

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 $k, k' = 1, \dots, K$ 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 $0 < \rho < 1$ 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.

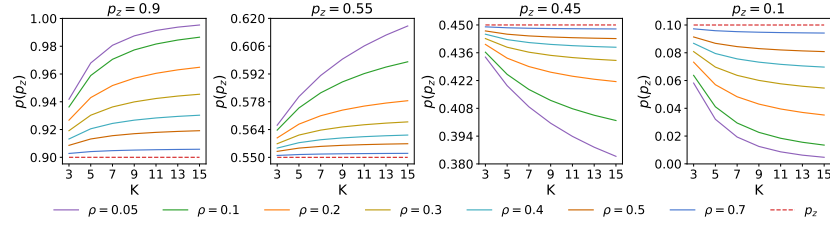


Fig. 1: The relationship of $p(p_z)$ and p_z .

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}_γ of an OOD-ENS algorithm, when $3 \leq K \leq n' - 1$ and $0 < \rho < 1$, 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}_γ of an OOD-ENS algorithm, the expectations of TP_γ , FP_γ , FN_γ and TN_γ are defined as follows.

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

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 $3 \leq K \leq n' - 1$ and $0 < \rho < 1$, 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}_γ 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 $0 < \rho < 1$, 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 a 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.

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

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

Under the condition of $0 < \rho < 1$, 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 a lower bound.