Inference, Fast and Slow: Reinterpreting VAEs for OOD Detection

Anonymous authors
Paper under double-blind review

Abstract

Unsupervised out-of-distribution (OOD) detection is critical for the safe deployment of machine learning systems, yet standard likelihood-based methods using deep generative models (DGMs) often fail, assigning deceptively high likelihoods to anomalous data. We attribute this failure, particularly within Variational Autoencoders (VAEs), to a phenomenon we term ***likelihood cancellation***: informative signals from the model's encoder and decoder can neutralize each other within the final scalar likelihood. To overcome this, we introduce the **Likelihood Path (LPath) Principle**, a new framework that extracts a robust OOD signal from the entire computational path of a VAE. We operationalize this principle by reinterpreting VAEs through the lens of *fast and slow weights*, enabling online, instance-wise inference without costly retraining. Our method extracts minimal sufficient statistics from the VAE's inference path and feeds them into a classical density estimator. On standard benchmarks (CIFAR-10, SVHN, CIFAR-100), our LPath method achieves state-of-the-art OOD detection, outperforming models with over 10x the parameters. Our lightweight 3M-parameter VAE provides a highly efficient and principled solution for real-world, streaming OOD detection.

1 Introduction

The assumption that training and test data are independent and identically distributed (IID) underpins much of machine learning's success. However, in real-world deployments, models inevitably encounter out-of-distribution (OOD) data, which can compromise their reliability and safety (Hendrycks & Gimpel, 2016). This challenge is most acute in unsupervised, streaming settings, where labeled data is absent and decisions must be made on-the-fly for each incoming sample. The goal of unsupervised OOD detection is to learn a scoring function from in-distribution (ID) data that can reliably identify anomalous inputs at test time.

A theoretically elegant approach is to use the likelihood $p_\theta(\mathbf{x})$ assigned by a deep generative model (DGM). Intuitively, ID samples should have high likelihood, while OOD samples should have low likelihood. Yet, this intuition famously fails in practice: high-capacity DGMs frequently assign higher likelihoods to OOD samples than to ID samples (Nalisnick et al., 2018; Choi et al., 2018). This paradox has been explored extensively, with studies showing that even perfect density models can be poor OOD indicators (Le Lan & Dinh, 2021; Zhang et al., 2021) and that perfect estimation is often infeasible for modern DGMs (Behrmann et al., 2021; Dai & Wipf, 2019). This leads to our first research question:

Research Question 1: Why does the likelihood score, a cornerstone of statistical modeling, systematically fail for OOD detection in high-capacity deep generative models?

We posit that this failure is particularly revealing in latent variable models like Variational Autoencoders (VAEs). Here, we identify a key culprit: the **Semantic-Texture Likelihood Cancellation Trap**. In a VAE, the final likelihood score is a marginalization of the product of components. For an OOD sample, the decoder might find the low-level texture easy to reconstruct (high conditional likelihood), while the encoder maps it to a semantically meaningless, low-probability latent code. These opposing signals can *cancel each*

other out, yielding a benign final likelihood that masks the anomaly. This insight motivates our second research question:

Research Question 2: Can we extract a more robust OOD signal from the *computational path* of a generative model, rather than from its final scalar output?

To answer this, we propose the **Likelihood Path (LPath) Principle**. It asserts that the intermediate statistics forming the computational path to the likelihood contain more robust information than the final score. We operationalize this principle by extracting the *minimal sufficient statistics* of a VAE's core components. This choice is fundamental to our method's success. Being *sufficient*, these statistics optimally preserve the information from the encoder and decoder distributions. Being *minimal*, they form a low-dimensional representation that is robust to the curse of dimensionality—a key advantage explaining why our method outperforms much larger models. By capturing these statistics *before* they are multiplied into a single likelihood score, our approach directly sidesteps the cancellation trap.

Our light-weight inference approach is particularly suitable for streaming settings, since the minimal sufficient statistics can be reinterpreted through the lens of *fast and slow weights* (Hinton & Plaut, 1987; Ba et al., 2016). The model's trained parameters (θ, ϕ) are the *slow weights*, learned offline. For each test sample $\mathbf{x}$, the VAE's encoder computes instance-dependent posterior parameters, which we view as *fast weights*. This enables efficient online inference without the retraining required by methods like Likelihood Regret (Xiao et al., 2020).

Our LPath algorithm is a two-stage process. We first uses the VAE for fast neural feature extraction of the minimal sufficient statistics, and then feeds them into a classical density estimator (e.g., COPOD (Li et al., 2020)) to generate the final OOD score.

This approach achieves state-of-the-art (SOTA) OOD detection performance on CIFAR-10, CIFAR-100, and SVHN benchmarks. Crucially, we achieve these results using a lightweight DC-VAE architecture (Xiao et al., 2020) with only **3M** parameters, a fraction of the **44M** for Glow-based DoSE (Morningstar et al., 2021) or **46M** for diffusion models (Liu et al., 2023). This remarkable efficiency makes our method ideal for low-latency, streaming applications.

Our contributions are threefold:

1. **Methodological:** We propose the **LPath Principle**, a novel framework for OOD detection that generalizes the classical likelihood principle by leveraging minimal sufficient statistics from the model's computational path to overcome likelihood cancellation.
2. **Practical:** We introduce a highly efficient OOD detection algorithm based on a fast-and-slow-weight reinterpretation of VAEs, enabling SOTA performance in streaming settings with a lightweight (3M parameter) model.
3. **Empirical:** We demonstrate SOTA performance on challenging OOD detection benchmarks, validating that our principled approach of "achieving more with less" is both effective and efficient.

2 Related Work

Our work is situated at the junction of likelihood-based OOD detection, its documented failures, and the subsequent paradigm shift towards probing internal model computations for more robust signals.

Likelihood-Based OOD Detection. The use of likelihood scores from DGMs like normalizing flows (Kingma & Dhariwal, 2018) and VAEs (Kingma & Welling, 2013) is a natural starting point. However, the seminal work of Nalisnick et al. (2018) demonstrated their surprising failure. Subsequent works have shown that even with perfect density models, likelihood may be a poor OOD indicator due to geometric factors and mismatched support (Le Lan & Dinh, 2021; Zhang et al., 2021), and that perfect estimation itself is often infeasible (Behrmann et al., 2021). Likelihood Regret (Xiao et al., 2020) attempted to salvage the likelihood by fine-tuning on test samples and measuring the change in likelihood, but this is computationally prohibitive for streaming applications. Our method avoids this by leveraging "fast weights."

Probing Internal Model Computations for OOD Signals. The failure of the marginal likelihood score catalyzed a shift in focus from a model's final output to its internal computational process. This has led to a diverse set of methods that extract OOD signals from deeper within the network. One successful branch of research sources signals from pre-trained *discriminative* models, such as using the Mahalanobis distance in a classifier's feature space (Lee et al., 2018). Another branch, more closely related to our work, probes the internal workings of *generative* models. This includes re-interpreting model outputs as unnormalized energy scores (Liu et al., 2020) or extracting various statistics from the DGM's computational graph, such as Jacobian norms or entropy terms (Morningstar et al., 2021; Graham et al., 2023). While effective, the selection of these statistics is often heuristic. The LPath principle provides a *principled* foundation for this process, grounding the choice of statistics in the classical principles of likelihood and sufficiency.

Theoretical Foundations. Our work is grounded in classical statistical theory, specifically the Likelihood Principle (Berger & Wolpert, 1988) and the Sufficiency Principle (Wasserman, 2006; Cvitkovic & Koliander, 2019). We extend these ideas to the context of imperfect deep generative models. Our reinterpretation of VAEs also draws inspiration from the concept of **fast and slow weights**, which has roots in meta-learning (Hinton & Plaut, 1987; Ba et al., 2016) and has recently been connected to attention mechanisms in Transformers (Schlag et al., 2021; Ha et al., 2022).

3 The Likelihood Path Method

Our method is built on a reinterpretation of VAEs through the lens of fast and slow weights, guided by our LPath Principle. To build the foundation for our approach, we first clarify the crucial distinction between using a model for static evaluation versus online inference, as this dichotomy is central to understanding both the limitations of prior work and the advantages of our method.

3.1 A Tale of Two Inferences: Evaluation vs. Online Adaptation

In the context of OOD detection, a trained deep generative model can be used in two fundamentally different ways at test time.

Evaluation Procedure (Static Scoring). The most common approach is a static *evaluation procedure*. Given a new sample $\mathbf{x}$ and a model with pre-trained parameters ψ_{trained}, we compute a scalar score, typically the log-likelihood:

$$(\mathbf{x}, \psi_{\text{trained}}) \longrightarrow p_{\psi_{\text{trained}}}(\mathbf{x}) \in \mathbb{R}. \tag{1}$$

Here, the model parameters ψ_{trained} are fixed. As discussed, this approach often fails because the scalar score can be misleading due to the likelihood cancellation trap.

