When AUC meets DRO: Optimizing Partial AUC for Deep Learning with Non-Convex Convergence Guarantee

Dixian Zhu, Gang Li, Bokun Wang, Xiaodong Wu, Tianbao Yang

Motivation

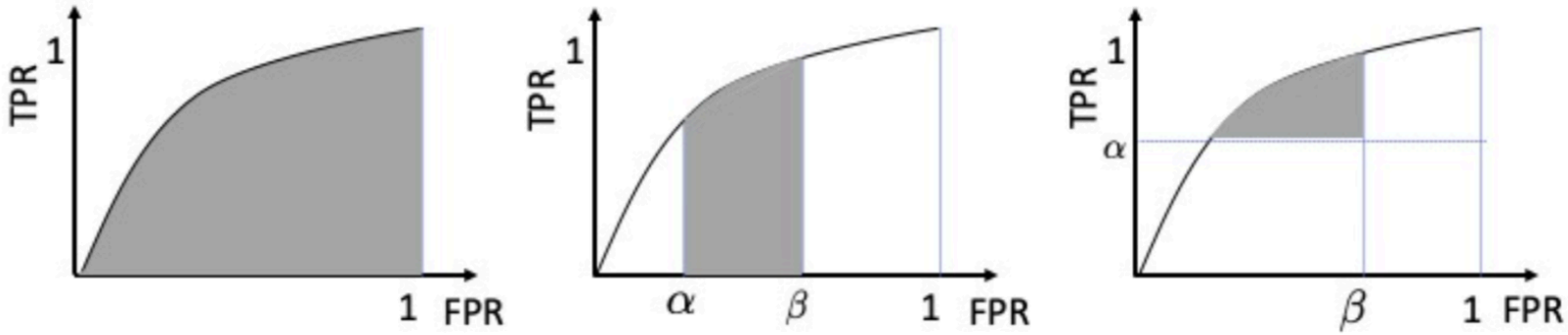


Figure 1: From left to right: AUC, one-way pAUC, two-way pAUC

There are few rigorous and efficient algorithms developed for pAUC maximization for deep learning. Our pAUC maximization method with distributional robust optimization (DRO) technique can provide the **exact&soft estimators** and **convergence guarantee**.

Preliminaries

- Non-parametric estimator
  - One way Partial AUC (OPAUC)

$$\widehat{\mathrm{OPAUC}}(h, \alpha_0, \alpha_1) = \frac{1}{n_+}\frac{1}{n_-} \sum_{\mathbf{x}_i \in \mathcal{S}_+} \sum_{\mathbf{x}_j \in \mathcal{S}_-^{\downarrow}[k_1+1, k_2]} \mathbb{I}(h(\mathbf{x}_i) > h(\mathbf{x}_j))$$

where $k_1 = \lceil n_- \alpha_0 \rceil, k_2 = \lfloor n_- \alpha_1 \rfloor$. In this work, we will focus on optimizing $\widehat{\mathrm{OPAUC}}(h, 0, \beta)$ for some $\beta \in (0, 1)$.

  - Two way Partial AUC (TPAUC)

$$\widehat{\mathrm{TPAUC}}(h, \alpha, \beta) = \frac{1}{n_+}\frac{1}{n_-} \sum_{\mathbf{x}_i \in \mathcal{S}_+^{\uparrow}[1, k_1]} \sum_{\mathbf{x}_j \in \mathcal{S}_-^{\downarrow}[1, k_2]} \mathbb{I}(h(\mathbf{x}_i) > h(\mathbf{x}_j))$$

where $k_1 = \lfloor n_+ \alpha \rfloor, k_2 = \lfloor n_- \beta \rfloor$.

