

OODD: Test-time Out-of-Distribution Detection with Dynamic Dictionary

Supplementary Material

A. Experiments

A.1. More Detailed Results

In Table 8, we provide more detailed experimental results on the CIFAR and ImageNet benchmarks across various types of outliers (C-Out, T-Out, D-Out, None).

A.2. Discussion of Computational Cost

In Table 4, we present the computational overhead of our method. Unlike the naive KNN detection, our approach relies solely on dot products after normalization, significantly reducing overhead, especially with parallel computation. This is equivalent to adding a single linear layer, introducing an additional matrix multiplication with complexity $\mathcal{O}(d \cdot l)$ per sample, where d is the feature dimension, and l denotes the priority queue size. Updating the priority queue has a complexity of $\mathcal{O}(\log l)$. Since $l \leq 2048$ in all experiments, the extra overhead when integrating our method with others (e.g., energy-based or maxlogits) remains negligible.

B. Theoretical Analysis

Setup. The decision function for OOD detection using KNN [31] is given by:

$$G(\mathbf{z}^*; k) = \mathbf{1}\{-r_k(\mathbf{z}^*) \geq \lambda\}, \quad (6)$$

where $r_k(\mathbf{z}^*) = \|\mathbf{z}^* - \mathbf{z}_{(k)}\|_2$ represents the Euclidean distance to the k -th nearest neighbor, λ is the threshold and $\mathbf{1}\{\cdot\}$ is the indicator function. According to Bayes' rule, the probability of $\mathbf{z}_i$ being ID data is:

$$\hat{p}(g_i = 1 | \mathbf{z}_i) = \frac{(1 - \varepsilon)\hat{p}_{in}(\mathbf{z}_i)}{(1 - \varepsilon)\hat{p}_{in}(\mathbf{z}_i) + \varepsilon\hat{p}_{out}(\mathbf{z}_i)}. \quad (7)$$

where $p(g_i = 0) = \varepsilon$, and the components are defined as: $\hat{p}_{in}(\mathbf{z}_i) = \frac{k}{c_b n (r_k(\mathbf{z}_i))^{m-1}}$, where c_b is constant, $\hat{p}_{out}(\mathbf{z}_i) = \hat{c}_0 \mathbf{1}\left\{\hat{p}_{in}(\mathbf{z}_i) < \frac{\beta \varepsilon \hat{c}_0}{(1-\beta)(1-\varepsilon)}\right\}$. If the OOD dictionary contains $\tilde{\varepsilon}$ proportion of OOD samples out of l total samples, the calibrated probability functions are defined as: $\tilde{p}_{in}(\mathbf{z}_i) = \hat{p}_{in}(\mathbf{z}_i) - \sigma_{in}\hat{p}_{in}(\mathbf{z}_i)$, $\tilde{p}_{out}(\mathbf{z}_i) = \hat{p}_{out}(\mathbf{z}_i) - \sigma_{out}\hat{p}_{out}(\mathbf{z}_i)$, where $\sigma_{in} = \eta_1(1 - \tilde{\varepsilon})\tilde{p}_{cal}(\mathbf{z}_i)$, $\sigma_{out} = \eta_2\tilde{\varepsilon}\tilde{p}_{cal}(\mathbf{z}_i)$, $\tilde{p}_{cal}(\mathbf{z}_i) = \frac{k}{c_b l (\tilde{r}_k(\mathbf{z}_i))^{m-1}}$, and $\tilde{r}(\mathbf{z}_i)$ is the distance obtained via KNN OOD detection using the OOD dictionary. $\eta_1, \eta_2, \tilde{k}$ are constants, and $\tilde{\varepsilon}$ is bounded by a function related to η_1 and η_2 .