Inferential Procedure (Online Adaptation). A more sophisticated approach is to perform an *inferential procedure* for each new test sample. In statistics, inference typically refers to estimating model parameters from data. In the context of OOD detection, this means updating the model parameters based on a new test sample $\mathbf{x}_{\text{test}}$:

$$(\mathbf{x}_{\text{test}}, \psi_{\text{trained}}) \longrightarrow \psi_{\text{online}} \in \Psi. \tag{2}$$

The likelihood differences resulted from changes in parameters, $|p_{\psi_{\text{online}}} - p_{\psi_{\text{trained}}}|$, can serve as an OOD score. This is precisely the strategy employed by Likelihood Regret (Xiao et al., 2020), where ψ_{trained} represents the VAE's network weights (the *slow weights*). While principled, this approach is computationally prohibitive for streaming applications, as it requires retraining by backpropagation for every single sample.

Our work carves out a third path. We perform an online inferential procedure not on the slow network weights, but on a set of instance-dependent *fast weights*. As we will show, VAEs are particularly suited for this, allowing us to gain the benefits of an inferential approach without the crippling computational cost of retraining.

3.2 VAEs as a Vehicle for Fast-Weight Inference

Variational Autoencoders (Kingma & Welling, 2013) are latent variable models that provide the ideal structure for our method. A VAE is defined by a decoder $p_\theta(\mathbf{x}|\mathbf{z})$ and an encoder $q_\phi(\mathbf{z}|\mathbf{x})$. The marginal likelihood $p_\theta(\mathbf{x})$ is approximated using the encoder as an importance sampler:

$$\log p_\theta(\mathbf{x}) \approx \frac{1}{N}\sum_{i=1}^{N}[\log p_\theta(\mathbf{x}|\mathbf{z}_i) + \log p(\mathbf{z}_i) - \log q_\phi(\mathbf{z}_i|\mathbf{x})], \quad \text{where} \quad \mathbf{z}_i \sim q_\phi(\mathbf{z}|\mathbf{x}). \tag{3}$$

This decomposition is the source of the likelihood cancellation trap. The reconstruction term ($\log p_\theta(\mathbf{x}|\mathbf{z})$) and the regularization terms ($\log p(\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})$) can contain conflicting OOD signals that are neutralized when summed. Our goal is to intercept the information from these components *before* they are combined.

Gaussian VAEs and Their Minimal Sufficient Statistics. A key to our approach lies in using Gaussian VAEs. Here, the prior, encoder, and decoder are all Gaussian distributions:

$$p(\mathbf{z}) = \mathcal{N}(\mathbf{z} \mid \mathbf{0}, \mathbf{I}), \tag{4}$$

$$q_\phi(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mathbf{z} \mid \boldsymbol{\mu}_z(\mathbf{x};\phi), \mathrm{diag}(\boldsymbol{\sigma}_z^2(\mathbf{x};\phi))), \tag{5}$$

$$p_\theta(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}_x(\mathbf{z};\theta), \mathrm{diag}(\boldsymbol{\sigma}_x^2(\mathbf{z};\theta))). \tag{6}$$

The parameters of these distributions—the means and variances—are not just arbitrary values; they are the **minimal sufficient statistics** for their respective Gaussian distributions. This property is fundamental to our method's effectiveness:

- **Sufficient:** They capture all the necessary information to define the encoder and decoder distributions for a given sample. Nothing is lost.
- **Minimal:** They represent this information in the most compact form possible. This low dimensionality makes them robust to the curse of dimensionality, enabling a small model to outperform larger ones that use less-principled features.

Reinterpreting VAE Inference: Fast and Slow Weights. We can now connect this back to our fast-and-slow-weight framework. The network weights ϕ and θ are the **slow weights**, learned offline. For any new sample $\mathbf{x}_{\text{test}}$, the encoder network performs a rapid, feed-forward pass to compute the parameters of the posterior:

$$(\mathbf{x}_{\text{test}}, \phi_{\text{trained}}) \longrightarrow (\boldsymbol{\mu}_z(\mathbf{x}_{\text{test}}), \boldsymbol{\sigma}_z(\mathbf{x}_{\text{test}}), \boldsymbol{\mu}_x(\mathbf{z}_{\text{test}}), \boldsymbol{\sigma}_x(\mathbf{z}_{\text{test}})). \tag{7}$$

These instance-dependent parameters are the **fast weights** we seek. They are the output of a cheap online *inferential* procedure. Because they are also the minimal sufficient statistics, they are the ideal candidates for an OOD signal that is both highly informative and compact, directly addressing the likelihood cancellation trap.

3.3 OOD Detection with VAE Fast Weights

Having established that VAEs provide a mechanism for efficient online inference via fast weights, which are also the minimal sufficient statistics of the model's core components, we now detail how we leverage this for OOD detection. Our goal is to design a scoring function that is effective (by intercepting information before it is lost to the cancellation trap), principled (by using minimal sufficient statistics), and efficient (by relying only on fast weights).

3.3.1 From Likelihood Components to Their Sufficient Statistics

Recall the finite sample approximation of the VAE log-likelihood from Equation (3):

$$\log p_\theta(\mathbf{x}) \approx \frac{1}{N}\sum_{i=1}^{N}[\underbrace{\log p_\theta(\mathbf{x}|\mathbf{z}_i)}_{\text{Decoder Term}} + \underbrace{\log p(\mathbf{z}_i)}_{\text{Prior Term}} - \underbrace{\log q_\phi(\mathbf{z}_i|\mathbf{x})}_{\text{Encoder Term}}]$$

The primary likelihood cancellation trap occurs when these three terms are summed. However, a more subtle cancellation can occur even *within* each term. For a multivariate Gaussian distribution with mean $\boldsymbol{\mu}$ and covariance $\boldsymbol{\Sigma}$, the log-likelihood of a sample $\mathbf{y}$ is:

$$\log \mathcal{N}(\mathbf{y} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = -\frac{1}{2}\left((\mathbf{y}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{y}-\boldsymbol{\mu}) + \log|\boldsymbol{\Sigma}| + k\log(2\pi)\right). \tag{8}$$

Consider the Mahalanobis distance term, $(\mathbf{y}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{y}-\boldsymbol{\mu})$. This single scalar value conflates two distinct sources of information: the magnitude of the residual error $(\mathbf{y}-\boldsymbol{\mu})$ and the model's uncertainty about that residual, encoded in $\boldsymbol{\Sigma}$. An OOD sample might produce a large residual but also high uncertainty, while an ID sample might have a small residual and low uncertainty. The final Mahalanobis distance could be similar in both cases, masking the underlying difference. Information about the absolute scale of the error and the uncertainty is lost. This information lost can be summarized as "cancellation behind cancellation".

Therefore, to create a maximally informative OOD score, we propose to bypass the computation of the log-likelihood value entirely. Instead of using the scalar outputs of the likelihood components, we directly use their underlying parameters—the minimal sufficient statistics $(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ that are computed as fast weights.

3.3.2 The LPath Statistics: Principled Features from Likelihood Components

The full set of fast weights—the vectors $(\boldsymbol{\mu}_z(\mathbf{x}), \boldsymbol{\sigma}_z(\mathbf{x}))$ from the encoder and $(\boldsymbol{\mu}_x(\mathbf{z}), \boldsymbol{\sigma}_x(\mathbf{z}))$ from the decoder—are minimal sufficient statistics, but they remain high-dimensional. A direct approach might be to use them directly, but this would be computationally intensive and susceptible to the curse of dimensionality in the second stage of our algorithm (Maciejewski et al., 2022).

Our key insight is that we do not need to summarize these vectors in an ad-hoc way. Instead, we can extract their fundamental properties that *directly determine* the value of the component likelihoods. Recall the log-likelihood of a multivariate Gaussian from Equation (8):

$$\log \mathcal{N}(\mathbf{y} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = -\frac{1}{2}\left(\underbrace{(\mathbf{y}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{y}-\boldsymbol{\mu})}_{\text{Mahalanobis Distance}} + \underbrace{\log|\boldsymbol{\Sigma}|}_{\text{Log-Determinant}} + k\log(2\pi)\right).$$

The two data-dependent terms are completely determined by the geometry of the residual vector $(\mathbf{y}-\boldsymbol{\mu})$ and the uncertainty vector(s) in $\boldsymbol{\Sigma}$. For the diagonal covariance matrices used in our VAE, these terms are functions of the L2 norms of the residual and the standard deviations. By extracting these norms directly, we are capturing the fundamental "ingredients" of the component likelihoods *before* they are combined and information is lost.

