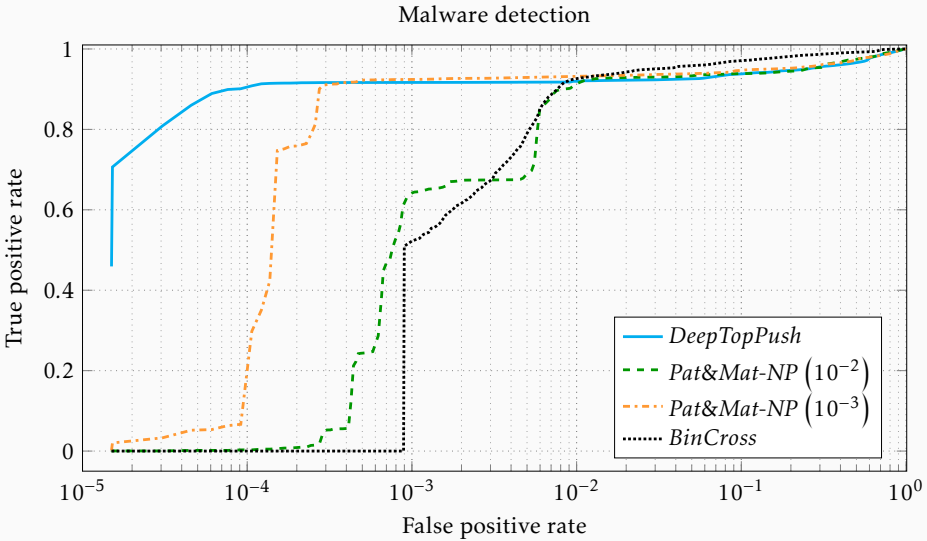

Thank you for your attention.