Preliminaries

Distributionally Robust Optimization (DRO). For a set of random loss functions $\ell_1(\cdot), \ldots, \ell_n(\cdot)$, a DRO loss can be written as

$$\hat{L}_\phi(\cdot) = \max_{\mathbf{p} \in \Delta} \sum_j p_j \ell_j(\cdot) - \lambda D_\phi(\mathbf{p}, 1/n), \tag{4}$$

Lemma 1. *By using KL divergence measure, we have*

$$\hat{L}_{kl}(\cdot; \lambda) = \lambda \log \left(\frac{1}{n} \sum_{i=1}^{n} \exp\left(\frac{\ell_i(\cdot)}{\lambda} \right) \right). \tag{5}$$

By using the CVaR divergence $\phi_c(t)$ for some γ such that $n\gamma$ is an integer, we have,

$$\hat{L}_{cvar}(\cdot; \gamma) = \frac{1}{n\gamma} \sum_{i=1}^{n\gamma} \ell_{[i]}(\cdot), \tag{6}$$

where $\ell_{[i]}(\cdot)$ denotes the i-th largest value in $\{\ell_1, \ldots, \ell_n\}$.

Methods for OPAUC

- Surrogate function:

$$\min_{\mathbf{w}} \frac{1}{n_+} \sum_{\mathbf{x}_i \in \mathcal{S}_+} \frac{1}{n_- \beta} \sum_{\mathbf{x}_j \in \mathcal{S}_-^{\downarrow}[1, n_- \beta]} L(\mathbf{w}; \mathbf{x}_i, \mathbf{x}_j), \tag{7}$$

- CVaR-based (exact) estimator:

$$\min_{\mathbf{w}} \frac{1}{n_+} \sum_{\mathbf{x}_i \in \mathcal{S}_+} \hat{L}_\phi(\mathbf{w}; \mathbf{x}_i). \tag{8}$$

Theorem 1. *By choosing* $\phi(\cdot) = \phi_c(\cdot) = \mathbb{I}(\cdot \in (0, 1/\beta])$, *then the problem (8) is equivalent to*

$$\min_{\mathbf{w}} \min_{\mathbf{s} \in \mathbb{R}^{n_+}} F(\mathbf{w}, \mathbf{s}) = \frac{1}{n_+} \sum_{\mathbf{x}_i \in \mathcal{S}_+} \left(s_i + \frac{1}{\beta} \psi_i(\mathbf{w}, s_i) \right), \tag{9}$$

where $\psi_i(\mathbf{w}, s_i) = \frac{1}{n_-} \sum_{\mathbf{x}_j \in \mathcal{S}_-} (L(\mathbf{w}; \mathbf{x}_i, \mathbf{x}_j) - s_i)_+$. *If* ℓ *is a monotonically decreasing function for* $\ell(\cdot) > 0$, *then the objective in (8) is equivalent to (7) of OPAUC.*

Methods for OPAUC

Algorithm 1 SOPA

1: Set $\mathbf{s}^1 = 0$ and initialize $\mathbf{w}$
2: **for** $t = 1, \ldots, T$ **do**
3: Sample two mini-batches $\mathcal{B}_+ \subset \mathcal{S}_+, \mathcal{B}_- \subset \mathcal{S}_-$
4: Let $p_{ij} = \mathbb{I}(\ell(h(\mathbf{w}_t, \mathbf{x}_i) - h(\mathbf{w}_t, \mathbf{x}_j)) - s_i^t > 0)$
5: Update $s_i^{t+1} = s_i^t - \frac{\eta_2}{n_+}(1 - \frac{\sum_j p_{ij}}{\beta|\mathcal{B}_-|})$ for $\mathbf{x}_i \in \mathcal{B}_+$
6: Compute a gradient estimator ∇_t by

$$\nabla_t = \frac{1}{\beta|\mathcal{B}_+||\mathcal{B}_-|} \sum_{\mathbf{x}_i \in \mathcal{B}_+} \sum_{\mathbf{x}_j \in \mathcal{B}_-} p_{ij} \nabla_{\mathbf{w}} L(\mathbf{w}_t; \mathbf{x}_i, \mathbf{x}_j)$$