This principled choice leads to our four LPath statistics. We apply this logic to both the encoder and decoder components of the VAE, yielding a practical, low-dimensional, and maximally informative feature vector $T(\mathbf{x}) = [u(\mathbf{x}), v(\mathbf{x}), w(\mathbf{x}), s(\mathbf{x})]^T$, where:

$$u(\mathbf{x}) = \|\mathbf{x} - \boldsymbol{\mu}_x(\boldsymbol{\mu}_z(\mathbf{x}))\|_2 \qquad \text{(Reconstruction Error Norm)} \tag{9}$$

$$v(\mathbf{x}) = \|\boldsymbol{\mu}_z(\mathbf{x})\|_2 \qquad \text{(Latent Mean Norm)} \tag{10}$$

$$w(\mathbf{x}) = \|\boldsymbol{\sigma}_z(\mathbf{x})\|_2 \qquad \text{(Latent Std Dev Norm)} \tag{11}$$

$$s(\mathbf{x}) = \|\boldsymbol{\sigma}_x(\boldsymbol{\mu}_z(\mathbf{x}))\|_2 \qquad \text{(Reconstruction Std Dev Norm)} \tag{12}$$

Each statistic is not only a building block of a likelihood term but is also directly interpretable in the context of the VAE's training objective. For an in-distribution (ID) sample, we expect:

- A small reconstruction error norm $u(\mathbf{x})$, as the model should reconstruct ID data well. We use the error norm rather than the norm of the reconstruction itself, $\|\boldsymbol{\mu}_x(\dots)\|_2$, to create a naturally centered statistic.
- A small latent mean norm $v(\mathbf{x})$, as the KL-divergence term in the VAE loss regularizes the posterior mean towards the prior mean of zero.

Algorithm 1 The LPath Algorithm for OOD Detection

Input: Training data $\mathcal{D}_{\text{ID}}$, test data $\mathcal{D}_{\text{Test}}$, classical OOD algorithm $\mathcal{A}_{\text{classical}}$.

Stage 1: Neural Feature Extraction (Offline Training)
Train VAE(s) on $\mathcal{D}_{\text{ID}}$ using a standard VAE loss.
Initialize feature set $\mathcal{T}_{\text{ID}} \leftarrow \emptyset$.
for each sample $\mathbf{x} \in \mathcal{D}_{\text{ID}}$ **do**
    Compute LPath statistics $T(\mathbf{x}) = (u(\mathbf{x}), v(\mathbf{x}), w(\mathbf{x}), s(\mathbf{x}))$ using Equations (9) to (12).
    Add the 4-dim vector $T(\mathbf{x})$ to $\mathcal{T}_{\text{ID}}$.
end for

Stage 2: Classical Density Estimation (Offline Training)
Train $\mathcal{A}_{\text{classical}}$ on the low-dimensional feature set $\mathcal{T}_{\text{ID}}$ to get a trained detector $\mathcal{A}_{\text{trained}}$. ▷ e.g., Estimate copulas for COPOD or mean/covariance for MD.

Inference (Online and Fast)
for each sample $\mathbf{x}_{\text{test}} \in \mathcal{D}_{\text{Test}}$ **do**
    Compute statistics $T_{\text{test}} = (u(\mathbf{x}_{\text{test}}), v(\mathbf{x}_{\text{test}}), w(\mathbf{x}_{\text{test}}), s(\mathbf{x}_{\text{test}}))$ via a single forward pass.
    Compute OOD score $S(\mathbf{x}_{\text{test}}) = \mathcal{A}_{\text{trained}}(T_{\text{test}})$.
end for
Output: OOD scores S for all samples in $\mathcal{D}_{\text{Test}}$.

- A latent standard deviation norm $w(\mathbf{x})$ close to a constant determined by the latent dimension, as the KL loss regularizes the posterior variance towards the prior's identity covariance.
- A small reconstruction standard deviation norm $s(\mathbf{x})$, reflecting the model's high confidence in its reconstruction of familiar ID data (Dai & Wipf, 2019).

Deviations from these expected values provide a strong, multi-faceted signal for OOD detection. This 4-dimensional feature vector, derived directly from the determinants of the likelihood components, forms the core of our LPath algorithm.

3.3.3 The Two-Stage LPath Algorithm

Our method combines deep representation learning with classical statistics in a two-stage process, as detailed in Algorithm 1. In the first stage, we use a trained VAE for neural feature extraction, computing the 4-dimensional LPath statistics for each data point. In the second stage, we use these low-dimensional features to train a classical, non-parametric OOD detection algorithm like COPOD (Li et al., 2020) or a simple Mahalanobis distance (MD) detector.

We propose two practical variants of this algorithm:

- **LPath-1M:** Uses a single VAE to extract all four statistics. This is the simplest and most efficient variant.
- **LPath-2M:** Uses two VAEs to resolve the inherent trade-off between encoder expressivity (which prefers a high-dimensional latent space) and decoder sensitivity (which prefers a low-dimensional one). We use a high-dimensional VAE for encoder statistics (v, w) and a low-dimensional VAE for decoder statistics (u, s). A detailed rationale is provided in Appendix B.

This two-stage design effectively leverages the strengths of both deep learning (for powerful, automatic feature extraction) and classical statistics (for robust, low-dimensional density estimation). In the next section, we will formalize the theoretical underpinnings of this approach with the Likelihood Path Principle.

4 The Likelihood Path Principle

In the previous section, we detailed *what* our method does: it extracts a set of four statistics derived from the fast weights of a VAE and uses them for OOD detection. In this section, we explain *why* this is the right approach. We formalize the intuition that the computational path to the likelihood contains more information than the final score by introducing the **Likelihood Path (LPath) Principle**. This principle generalizes classical statistical ideas to the setting of modern, high-capacity, and imperfectly trained deep generative models.

4.1 Foundations: The Classical Likelihood and Sufficiency Principles

To understand our contribution, we first revisit two cornerstones of classical statistical inference.

The Likelihood Principle. A central tenet of statistical inference is the *Likelihood Principle* (Berger & Wolpert, 1988). It states that all the evidence in an observed sample $\mathbf{x}$ relevant to the model parameters ψ is contained entirely within the likelihood function, $\ell(\psi|\mathbf{x}) \equiv p(\mathbf{x}|\psi)$. The standard practice of training generative models via Maximum Likelihood Estimation (MLE) directly adheres to this principle, as the choice of optimal parameters ψ_{MLE} depends only on this function. Many likelihood-based OOD detection methods (Nalisnick et al., 2018; Xiao et al., 2020) implicitly follow this principle by using the final likelihood score, which is a functional of $\ell(\psi|\mathbf{x})$, as their OOD signal.

The Sufficiency Principle. While the likelihood function contains all the information, it is often a complex, high-dimensional object. The *Sufficiency Principle* provides a formal way to compress this information without loss. A statistic $T(\mathbf{x})$ is called a *sufficient statistic* for ψ if the conditional distribution of the data given the statistic, $p(\mathbf{x}|T(\mathbf{x}), \psi)$, does not depend on ψ. In other words, once $T(\mathbf{x})$ known, the original data $\mathbf{x}$ provides no further information about the parameters ψ. A sufficient statistic is *minimal* if it is the most compressed representation possible without losing information (Cvitkovic & Koliander, 2019). Minimal sufficient statistics provide the ideal trade-off: they are maximally informative yet minimally complex, helping to avoid the curse of dimensionality that plagues methods using less-principled, high-dimensional features.

4.2 An Information-Theoretic View of the Likelihood Path

These classical principles provide a powerful lens. Figure 1 illustrates this classical view, showing a sequence of steps where information about the data is progressively compressed, from the raw data $\mathbf{x}$ to the likelihood function and finally to a sufficient statistic $T(\mathbf{x})$. To formalize this notion of information reduction and apply it to our VAE context, we turn to information theory. The relationship between data, statistics, and parameters can be quantified using mutual information, $\mathrm{I}(\cdot, \cdot)$. A statistic $T(\mathbf{x})$ is sufficient for parameters ψ if and only if it preserves all the mutual information between the data and the parameters: $\mathrm{I}(\psi; T(\mathbf{x})) = \mathrm{I}(\psi; \mathbf{x})$.