Theorem 1 Given the setup above, if $\hat{p}_{out}(\mathbf{z}_i) = \hat{c}_0 \mathbf{1}\left\{\hat{p}_{in}(\mathbf{z}_i) < \frac{\beta \varepsilon \hat{c}_0}{(1-\beta)(1-\varepsilon)}\right\}$, $\tilde{\varepsilon} > \frac{\eta_1}{\eta_1 + \eta_2}$ and $\lambda = -\frac{m-1}{\sqrt{\frac{(1-\beta)(1-\varepsilon)k}{\beta \varepsilon c_b n \hat{c}_0}}}$, then there exists $\delta > 0$ such that:

$$\mathbf{1}\{-r_k(\mathbf{z}_i) \geq \lambda\} = \mathbf{1}\{\tilde{p}(g_i = 1 | \mathbf{z}_i) \geq \beta + \delta\} \quad (8)$$

Lemma 1 With the setup specified above and the premise of Theorem 1, the decision boundary can be rewritten as:

$$\begin{aligned} \mathbf{1}\{-r_k(\mathbf{z}_i) \geq \lambda\} &= \mathbf{1}\{\hat{p}(g_i = 1 | \mathbf{z}_i) \geq \beta\} \\ &= \mathbf{1}\left\{\frac{k(1 - \varepsilon)}{k(1 - \varepsilon) + \varepsilon c_b n \hat{p}_{out}(\mathbf{z}_i) (r_k(\mathbf{z}_i))^{m-1}} \geq \beta\right\}. \end{aligned} \quad (9)$$

The proof of Lemma 1 is given in [31].

Proof. The calibrated probability of $\mathbf{z}_i$ being ID data is:

$$\begin{aligned} \tilde{p}(g_i = 1 | \mathbf{z}_i) &= \frac{(1 - \varepsilon)\tilde{p}_{in}(\mathbf{z}_i)}{(1 - \varepsilon)\tilde{p}_{in}(\mathbf{z}_i) + \varepsilon\tilde{p}_{out}(\mathbf{z}_i)} \\ &= \frac{(1 - \varepsilon)\hat{p}_{in}(\mathbf{z}_i)}{(1 - \varepsilon)\hat{p}_{in}(\mathbf{z}_i) + \frac{1 - \sigma_{out}}{1 - \sigma_{in}} \varepsilon \hat{p}_{out}(\mathbf{z}_i)}. \end{aligned} \quad (10)$$

Since $\tilde{\varepsilon} > \frac{\eta_1}{\eta_1 + \eta_2}$, using $\frac{1 - \sigma_{out}}{1 - \sigma_{in}} = \frac{1 - \eta_2 \tilde{\varepsilon} \tilde{p}_{cal}}{1 - \eta_1 (1 - \tilde{\varepsilon}) \tilde{p}_{cal}} < \frac{1 - \eta_2 \frac{\eta_1}{\eta_1 + \eta_2} \tilde{p}_{cal}}{1 - \eta_1 (1 - \frac{\eta_1}{\eta_1 + \eta_2}) \tilde{p}_{cal}} = 1$, and combining with Lemma 1, we obtain:

$$\begin{aligned} \tilde{p}(g_i = 1 | \mathbf{z}_i) &> \frac{(1 - \varepsilon)\hat{p}_{in}(\mathbf{z}_i)}{(1 - \varepsilon)\hat{p}_{in}(\mathbf{z}_i) + \varepsilon\hat{p}_{out}(\mathbf{z}_i)} \\ &= \frac{k(1 - \varepsilon)}{k(1 - \varepsilon) + \varepsilon c_b n \hat{p}_{out}(\mathbf{z}_i) (r_k(\mathbf{z}_i))^{m-1}} \geq \beta. \end{aligned} \quad (11)$$

Finally, there exists $\delta > 0$ such that:

$$\mathbf{1}\{-r_k(\mathbf{z}_i) \geq \lambda\} = \mathbf{1}\{\tilde{p}(g_i = 1 | \mathbf{z}_i) \geq \beta + \delta\}$$