7: Update $\mathbf{w}_{t+1} = \mathbf{w}_t - \eta_1 \nabla_t$
8: **end for**

Methods for OPAUC

- KLDRO-based (soft) estimator:

$$\min_{\mathbf{w}} \frac{1}{n_+} \sum_{\mathbf{x}_i \in \mathcal{S}_+} \hat{L}_\phi(\mathbf{w}; \mathbf{x}_i). \tag{8}$$

Theorem 2. *By choosing $\phi(\cdot) = \phi_{kl}(\cdot)$, then the problem (8) becomes*

$$\min_{\mathbf{w}} \frac{1}{n_+} \sum_{\mathbf{x}_i \sim \mathcal{S}_+} \lambda \log \mathrm{E}_{\mathbf{x}_j \in \mathcal{S}_-} \exp\left(\frac{L(\mathbf{w}; \mathbf{x}_i, \mathbf{x}_j)}{\lambda}\right). \tag{10}$$

If $\ell(\cdot)$ is a monotonically decreasing function for $\ell(\cdot) > 0$, when $\lambda = 0$, the above objective is a surrogate of $\widehat{OPAUC}(h_{\mathbf{w}}, 0, \frac{1}{n_-})$; and when $\lambda = +\infty$, the above objective is a surrogate of $\widehat{OPAUC}(h_{\mathbf{w}}, 0, 1)$, i.e., the AUC.

Methods for OPAUC

Algorithm 2 SOPA-s

1: Set $\mathbf{u}^1 = 0$ and initialize $\mathbf{w}$
2: **for** $t = 1, \ldots, T$ **do**
3: Sample two mini-batches $\mathcal{B}_+ \subset \mathcal{S}_+, \mathcal{B}_- \subset \mathcal{S}_-$
4: For each $\mathbf{x}_i \in \mathcal{B}_+$, update $u_i^{t+1} = (1-\gamma_0)u_i^t + \gamma_0 \frac{1}{|\mathcal{B}_-|} \sum_{\mathbf{x}_j \in \mathcal{B}_-} \exp\left(\frac{L(\mathbf{w}_t;\mathbf{x}_i,\mathbf{x}_j)}{\lambda}\right)$
5: Let $p_{ij} = \exp(L(\mathbf{w}_t;\mathbf{x}_i,\mathbf{x}_j)/\lambda)/u_i^t$
6: Compute a gradient estimator ∇_t by

$$\nabla_t = \frac{1}{|\mathcal{B}_+|}\frac{1}{|\mathcal{B}_-|}\sum_{\mathbf{x}_i \in \mathcal{B}_+}\sum_{\mathbf{x}_j \in \mathcal{B}_-} p_{ij}\nabla L(\mathbf{w}_t;\mathbf{x}_i,\mathbf{x}_j)$$

7: Update $\mathbf{v}_t = (1-\gamma_1)\mathbf{v}_{t-1} + \gamma_1 \nabla_t$
8: Update $\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \mathbf{v}_t$ (or Adam-style)
9: **end for**

Methods for OPAUC

Theorem 3. *Under Assumption 2, Algorithm 1 ensures that after* $T = O(1/(\beta\epsilon^4))$ *iterations we can find an* ϵ *nearly stationary solution of* $F(\mathbf{w}, \mathbf{s})$*, i.e.,* $\mathrm{E}\|\nabla F_{\hat{\rho}}(\mathbf{w}_\tau, \mathbf{s}_\tau)\|^2 \leq \epsilon^2$ *for a randomly selected* $\tau \in \{1, \ldots, T\}$ *and* $\hat{\rho} = 1.5\rho$.

Theorem 4. *Under Assumption 2, Algorithm 2 with* $\gamma_0 = O(B_-\epsilon^2)$, $\gamma_1 = O(\min\{B_-, B_+\}\epsilon^2)$, $\eta = O(\min\{\gamma_0 B_1/n_+, \gamma_1\})$ *ensures that after* $T = O(\frac{1}{\min(B_+, B_-)\epsilon^4} + \frac{n_+}{B_+ B_- \epsilon^4})$ *iterations we can find an* ϵ*-stationary solution of* $F(\mathbf{w})$*, i.e.,* $\mathrm{E}[\|\nabla F(\mathbf{w}_\tau)\|^2] \leq \epsilon^2$ *for a randomly selected* $\tau \in \{1, \ldots, T\}$*, where* $B_+ = |\mathcal{B}_+|$ *and* $B_- = |\mathcal{B}_-|$.