The abstract information pathway in Figure 1 finds a concrete analogue in the computational process of a VAE. Recall the VAE likelihood calculation:

$$p_\theta(\mathbf{x}) = \int_{\mathbf{z}\sim P(\mathbf{z})} p_\theta(\mathbf{x} \mid \mathbf{z}) p(\mathbf{z})\, \mathrm{d}\mathbf{z} = \int_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})} \frac{p_\theta(\mathbf{x} \mid \mathbf{z}) p(\mathbf{z})}{q_\phi(\mathbf{z} \mid \mathbf{x})}\, \mathrm{d}\mathbf{z}, \tag{13}$$

For any given sample $\mathbf{x}$ and any latent variable $\mathbf{z}$, the VAE likelihood computation process can be viewed as an integral of Markov chain of information processing:

$$\mathbf{x} \longrightarrow \underbrace{\{(\boldsymbol{\mu}_z(\mathbf{x}), \boldsymbol{\sigma}_z(\mathbf{x})), (\boldsymbol{\mu}_x(\mathbf{z}), \boldsymbol{\sigma}_x(\mathbf{z}))\}}_{\text{Minimal Sufficient Statistics (Fast Weights)}} \longrightarrow \underbrace{\{q_\phi(\mathbf{z}|\mathbf{x}), p_\theta(\mathbf{x}|\mathbf{z}), p(\mathbf{z})\}}_{\text{Component Distributions}} \longrightarrow \underbrace{p_\theta(\mathbf{x})}_{\text{Final Likelihood Score}} \tag{14}$$

where $\mathbf{z} \sim q_\phi(\mathbf{z}|\mathbf{x})$. The above naturally admits the following sampling version, where we sample N latent codes:

$$\mathbf{x} \longrightarrow \underbrace{\{(\boldsymbol{\mu}_z(\mathbf{x}), \boldsymbol{\sigma}_z(\mathbf{x})), (\boldsymbol{\mu}_x(\mathbf{z}_i), \boldsymbol{\sigma}_x(\mathbf{z}_i))\}_{i=1}^N}_{\text{Sampling Minimal Sufficient Statistics}} \longrightarrow \underbrace{\{q_\phi(\mathbf{z}_i|\mathbf{x}), p_\theta(\mathbf{x}|\mathbf{z}_i), p(\mathbf{z}_i)\}_{i=1}^N}_{\text{Component Sampling Distributions}} \longrightarrow \underbrace{p_\theta(\mathbf{x})}_{\text{Estimated Likelihood}} \tag{15}$$

The sampling version is rigorously a Markov chain of information processing. Let's denote the minimal sufficient statistics as $\mathcal{T}(\mathbf{x}) = \{(\boldsymbol{\mu}_z(\mathbf{x}), \boldsymbol{\sigma}_z(\mathbf{x})), (\boldsymbol{\mu}_x(\mathbf{z}), \boldsymbol{\sigma}_x(\mathbf{z}))\}$ and the set of component sampling distributions as $\mathcal{P}(\mathbf{x})$. By the Data Processing Inequality, any processing step cannot increase information. This gives us a chain of inequalities that mirrors the information reduction shown in Figure 1:

$$\mathrm{I}(\mathbf{x}; \mathcal{T}(\mathbf{x})) \geq \mathrm{I}(\mathbf{x}; \mathcal{P}(\mathbf{x})) \geq \mathrm{I}(\mathbf{x}; p_\theta(\mathbf{x})). \tag{16}$$

Let's analyze these inequalities.

1. $\mathrm{I}(\mathbf{x}; \mathcal{T}(\mathbf{x})) \geq \mathrm{I}(\mathbf{x}; \mathcal{P}(\mathbf{x}))$: Since the component distributions $\mathcal{P}(\mathbf{x})$ are completely determined by the minimal sufficient statistics $\mathcal{T}(\mathbf{x})$, no information is lost in this step. Therefore, $\mathrm{I}(\mathbf{x}; \mathcal{T}(\mathbf{x})) = \mathrm{I}(\mathbf{x}; \mathcal{P}(\mathbf{x}))$. The fast weights contain exactly as much information as the full distributions they parameterize.

2. $\mathrm{I}(\mathbf{x}; \mathcal{P}(\mathbf{x})) \geq \mathrm{I}(\mathbf{x}; p_\theta(\mathbf{x}))$: This is the crucial step. The final likelihood $p_\theta(\mathbf{x})$ is computed by integrating/multiplying the component distributions in $\mathcal{P}(\mathbf{x})$. If the model were a perfect representation of the data generating process, this step might also preserve information. However, for a real-world, imperfectly trained DGM, this is where the **likelihood cancellation** occurs. As opposing signals from the encoder and decoder are combined, information about the anomaly is irreversibly destroyed.

This leads to the central theoretical claim of our work: under imperfect density estimation, the second inequality becomes strict:

$$\mathrm{I}(\mathbf{x}; \mathcal{P}(\mathbf{x})) > \mathrm{I}(\mathbf{x}; p_\theta(\mathbf{x})). \tag{17}$$

The core of our method is to exploit this information gap. By extracting statistics from the components *before* they are combined, we access a richer, more reliable source of information for OOD detection.

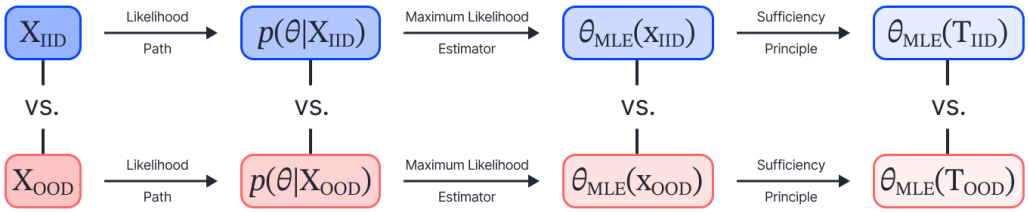


Figure 1: A conceptual diagram of the classical statistical inference pipeline, contrasting the paths for in-distribution ($\mathbf{x}_{\mathrm{ID}}$, top) and out-of-distribution ($\mathbf{x}_{\mathrm{OOD}}$, bottom) data. The diagram illustrates the progressive information reduction from left to right by applying the Likelihood Principle (LP), Maximum Likelihood Estimation (MLE), and the Sufficiency Principle (SP). T denotes the sufficient statistic. The LPath method is inspired by analyzing the differences between these two paths.

4.3 The LPath Principle as a Generalization

This analysis allows us to formally define our principle.

Definition 4.1 (The Likelihood Path (LPath) Principle)**.** For a latent variable model under imperfect density estimation, the minimal sufficient statistics of the likelihood's factorization components contain strictly more information about the input data for OOD detection than the final scalar marginal likelihood, which is subject to information loss via cancellation.

The LPath Principle is a natural generalization of the classical Likelihood Principle for the modern era of deep generative models. The likelihood principle assumes a perfect, well-specified model and suggests using the likelihood function. Our principle acknowledges the reality of imperfect models and suggests using the more informative building blocks of that likelihood function. The path of minimal sufficient statistics, $\mathcal{T}(\mathbf{x})$, is the optimal compromise: it is maximally informative about the components of the likelihood, minimally complex, and avoids the information destruction of the final integration step. This is why our method, which is based on simple L2 norms of these statistics, can be so effective.

4.4 The Mechanism of Likelihood Cancellation

While Section 4 provides a **statistical** view on information loss, a **combinatorial** perspective offers a more concrete mechanism: **arithmetic cancellation**. In a VAE, the final likelihood score is a product of components that can carry opposing signals for OOD detection. An anomalous signal from one component can be neutralized by a benign signal from another, masking the OOD nature of the input.

This phenomenon is rooted in the VAE's approximate log-likelihood, $\log p_\theta(\mathbf{x}) \approx \log p_\theta(\mathbf{x} \mid \mathbf{z}) + \log p(\mathbf{z}) - \log q_\phi(\mathbf{z} \mid \mathbf{x})$. We can interpret this cancellation through the lens of a texture-semantic conflict:

- The **decoder's conditional likelihood**, $p_\theta(\mathbf{x} \mid \mathbf{z})$, often focuses on reconstructing low-level **pixel textures**.
- The **prior evaluated at the latent code**, $p(\mathbf{z})$ for $\mathbf{z} \sim q_\phi(\mathbf{z} \mid \mathbf{x})$, captures higher-level **semantics**.

This is the **Semantic-Texture Likelihood Cancellation Trap** mentioned in Section 1, leading to two common failure modes. First, consider an OOD sample that is semantically different but has familiar textures (e.g., an image of a dog with the texture of cat fur). The decoder may reconstruct it well (high $p_\theta(\mathbf{x} \mid \mathbf{z})$), while the encoder maps it to an unlikely, semantically incorrect latent code (low $p(\mathbf{z})$). As noted by Havtorn et al. (2021), the final likelihood is often dominated by low-level texture information, so the strong reconstruction signal can overwhelm the weak semantic signal. Conversely, consider an OOD sample with unfamiliar textures, leading to a large reconstruction error (low $p_\theta(\mathbf{x} \mid \mathbf{z})$). This provides a strong OOD signal. However, if the sample happens to map to a region of unusually high prior density, this can partially offset the low reconstruction likelihood, making the sample appear less anomalous than it is.

