OOD-ENS: Cross-Validated Out-of-Distribution Ensemble Detector

A The relationship of $p(p_z)$ and p_z.

Before providing the relationship of $p(p_z)$ and p_z, we introduce Eq. (7) in the submitted paper as follows.

$$p(p_z) = \int_{0.5}^{1} Be((m_e - 1)p_z, (m_e - 1)(1 - p_z))dx.$$

where $m_e = \frac{K}{1+(K-1)\rho}$ and $\rho = Corr(\hat{g}_k, \hat{g}_{k'})$ with $k, k' = 1, \ldots, K$ and $k \neq k'$.

According to the above formula, we calculate the values of $p(p_z)$ for different p_z, K, and ρ under the condition of $0 \leq \rho < 1$ and $3 \leq K \leq n-1$, and plot the variance of $p(p_z)$ along with an increases K. The results are shown in Figure 1.

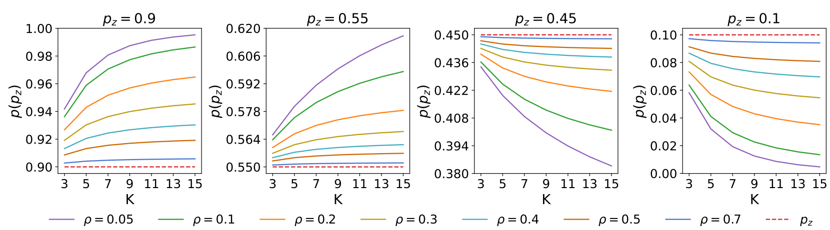

Fig. 1. The relationship of $p(p_z)$ and p_z.

From the Figure, it is clear that $p(p_z) > p_z$, and $p(p_z)$ is an increasing function with regard to K when $p_z > 0.5$. On contrary, when $p_z < 0.5$, $p(p_z) < p_z$, and $p(p_z)$ is an decreasing function with regard to K. For example, $p(p_z)$ is larger than 0.9 in the left-top subfigure when $p_z = 0.9$, and $p(p_z)$ is smaller than 0.45 in the left-bottom subfigure when $p_z = 0.45$. Therefore, the relationship of $p(p_z)$ and p_z is as follows.

- When $p_z > 0.5$, $p(p_z) > p_z$ and $p(p_z)$ is increasing with an increasing K.
- When $p_z < 0.5$, $p(p_z) < p_z$ and $p(p_z)$ is decreasing with an increasing K.

B The proof of Lemma 1.

Lemma 3.1 *For the confusion matrix $\mathcal{H}_\gamma$ of an OOD-ENS algorithm, when $0 \leq \rho < 1$ and $3 \leq K \leq n-1$, the expectations of TP_γ and TN_γ monotonically* *increase with an increasing K; the expectations of FP_γ and FN_γ monotonically decrease.*

Proof. For the confusion matrix $\mathcal{H}_\gamma$ of an OOD-ENS algorithm, the expectations of TP_γ, FP_γ, FN_γ and TN_γ are defined as follows.

$$\begin{aligned}\mathbb{E}(\mathrm{TP}_\gamma) &= \mathbb{E}\Big(\sum_{j=1}^{n'} \mathbf{1}\big(p(\hat{g}_{oe}=1) \geq \gamma, g_j=1\big)\Big)\\ &= \sum_{j=1}^{n'} P\big(p(\hat{g}_{oe}=1) \geq \gamma, g_j=1\big)\\ &= \sum_{j=1}^{n'} P(g_j=1)\cdot P\big(p(\hat{g}_{oe}=1) \geq \gamma | g_j=1\big)\end{aligned}$$

$$\begin{aligned}\mathbb{E}(\mathrm{FP}_\gamma) &= \sum_{j=1}^{n'} P(g_j=0)\cdot P\big(p(\hat{g}_{oe}=1) \geq \gamma | g_j=0\big)\\ \mathbb{E}(\mathrm{FN}_\gamma) &= \sum_{j=1}^{n'} P(g_j=1)\cdot P\big(p(\hat{g}_{oe}=0) \geq \gamma | g_j=1\big)\\ \mathbb{E}(\mathrm{TN}_\gamma) &= \sum_{j=1}^{n'} P(g_j=0)\cdot P\big(p(\hat{g}_{oe}=0) \geq \gamma | g_j=0\big),\end{aligned}$$

where $\hat{g}_{oe}$ denotes the majority-voting prediction and g_j denotes a gold label. Without loss of generality, we assume that an algorithm is at least a weak learning algorithm, which indicates $p_z > 0.5$ for the records of $g_j = 1$, and $p_z < 0.5$ for the records of $g_j = 0$, where $p_z = P(\hat{g}_k = 1)$.

According to the Appendix A, when $0 \leq \rho < 1$ and $3 \leq K \leq n-1$, the following analyses can be obtained.

- For TP_γ and TN_γ, we have $P(p(\hat{g}_{oe}=1) \geq \gamma | g_j=1)$ and $P(p(\hat{g}_{oe}=0) \geq \gamma | g_j=0)$ is an increasing function with regard to K.
- For FP_γ and FN_γ, we have $P(p(\hat{g}_{oe}=1) \geq \gamma | g_j=0)$ and $P(p(\hat{g}_{oe}=0) \geq \gamma | g_j=1)$ is a decreasing function with regard to K.

On this basis, the confusion matrix $\mathcal{H}_\gamma$ has the optimal properties that the expectations of TP_γ and TN_γ monotonically increase with an increasing K; the expectations of FP_γ and FN_γ monotonically decrease.

C The proof of Theorem 1

Theorem 3.2 *Under the condition of $0 \leq \rho < 1$ and $3 \leq K \leq n-1$, the expectation of the evaluation measure ACC of an OOD-ENS algorithm increases with an increasing K and owns an upper bound when K equals to $n-1$, while those of estimators α and β decrease and own an lower bound.*

Proof. The expectations of the evaluation measure ACC, the Type I error α and the type II error β of an OOD-ENS algorithm are defined as follows.

$$\mathbb{E}(\mathrm{ACC}) = \mathbb{E}\left(\frac{\mathrm{TP}_\gamma + \mathrm{TN}_\gamma}{n'}\right) = \frac{\mathbb{E}(\mathrm{TP}_\gamma) + \mathbb{E}(\mathrm{TN}_\gamma)}{n'},$$
$$\mathbb{E}(\alpha) = \mathbb{E}\left(\frac{\mathrm{FP}_\gamma}{\mathrm{FP}_\gamma + \mathrm{TN}_\gamma}\right) = \frac{\mathbb{E}(\mathrm{FP}_\gamma)}{\sum_j \mathbf{1}(g_j = 0)},$$
$$\mathbb{E}(\beta) = \mathbb{E}\left(\frac{\mathrm{FN}_\gamma}{\mathrm{FN}_\gamma + \mathrm{TP}_\gamma}\right) = \frac{\mathbb{E}(\mathrm{FN}_\gamma)}{\sum_j \mathbf{1}(g_j = 1)},$$

where $n' = \mathrm{TP}_\gamma + \mathrm{FP}_\gamma + \mathrm{FN}_\gamma + \mathrm{TN}_\gamma$ is a constant and $\mathbf{1}(\cdot)$ is an indicator function.

Under the condition of $0 \leq \rho < 1$ and $3 \leq K \leq n-1$, according to the Lemma 1, the expectations of ACC increases with an increasing K and owns an upper bound when K equals to $n-1$, while those of estimators α and β decrease and own an lower bound.