Methods for TPAUC

- KLDRO-based (soft) estimator:

$$F(\mathbf{w};\phi,\phi') = \max_{\mathbf{p}\in\Delta} \sum_{\mathbf{x}_i\in\mathcal{S}_+} p_i \hat{L}_\phi(\mathbf{x}_i,\mathbf{w}) - \lambda' D_{\phi'}(\mathbf{p}, \frac{1}{n_+}).$$

Lemma 3. *When $\phi = \phi' = \phi_{kl}$, we have*

$$F(\mathbf{w};\phi_{kl},\phi_{kl})$$

$$= \lambda' \log \mathrm{E}_{\mathbf{x}_i\sim\mathcal{S}_+} \left(\mathrm{E}_{\mathbf{x}_j\sim\mathcal{S}_-} \exp(\frac{\ell(\mathbf{w};\mathbf{x}_i,\mathbf{x}_j)}{\lambda}) \right)^{\frac{\lambda}{\lambda'}}.$$

For minimizing this function, we formulate the problem as a novel three-level compositional stochastic optimization:

$$\min_{\mathbf{w}} f_1(\frac{1}{n_+} \sum_{\mathbf{x}_i\in\mathcal{S}_+} f_2(g_i(\mathbf{w}))),$$

Methods for TPAUC

Algorithm 3 SOTA-s

Set $\mathbf{u}_0 = 0, v_0 = 0, \mathbf{m}_0 = 0$ and initialize $\mathbf{w}$

for $t = 1, \ldots, T$ **do**

  Sample two mini-batches $\mathcal{B}_+ \subset \mathcal{S}_+, \mathcal{B}_- \subset \mathcal{S}_-$

  For each $\mathbf{x}_i \in \mathcal{B}_+$ compute $u_t^i = (1-\gamma_0)u_{t-1}^i + \gamma_0 \frac{1}{|\mathcal{B}_-|} \sum_{\mathbf{x}_j \in \mathcal{B}_-} L(\mathbf{w}_t; \mathbf{x}_i, \mathbf{x}_j)$

  Let $v_t = (1-\gamma_1)v_{t-1} + \gamma_1 \frac{1}{|\mathcal{B}_+|} \sum_{\mathbf{x}_i \in \mathcal{B}_+} f_2(u_{t-1}^i)$

  Let $p_{ij} = (u_{t-1}^i)^{\lambda/\lambda'-1} \exp(L(\mathbf{w}_t, \mathbf{x}_i, \mathbf{x}_j)/\lambda)/v_t$

  Compute a gradient estimator ∇_t by

$$\nabla_t = \frac{1}{|\mathcal{B}_+|} \frac{1}{|\mathcal{B}_-|} \sum_{\mathbf{x}_i \in \mathcal{B}_+} \sum_{\mathbf{x}_j \in \mathcal{B}_-} p_{ij} \nabla L(\mathbf{w}_t; \mathbf{x}_i, \mathbf{x}_j)$$

  Update $\mathbf{m}_t = (1-\gamma_2)\mathbf{m}_{t-1} + \gamma_2 \nabla_t$

  Update $\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \mathbf{m}_t$ (or Adam-style)