We conceptualize these different interactions as distinct **likelihood paths**, which are illustrated conceptually in Figure 2. This cancellation effect is not merely theoretical; it is directly observable in the data. Figure 3 provides a striking empirical demonstration. The distributions of the individual LPath statistics—the reconstruction error in Figure 3(b) and the latent norm in Figure 3(a)—show a relatively clear separation between the ID (CIFAR-10) and OOD (SVHN) data. However, when these signals are combined into the final ELBO score, shown in Figure 3(c), the separation is visibly diminished. The distinct OOD signals have been diluted.

This observation is quantified in our experimental analysis in Section 5.3, where we map the four conceptual cases from Figure 2 to these component behaviors and show that the ELBO's performance degrades significantly in precisely the scenarios where cancellation is expected (Table 2). The LPath method is designed to circumvent this problem by capturing the rich, multi-faceted information from the component statistics *before* they are collapsed into a single, less informative score.

5 Experiments

We conduct a series of experiments to validate the LPath method. First, we compare its OOD detection performance against state-of-the-art methods on standard benchmarks. Second, we perform a targeted analysis to empirically demonstrate the likelihood cancellation phenomenon and show how the LPath statistics overcome it.

5.1 Experimental Setup

Baselines and Setting. We compare our LPath method with a suite of state-of-the-art OOD detection methods, including those based on likelihood-regret (LR), hierarchical VAEs (BIVA), normalizing flows (DoSE), diffusion models (DDPM), and other feature-based approaches (Xiao et al., 2020; Havtorn et al., 2021; Morningstar et al., 2021; Bergamin et al., 2022; Liu et al., 2023; Graham et al., 2023). All experiments are conducted under a challenging and realistic setting: unsupervised, single-sample, and without any inductive bias about the nature of the OOD data.

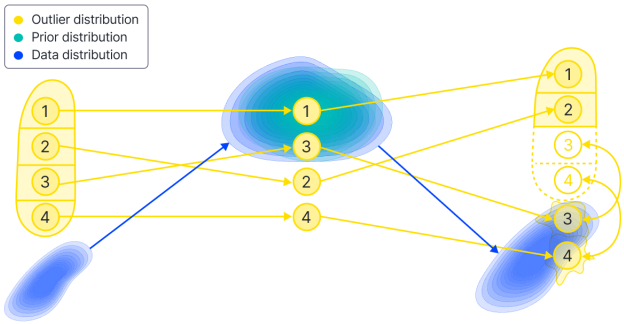
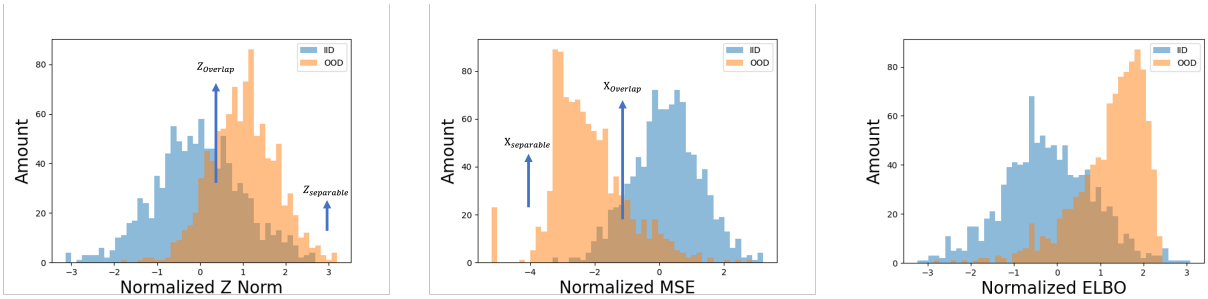


Figure 2: **Conceptual illustration of different likelihood paths.** This figure traces in-distribution ($\mathbf{x}_{\text{ID}}$, blue) and out-of-distribution ($\mathbf{x}_{\text{OOD}}$, yellow) data through a VAE's computational path: from the input space (left), through the latent space (middle), to the reconstruction space (right). We identify four distinct cases for OOD data based on their interaction with the prior (turquoise) and their final reconstruction quality. Cases (1) and (2) are well-reconstructed, while Cases (3) and (4) are poorly reconstructed (visualized as 'fried egg' shapes), revealing a strong OOD signal from the decoder. The grey areas highlight *atypical sets* (Nalisnick et al., 2019)—pathological regions of high density but low volume that can mislead likelihood-based OOD detectors.



(a) (b) (c)

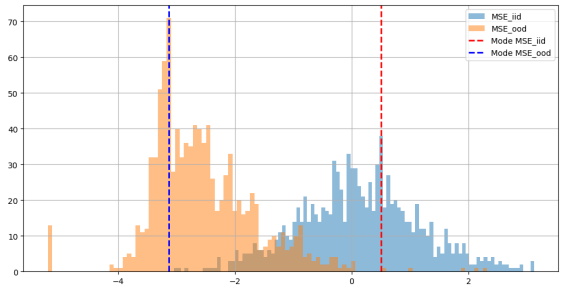
Figure 3: Histograms demonstrating the **likelihood cancellation effect** on a VAE with a 100-dimensional latent space, trained on CIFAR-10 (ID) vs. SVHN (OOD). The plots show distributions for three components of the VAE log-likelihood from Equation (3): (a) the latent code norm, $\|\mathbf{z}\|_2$, related to the prior term; (b) the reconstruction error (MSE), $\|\mathbf{x} - \hat{\mathbf{x}}\|_2$, related to the decoder's conditional likelihood; and (c) the final ELBO score. The four conceptual cases from Figure 2 map to combinations of separability in these components: Case (1) is $Z_{\text{overlap}} + X_{\text{overlap}}$; Case (2) is $Z_{\text{separable}} + X_{\text{overlap}}$; Case (3) is $Z_{\text{overlap}} + X_{\text{separable}}$; and Case (4) is $Z_{\text{separable}} + X_{\text{separable}}$. Note that the separation between ID and OOD data is much clearer in the individual components (a, b) than in the final ELBO (c), illustrating how information is lost. All values are normalized; see Appendix D for details.

Datasets and Metrics. Following convention, we use several common image benchmarks. We evaluate performance using CIFAR-10, SVHN, MNIST, and FashionMNIST (FMNIST) as in-distribution (ID) datasets. For OOD data, we use these datasets against each other, as well as CIFAR-100 and synthetically challenging variants like horizontally-flipped (Hflip) and vertically-flipped (Vflip) images. Performance is measured using the Area Under the Receiver Operating Characteristic curve (AUROC). Further details on the VAE architecture and training are in Appendix D.

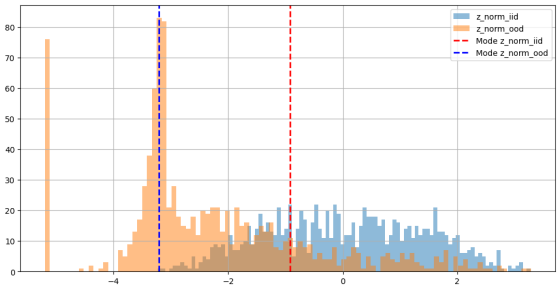
5.2 Main Results: State-of-the-Art OOD Detection

SOTA Performance with a Lightweight Model. As shown in Table 1, our LPath method (in both its 1-Model and 2-Model variants) achieves state-of-the-art or competitive performance across all benchmark settings. The method excels on difficult pairs like CIFAR-10 vs. SVHN and demonstrates strong performance on the subtle Hflip/Vflip tasks, where many prior methods perform near chance. This is particularly

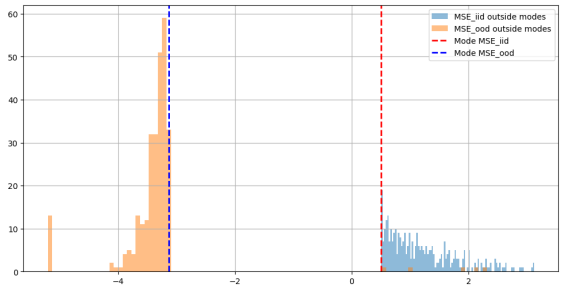
Figure 4: **Visualization of the data partitioning method for the four-case analysis.** This figure illustrates how we define the 'separable' and 'overlap' regions for the experiment in Section 5.3. The partitioning is based on the modes (dashed vertical lines) of the in-distribution (ID, blue) and out-of-distribution (OOD, orange) data for the reconstruction error ($u(\mathbf{x})$) and latent norm ($v(\mathbf{x})$). **Top Row (a, b):** The original, full distributions of the two statistics. **Middle Row (c, d):** The 'separable' regions, containing data points that fall outside the modes of the opposing distribution. **Bottom Row (e, f):** The 'overlap' regions, containing data points that fall between the two modes. This partitioning creates the four scenarios analyzed in Table 2.