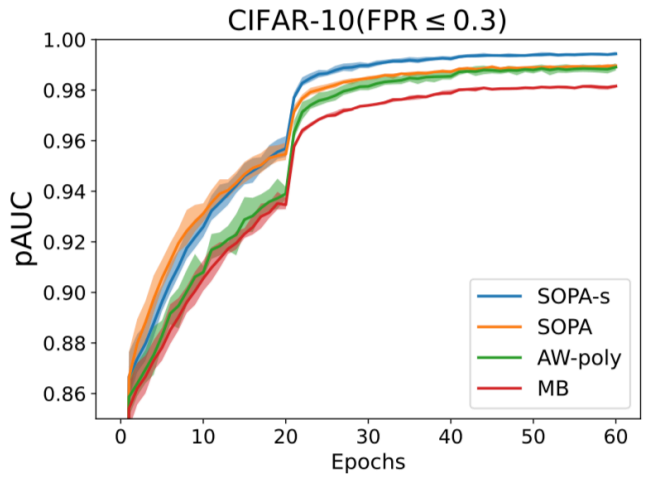
end for

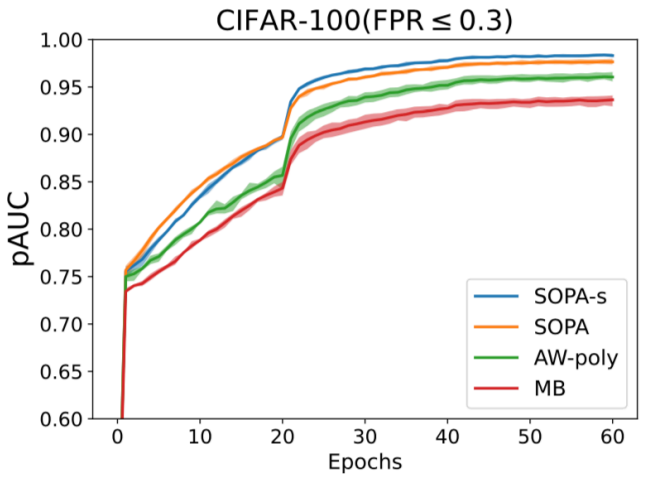
Methods for TPAUC

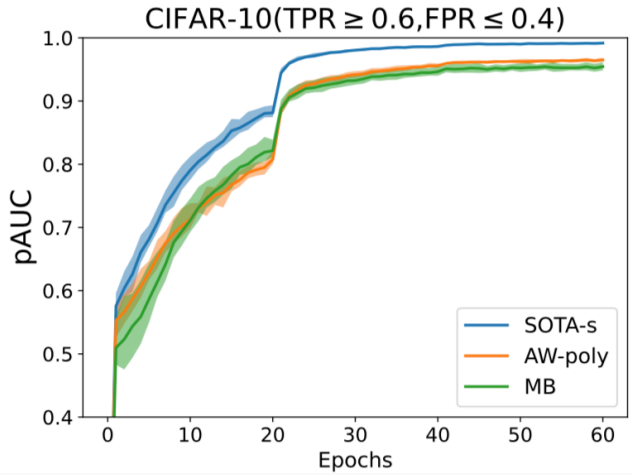
Theorem 5. *Under Assumption 2, Algorithm 3 with* $\gamma_0 = O(B_-\epsilon^2)$, $\gamma_1 = O(B_+\epsilon^2)$, $\gamma_2 = O(\min\{B_-, B_+\}\epsilon^2)$, $\eta = O(\min\{\gamma_0 B_1/n_+, \gamma_1, \gamma_2\})$ *ensures that after* $T = O(\frac{1}{\min(B_+, B_-)\epsilon^4} + \frac{n_+}{B_+ B_- \epsilon^4})$ *iterations we can find an* ϵ *nearly stationary solution of* $F(\mathbf{w})$, *where* $B_+ = |\mathcal{B}_+|$ *and* $B_- = |\mathcal{B}_-|$.