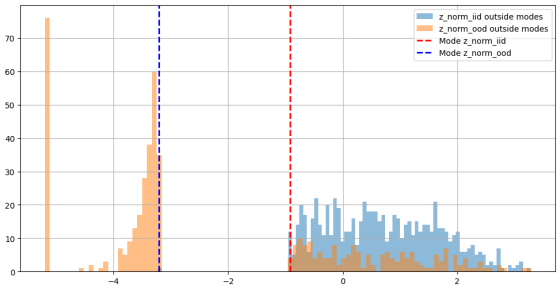
(a) Histogram of $u(\mathbf{x})$ (MSE)



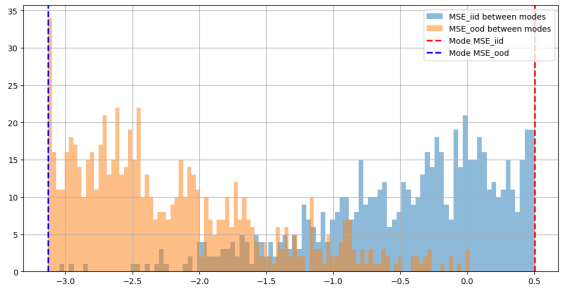
(b) Histogram of $v(\mathbf{x})$ (z_norm)



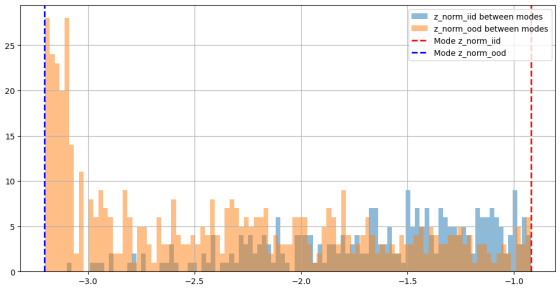
(c) $\mathbf{x}_{\text{separable}}$: Outside regions of $u(\mathbf{x})$



(d) $\mathbf{z}_{\text{separable}}$: Outside regions of $v(\mathbf{x})$



(e) $\mathbf{x}_{\text{overlap}}$: Overlap region of $u(\mathbf{x})$



(f) $\mathbf{z}_{\text{overlap}}$: Overlap region of $v(\mathbf{x})$

noteworthy because these flipped datasets differ from the ID data by only one latent dimension, making them a stringent test of a method's sensitivity.

Achieving More with Less. This improvement is particularly significant given that we use a very small VAE architecture. Compared to other SOTA methods, our approach relies on a much smaller model (a DC-VAE from Xiao et al. (2020)'s architecture) with a parameter count of only **3M**. This is a fraction of the **44M** parameters required for the Glow model (Kingma & Dhariwal, 2018) used in DoSE (Morningstar et al., 2021) or the **46M** parameters for the diffusion model used in recent work (Rombach et al., 2022; Liu et al., 2023). Our method clearly exceeds other VAE-based approaches (Xiao et al., 2020; Havtorn et al., 2021) and is the only one that is competitive with these much larger models.

Table 1: **Our LPath method achieves state-of-the-art OOD detection performance while using a fraction of the model parameters.** This table presents the Area Under the Receiver Operating Characteristic curve (AUROC) for various methods on common OOD detection benchmarks. The highest score in each column is bolded. Our methods are presented in three variants: 'LPath-1M' uses a single VAE, while 'LPath-2M' uses a pair of VAEs with different latent dimensions (see Appendix D). 'COPOD' and 'MD' refer to the classical density estimator used in the second stage of our algorithm. Notably, our lightweight VAE-based approach consistently matches or exceeds the performance of much larger models like DoSE (Glow-based) and DDPM, highlighting the effectiveness of our principled feature selection.

ID	**CIFAR10**				**SVHN**			**FMNIST**			**MNIST**		
OOD	**SVHN**	**CIFAR100**	**Hflip**	**Vflip**	**CIAFR10**	**Hflip**	**Vflip**	**MNIST**	**Hflip**	**Vflip**	**FMNIST**	**Hflip**	**Vflip**
ELBO	0.08	0.54	0.5	0.56	**0.99**	0.5	0.5	0.87	0.63	0.83	**1.00**	0.59	0.6
LR (Xiao et al., 2020)	0.88	N/A	N/A	N/A	0.92	N/A	N/A	0.99	N/A	N/A	N/A	N/A	N/A
BIVA (Havtorn et al., 2021)	0.89	N/A	N/A	N/A	**0.99**	N/A	N/A	0.98	N/A	N/A	**1.00**	N/A	N/A
DoSE (Morningstar et al., 2021)	0.97	0.57	0.51	0.53	**0.99**	0.52	0.51	**1.00**	0.66	0.75	**1.00**	**0.81**	0.83
Fisher (Bergamin et al., 2022)	0.87	0.59	N/A	N/A	N/A	N/A	N/A	0.96	N/A	N/A	N/A	N/A	N/A
DDPM (Liu et al., 2023)	0.98	N/A	0.51	0.63	**0.99**	**0.62**	**0.58**	0.97	0.65	**0.89**	N/A	N/A	N/A
LMD (Graham et al., 2023)	**0.99**	0.61	N/A	N/A	0.91	N/A	N/A	0.99	N/A	N/A	**1.00**	N/A	N/A
LPath-1M-COPOD (Ours)	**0.99**	**0.62**	**0.53**	0.61	**0.99**	0.55	0.56	**1.00**	0.65	0.81	**1.00**	0.65	**0.87**
LPath-2M-COPOD (Ours)	0.98	**0.62**	**0.53**	**0.65**	0.96	0.56	0.55	0.95	**0.67**	0.87	**1.00**	0.77	0.78
LPath-1M-MD (Ours)	**0.99**	0.58	0.52	0.60	0.95	0.52	0.52	0.97	0.63	0.82	**1.00**	0.75	0.76

Table 2: **LPath method excels across all OOD scenarios, especially in the most difficult case.** This table shows the OOD detection performance (AUROC) of different statistics across the four conceptual cases defined in Section 4.4. The cases range from most difficult (Case 1, where ID/OOD distributions overlap in both reconstruction and latent spaces) to easiest (Case 4, where they are separable). The LPath method ("Ours") consistently outperforms the individual component statistics ($u(\mathbf{x})$, $v(\mathbf{x})$) and the final ELBO score, demonstrating its ability to overcome the likelihood cancellation that degrades ELBO's performance in Case 1.

Statistic Used for OOD Detection	**Case 1**	**Case 2**	**Case 3**	**Case 4**
Latent Norm ($v(\mathbf{x})$)	0.75	0.74	0.93	0.96
Reconstruction Error ($u(\mathbf{x})$)	0.93	0.98	1.00	0.98
ELBO (Final Likelihood Score)	0.83	0.87	1.00	0.96
LPath Statistics (Ours)	**0.99**	**0.99**	**1.00**	**0.99**

The comparison with DoSE is especially revealing. The authors of DoSE reported results using a VAE for simpler datasets like MNIST/FMNIST but switched to the larger Glow model for more complex datasets like CIFAR-10 and SVHN. This suggests that their heuristically chosen statistics were not sufficiently powerful to achieve SOTA performance on a VAE with challenging data. In contrast, our LPath method, guided by the principled selection of minimal sufficient statistics, surpasses their Glow-based results using our lightweight VAE. While Glow's likelihood estimation is arguably superior to our small VAE's, and DoSE's chosen statistics are sophisticated, our simpler and more principled method proves more effective and vastly more efficient. This showcases that the power of the LPath method lies not in model scale, but in its information-theoretic foundation. This answers RQ2.

5.3 Analysis: Overcoming Likelihood Cancellation

To empirically validate our central claim that the final likelihood score suffers from information loss, we conduct an experiment based on the four conceptual OOD cases illustrated in Figure 2.

Experimental Design. We partition the OOD data (SVHN) into four cases based on whether their LPath statistics fall into regions of high overlap with the ID data (CIFAR-10). We define "overlap" and "separable"

regions based on the distributions of the reconstruction error ($u(\mathbf{x})$) and the latent norm ($v(\mathbf{x})$), as visualized in Figure 4. This creates four scenarios of increasing difficulty:

- **Case 1 (Hardest):** Overlap in both reconstruction and latent spaces ($X_{\text{overlap}} + Z_{\text{overlap}}$).
- **Case 2:** Separable in latent space, overlap in reconstruction ($X_{\text{overlap}} + Z_{\text{separable}}$).
- **Case 3:** Overlap in latent space, separable in reconstruction ($X_{\text{separable}} + Z_{\text{overlap}}$).
- **Case 4 (Easiest):** Separable in both spaces ($X_{\text{separable}} + Z_{\text{separable}}$).

Results. The results, shown in Table 2, provide clear evidence for likelihood cancellation. In the most challenging scenario, **Case 1**, the individual statistics $u(\mathbf{x})$ (AUROC 0.93) and $v(\mathbf{x})$ (AUROC 0.75) both contain a useful OOD signal. However, the final ELBO score, which combines them, sees its performance degraded to 0.83—worse than the reconstruction error alone. This is a direct demonstration of the arithmetic cancellation discussed in Section 4.4. In contrast, our LPath method, which combines the statistics in a principled manner, achieves a near-perfect AUROC of 0.99. This confirms that the LPath method successfully integrates the information from the full computational path, avoiding the information loss that plagues the final likelihood score. This answers RQ1.

6 Conclusion

This work confronts a fundamental paradox in unsupervised OOD detection: the systematic failure of likelihood scores from powerful deep generative models. We identified a key mechanism for this failure in VAEs, a phenomenon we term **likelihood cancellation**, where informative OOD signals from the encoder and decoder neutralize each other in the final scalar likelihood.

To overcome this, we introduced the **Likelihood Path (LPath) Principle**, a new framework that moves beyond the final likelihood score to extract a richer signal from the model's entire computational path. We provided a multi-faceted analysis of this principle, grounding it in the statistical theories of likelihood and sufficiency, reinterpreting VAE inference through the neural lens of fast and slow weights, and demonstrating the cancellation effect from a combinatorial perspective.

Our resulting LPath method is not only principled but also remarkably effective and efficient. On standard benchmarks, our approach achieves state-of-the-art results, outperforming methods that rely on models over ten times larger. By using a lightweight 3M-parameter VAE, we validate our core thesis of "achieving more with less," offering a practical solution for real-world, streaming OOD detection where efficiency is paramount.

The LPath Principle offers a new perspective on OOD detection in generative models. Future work will involve extending this principled framework beyond VAEs to more powerful DGMs, such as normalizing flows and diffusion models, to explore its full potential as a general tool for building more reliable and robust machine learning systems.

References

Jimmy Ba, Geoffrey E Hinton, Volodymyr Mnih, Joel Z Leibo, and Catalin Ionescu. Using fast weights to attend to the recent past. *Advances in neural information processing systems*, 29, 2016.

Dara Bahri, Heinrich Jiang, Yi Tay, and Donald Metzler. Label smoothed embedding hypothesis for out-of-distribution detection, 2021.

Jens Behrmann, Paul Vicol, Kuan-Chieh Wang, Roger Grosse, and Jörn-Henrik Jacobsen. Understanding and mitigating exploding inverses in invertible neural networks. In *International Conference on Artificial Intelligence and Statistics*, pp. 1792–1800. PMLR, 2021.

Federico Bergamin, Pierre-Alexandre Mattei, Jakob Drachmann Havtorn, Hugo Senetaire, Hugo Schmutz, Lars Maaløe, Soren Hauberg, and Jes Frellsen. Model-agnostic out-of-distribution detection using combined statistical tests. In *International Conference on Artificial Intelligence and Statistics*, pp. 10753–10776. PMLR, 2022.

James O Berger and Robert L Wolpert. The likelihood principle. IMS, 1988.

Hyunsun Choi, Eric Jang, and Alexander A Alemi. Waic, but why? generative ensembles for robust anomaly detection. *arXiv preprint arXiv:1810.01392*, 2018.

Milan Cvitkovic and Günther Koliander. Minimal achievable sufficient statistic learning. In *International Conference on Machine Learning*, pp. 1465–1474. PMLR, 2019.

Bin Dai and David Wipf. Diagnosing and enhancing vae models. *arXiv preprint arXiv:1903.05789*, 2019.

Bin Dai, Li Kevin Wenliang, and David Wipf. On the value of infinite gradients in variational autoencoder models. In *Advances in Neural Information Processing Systems*.

Nicholas Frosst, Nicolas Papernot, and Geoffrey Hinton. Analyzing and improving representations with the soft nearest neighbor loss, 2019.

Mark S Graham, Walter HL Pinaya, Petru-Daniel Tudosiu, Parashkev Nachev, Sebastien Ourselin, and Jorge Cardoso. Denoising diffusion models for out-of-distribution detection. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 2947–2956, 2023.

Arthur Gretton, Karsten M Borgwardt, Malte J Rasch, Bernhard Schölkopf, and Alexander Smola. A kernel two-sample test. *The Journal of Machine Learning Research*, 13(1):723–773, 2012.

Théo Guénais, Dimitris Vamvourellis, Yaniv Yacoby, Finale Doshi-Velez, and Weiwei Pan. Bacoun: Bayesian classifers with out-of-distribution uncertainty. *arXiv preprint arXiv:2007.06096*, 2020.

David Ha, Andrew M Dai, and Quoc V Le. Hypernetworks. In *International Conference on Learning Representations*, 2022.

Jakob D Drachmann Havtorn, Jes Frellsen, Soren Hauberg, and Lars Maaløe. Hierarchical vaes know what they don't know. In *International Conference on Machine Learning*, pp. 4117–4128. PMLR, 2021.

Dan Hendrycks and Kevin Gimpel. A baseline for detecting misclassified and out-of-distribution examples in neural networks. *arXiv preprint arXiv:1610.02136*, 2016.

Geoffrey E Hinton and David C Plaut. Using fast weights to deblur old memories. In *Proceedings of the ninth annual conference of the Cognitive Science Society*, pp. 177–186, 1987.

Agnan Kessy, Alex Lewin, and Korbinian Strimmer. Optimal whitening and decorrelation. *The American Statistician*, 72(4):309–314, 2018.

Diederik P Kingma and Max Welling. Auto-encoding variational bayes. *arXiv preprint arXiv:1312.6114*, 2013.

Durk P Kingma and Prafulla Dhariwal. Glow: Generative flow with invertible 1x1 convolutions. *Advances in neural information processing systems*, 31, 2018.

Balaji Lakshminarayanan, Alexander Pritzel, and Charles Blundell. Simple and scalable predictive uncertainty estimation using deep ensembles. *arXiv preprint arXiv:1612.01474*, 2016.

Charline Le Lan and Laurent Dinh. Perfect density models cannot guarantee anomaly detection. *Entropy*, 23 (12):1690, 2021.

Kimin Lee, Kibok Lee, Honglak Lee, and Jinwoo Shin. A simple unified framework for detecting out-of-distribution samples and adversarial attacks. *Advances in neural information processing systems*, 31, 2018.

Zheng Li, Yue Zhao, Nicola Botta, Cezar Ionescu, and Xiyang Hu. Copod: copula-based outlier detection. In *2020 IEEE International Conference on Data Mining (ICDM)*, pp. 1118–1123. IEEE, 2020.

Weitang Liu, Xiaoyun Wang, John Owens, and Yixuan Li. Energy-based out-of-distribution detection. *Advances in Neural Information Processing Systems*, 33, 2020.

Zhenzhen Liu, Jin Peng Zhou, Yufan Wang, and Kilian Q Weinberger. Unsupervised out-of-distribution detection with diffusion inpainting. *arXiv preprint arXiv:2302.10326*, 2023.

Henryk Maciejewski, Tomasz Walkowiak, and Kamil Szyc. Out-of-distribution detection in high-dimensional data using mahalanobis distance-critical analysis. In *Computational Science–ICCS 2022: 22nd International Conference, London, UK, June 21–23, 2022, Proceedings, Part I*, pp. 262–275. Springer, 2022.

Warren Morningstar, Cusuh Ham, Andrew Gallagher, Balaji Lakshminarayanan, Alex Alemi, and Joshua Dillon. Density of states estimation for out of distribution detection. In *International Conference on Artificial Intelligence and Statistics*, pp. 3232–3240. PMLR, 2021.

Eric Nalisnick, Akihiro Matsukawa, Yee Whye Teh, Dilan Gorur, and Balaji Lakshminarayanan. Do deep generative models know what they don't know? *arXiv preprint arXiv:1810.09136*, 2018.

Eric Nalisnick, Akihiro Matsukawa, Yee Whye Teh, and Balaji Lakshminarayanan. Detecting out-of-distribution inputs to deep generative models using typicality. *arXiv preprint arXiv:1906.02994*, 2019.

Kazuki Osawa, Siddharth Swaroop, Anirudh Jain, Runa Eschenhagen, Richard E Turner, Rio Yokota, and Mohammad Emtiyaz Khan. Practical deep learning with bayesian principles. *arXiv preprint arXiv:1906.02506*, 2019.