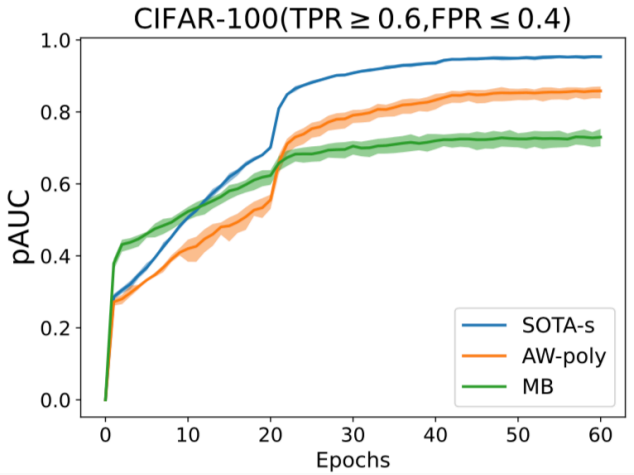
Remark: It is notable that SOTA-s has an iteration complexity in the same order of SOPA-s for OPAUC maximization.

Experiments: training

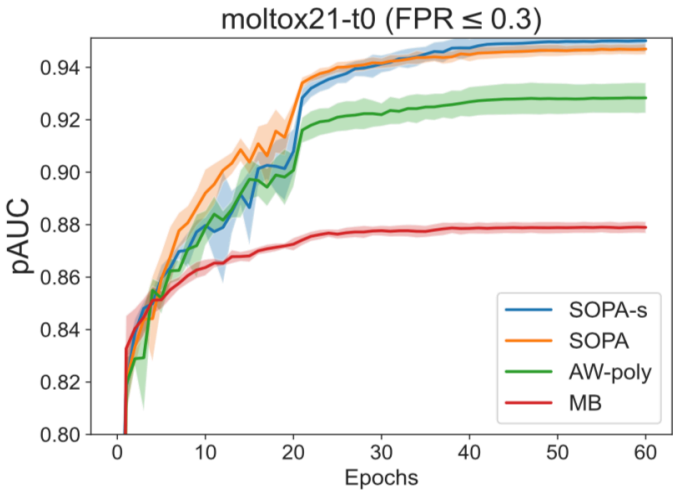


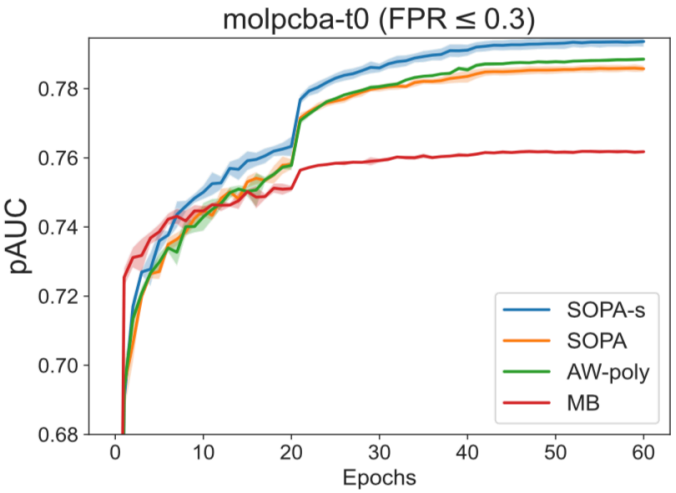


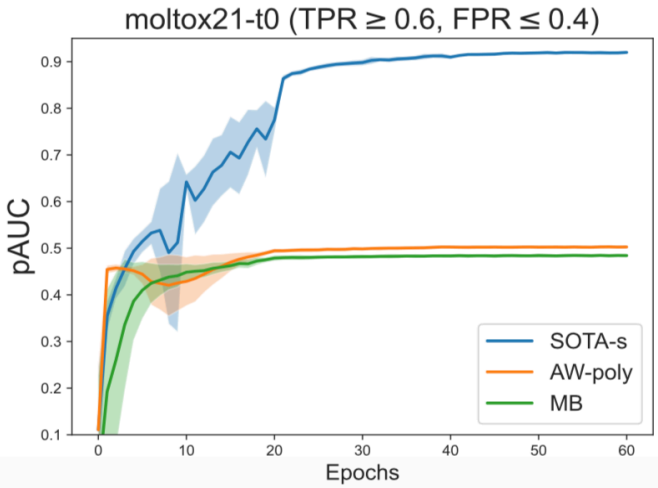


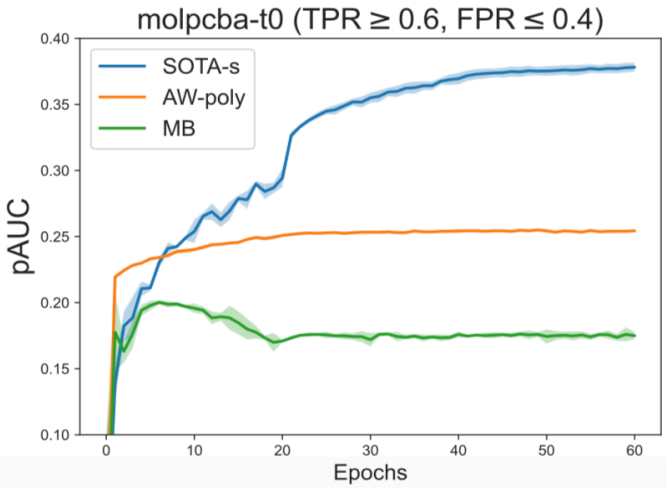


Experiments: training









Experiments: testing

Table 1. One way partial AUC on testing data of three image datasets

	CIFAR-10		CIFAR-100		Melanoma	
Methods	FPR≤0.3	FPR≤0.5	FPR≤0.3	FPR≤0.5	FPR≤0.3	FPR≤0.5
CE	0.8446(0.0018)	0.8777(0.0014)	0.7338(0.0047)	0.7787(0.0044)	0.7651(0.0135)	0.8151(0.0028)
AUC-SH	0.8657(0.0056)	0.8948(0.0036)	0.7467(0.0047)	0.7930(0.0027)	0.7824(0.0138)	0.8176(0.0160)
AUC-M	0.8678(0.0016)	0.8934(0.0022)	0.7371(0.0031)	0.7828(0.0005)	0.7788(0.0068)	0.8249(0.0141)
P-push	0.8610(0.0007)	0.8889(0.0021)	0.7445(0.0025)	0.7930(0.0029)	0.7440(0.0130)	0.8028(0.0170)
MB	0.8690(0.0016)	0.8931(0.0015)	0.7487(0.0017)	0.7930(0.0014)	0.7683(0.0303)	0.8184(0.0278)
AW-poly	0.8664(0.0052)	0.8915(0.0075)	0.7490(0.0058)	0.7909(0.0068)	0.7936(0.0238)	0.8355(0.0067)
SOPA	**0.8766(0.0034)**	**0.9028(0.0031)**	**0.7551(0.0044)**	**0.7999(0.0028)**	**0.8093(0.0248)**	**0.8585(0.0210)**
SOPA-s	0.8691(0.0036)	0.8961(0.0036)	0.7468(0.0056)	0.7877(0.0053)	0.7775(0.0076)	0.8401(0.0206)

Table 2. Two way partial AUC on testing data of three image datasets; (α,β) represents TPR$\geq \alpha$ and FPR $\leq \beta$.

	CIFAR-10		CIFAR-100		Melanoma	
Methods	(0.6,0.4)	(0.5,0.5)	(0.6,0.4)	(0.5,0.5)	(0.6,0.4)	(0.5,0.5)
CE	0.4981(0.0078)	0.6414(0.0080)	0.2178(0.0136)	0.4011(0.0118)	0.3399(0.0135)	0.5150(0.0038)
AUC-SH	0.5622(0.0064)	0.6923(0.0071)	0.2599(0.0061)	0.4397(0.0062)	0.3640(0.0354)	0.5291(0.0312)
AUC-M	0.5691(0.0021)	0.6907(0.0125)	0.2336(0.0041)	0.4153(0.0022)	0.3665(0.0646)	0.5404(0.0545)
P-push	0.5477(0.0077)	0.6781(0.0055)	0.2623(0.0042)	0.4417(0.0092)	0.3317(0.0304)	0.4870(0.0443)
MB	0.5404(0.0041)	0.6724(0.0011)	0.2207(0.0033)	0.4017(0.0149)	0.3330(0.0258)	0.4981(0.0252)
AW-poly	0.5536(0.0196)	0.6814(0.0203)	0.2489(0.0166)	0.4342(0.0112)	0.3878(0.0292)	0.5216(0.0288)
SOTA-s	**0.5799(0.0202)**	**0.7074(0.0145)**	**0.2708(0.0055)**	**0.4528(0.0069)**	**0.4198(0.0825)**	**0.5865(0.0664)**

Experiments: testing

Table 3. One way partial AUC on testing data of three molecular datasets

	moltox21(t0)		molmuv(t1)		molpcba(t0)	
Methods	FPR≤0.3	FPR≤0.5	FPR≤0.3	FPR≤0.5	FPR≤0.3	FPR≤0.5
CE	0.6671(0.0009)	0.6954(0.005)	0.8008(0.0090)	0.8201(0.0061)	0.6802(0.0002)	0.7169(0.0002)
AUC-SH	0.7161(0.0043)	0.7295(0.0036)	0.7880(0.0382)	0.8025(0.0437)	0.6939(0.0009)	0.7350(0.0015)
AUC-M	0.6866(0.0048)	0.7080(0.0020)	0.7960(0.0123)	0.8076(0.0175)	0.6985(0.0016)	0.7399(0.0005)
P-push	0.6946(0.0107)	0.7160(0.0073)	0.7832(0.0220)	0.7940(0.0321)	0.6841(0.0007)	0.7293(0.0043)
MB	**0.7398(0.0131)**	0.7329(0.0099)	0.7672(0.0563)	0.7772(0.0547)	0.6899(0.0002)	0.7253(0.0006)
AW-poly	0.7227(0.0024)	0.7271(0.0112)	0.7754(0.0372)	0.7883(0.0431)	0.6975(0.0006)	0.7350(0.0015)
SOPA	0.7209(0.0063)	0.7318(0.0084)	0.8187(0.0319)	0.8245(0.0312)	0.6989(0.0022)	0.7371(0.0011)
SOPA-s	0.7309(0.0151)	**0.7330(0.0073)**	**0.8449(0.0399)**	**0.8412(0.0447)**	**0.7027(0.0018)**	**0.7416(0.0006)**

Table 4. Two way partial AUC on testing data of three molecular datasets; (α,β) represents TPR$\geq \alpha$ and FPR $\leq \beta$.

	moltox21(t0)		molmuv(t1)		molpcba(t0)	
Methods	(0.6,0.4)	(0.5,0.5)	(0.6,0.4)	(0.5,0.5)	(0.6,0.4)	(0.5,0.5)
CE	0.0674(0.0014)	0.2082(0.0011)	0.1613(0.0337)	0.4691(0.0183)	0.0949(0.0006)	0.2639(0.0006)
AUC-SH	0.0640(0.0080)	0.2170(0.0140)	0.2600(0.1300)	0.4440(0.1280)	0.1400(0.0030)	0.3120(0.0030)
AUC-M	0.0660(0.0090)	0.2090(0.0100)	0.1140(0.0790)	0.4330(0.0530)	0.1420(0.0090)	0.3130(0.0030)
P-push	0.0610(0.0180)	0.2070(0.0120)	0.1860(0.1520)	0.4170(0.1080)	0.1350(0.0020)	0.3000(0.0120)
MB	0.0670(0.0150)	0.2150(0.0230)	0.1730(0.1530)	0.4260(0.1180)	0.0950(0.0020)	0.2620(0.0030)
AW-poly	0.0640(0.0100)	0.2060(0.0250)	0.1720(0.1440)	0.3930(0.1230)	0.1100(0.0010)	0.2810(0.0020)
SOTA-s	**0.0680(0.0180)**	**0.2300(0.0210)**	**0.3270(0.1640)**	**0.5260(0.1220)**	**0.1430(0.0010)**	**0.3140(0.0020)**

Thank you!