Nicolas Papernot and Patrick McDaniel. Deep k-nearest neighbors: Towards confident, interpretable and robust deep learning, 2018.

Tim Pearce, Felix Leibfried, and Alexandra Brintrup. Uncertainty in neural networks: Approximately bayesian ensembling. In *International conference on artificial intelligence and statistics*, pp. 234–244. PMLR, 2020.

Jie Ren, Peter J Liu, Emily Fertig, Jasper Snoek, Ryan Poplin, Mark Depristo, Joshua Dillon, and Balaji Lakshminarayanan. Likelihood ratios for out-of-distribution detection. In *Advances in Neural Information Processing Systems*, pp. 14707–14718, 2019.

Robin Rombach, Andreas Blattmann, Dominik Lorenz, Patrick Esser, and Björn Ommer. High-resolution image synthesis with latent diffusion models. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, pp. 10684–10695, 2022.

Chandramouli Shama Sastry and Sageev Oore. Detecting out-of-distribution examples with Gram matrices. In Hal Daumé III and Aarti Singh (eds.), *Proceedings of the 37th International Conference on Machine Learning*, volume 119 of *Proceedings of Machine Learning Research*, pp. 8491–8501. PMLR, 13–18 Jul 2020.

Imanol Schlag, Kazuki Irie, and Jürgen Schmidhuber. Linear transformers are secretly fast weight programmers. In *International Conference on Machine Learning*, pp. 9355–9366. PMLR, 2021.

Joan Serrà, David Álvarez, Vicenç Gómez, Olga Slizovskaia, José F Núñez, and Jordi Luque. Input complexity and out-of-distribution detection with likelihood-based generative models. In *International Conference on Learning Representations*, 2019.

Larry Wasserman. *All of nonparametric statistics*. Springer Science & Business Media, 2006.

Zhisheng Xiao, Qing Yan, and Yali Amit. Likelihood regret: An out-of-distribution detection score for variational auto-encoder. *Advances in neural information processing systems*, 33:20685–20696, 2020.

Lily Zhang, Mark Goldstein, and Rajesh Ranganath. Understanding Failures in Out-of-Distribution Detection with Deep Generative Models. In *Proceedings of the 38th International Conference on Machine Learning*, pp. 12427–12436. PMLR, July 2021. URL `https://proceedings.mlr.press/v139/zhang21g.html`. ISSN: 2640-3498.

A More Related Works

Prior works have approached OOD detection from various perspectives and with different data assumptions, e.g., with or without access to training labels, batches of test data, or single test data points in a streaming fashion, and with or without knowledge and inductive bias of the data. In the following, we give an overview organized by different data assumptions with a focus on where our method fits.

The first assumption is whether the method has access to training labels. There has been extensive work on classifier-based methods that assume access to training labels (Hendrycks & Gimpel, 2016; Frosst et al., 2019; Sastry & Oore, 2020; Bahri et al., 2021; Papernot & McDaniel, 2018; Osawa et al., 2019; Guénais et al., 2020; Lakshminarayanan et al., 2016; Pearce et al., 2020). Within this category, there are different assumptions as well, such as access to a pretrained network or knowledge of OOD test examples. See Table 1 of Sastry & Oore (2020) for a summary of such methods.

When we do not assume access to the training labels, the problem becomes more general and also harder. Under this category, some methods assume access to a batch of test data where either all the data points are OOD or not (Nalisnick et al., 2019). A more general setting does not assume OOD data would come in batches. Under this setup, there are methods that implicitly assume prior knowledge of the data, such as the input complexity method (Serrà et al., 2019), where the use of image compressors implicitly assumes an image-like structure, or the likelihood ratio method (Ren et al., 2019), where a noisy background model is trained with the assumption of a background-object structure.

B Overcoming the Latent Dimensionality Trade-off

The ‘LPath-2M‘ variant of our method is designed to resolve a fundamental trade-off inherent in using a single VAE for OOD detection. This section details this trade-off and explains how our two-model approach provides an effective solution.

The Inherent Trade-off of a Single VAE. When using a single VAE, the choice of the latent dimension creates a conflict between the needs of the encoder and the decoder for effective OOD detection:

- **A Higher Latent Dimension Benefits the Encoder (q_ϕ):** A large latent space provides the encoder with more capacity to capture complex features. This allows it to map in-distribution (ID) and OOD data to more distinct, separable regions, improving the discriminative power of statistics derived from the latent code (e.g., $v(\mathbf{x})$ and $w(\mathbf{x})$).
- **A Lower Latent Dimension Benefits the Decoder (p_θ):** A small, bottlenecked latent space constrains the decoder's ability to generalize. It learns to reconstruct ID data well but struggles to accurately reconstruct unfamiliar OOD samples. This constraint is beneficial for OOD detection, as it leads to larger, more easily detectable reconstruction errors (i.e., a stronger signal from $u(\mathbf{x})$).

This trade-off means that any single choice of latent dimension is a compromise. Optimizing for the encoder's discriminative power (with a high dimension) weakens the decoder's reconstruction-based OOD signal, and vice-versa.

The Two-Model Solution. To overcome this trade-off, the ‘LPath-2M‘ method uses two specialized VAEs in parallel:

1. **A High-Dimensional VAE:** This model has an overparameterized (large) latent dimension, optimized for the encoder. It excels at capturing complex features and producing informative latent statistics ($v(\mathbf{x})$ and $w(\mathbf{x})$) that effectively discriminate between ID and OOD data.
2. **A Low-Dimensional VAE:** This model has an underparameterized (small) latent dimension, optimized for the decoder. Its constrained nature amplifies reconstruction errors for OOD samples, providing a strong OOD signal via the decoder-based statistics ($u(\mathbf{x})$ and $s(\mathbf{x})$).

By combining the complementary strengths of these two models, we can leverage the best of both worlds without being limited by the conflicting requirements of a single architecture.

Implementation and Empirical Validation. In practice, we implement the 'LPath-2M' method by extracting the LPath statistics from their respective specialist models:

- **From the High-Dimensional VAE**, we extract the encoder-based statistics:

$$v(\mathbf{x}) = \|\boldsymbol{\mu}_{\mathbf{z}}(\mathbf{x})\|_2, \tag{18}$$
$$w(\mathbf{x}) = \|\boldsymbol{\sigma}_{\mathbf{z}}(\mathbf{x})\|_2. \tag{19}$$

- **From the Low-Dimensional VAE**, we extract the decoder-based statistics:

$$u(\mathbf{x}) = \|\mathbf{x} - \widehat{\mathbf{x}}\|_2, \tag{20}$$
$$s(\mathbf{x}) = \|\boldsymbol{\sigma}_{\mathbf{x}}(\boldsymbol{\mu}_{\mathbf{z}}(\mathbf{x}))\|_2. \tag{21}$$

This integrated feature set provides a comprehensive signal for OOD detection. As shown in our main results (Table 1), this two-model approach yields state-of-the-art performance on challenging OOD scenarios (e.g., CIFAR-10 vs. VFlip). This is achieved even though each VAE, considered individually, has potential limitations (e.g., the high-dimensional VAE may overfit, while the low-dimensional one may underfit). By combining their complementary strengths, the 'LPath-2M' method demonstrates that it can be more effective to use two specialized, simple models than a single, compromised one, achieving one plus one greater than two.

C Sufficient Statistics and Where to Find Them

Though in the case of the Guassian parameterized VAE decoder and encoder, it is easy to find the corresponding minimal sufficient statistics, the same might not be true for more complicated distributions. Here we briefly overview the Fisher-Neyman factorization perspective on the sufficiency principle which can help find sufficient statistics in more complicated distributions. A sufficiency statistics is also characterized by Fisher-Neyman factorization theorem (Wasserman, 2006): $T(\mathbf{x})$ is a sufficient statistics for $p(\mathbf{x}|\psi)$ parameterized by ψ if and only if:

$$\ell(\psi|\mathbf{x}) = p(\mathbf{x}|\psi) = f(\mathbf{x})g_\psi(T(\mathbf{x})) \tag{22}$$

i.e. the density $p(\mathbf{x}|\psi)$ can be factored into a product such that f, does not depend on ψ and g that does depend on ψ *but who depends on* $\mathbf{x}$ *only through* $T(\mathbf{x})$. For example, if we perform inference by maximum likelihood:

$$\psi_{\text{MLE}} = \arg\max_\psi \ell(\psi|\mathbf{x}) = \arg\max_\psi f(\mathbf{x})g_\psi(T(\mathbf{x})) = \arg\max_\psi g_\psi(T) \tag{23}$$

T is sufficient for MLE procedure, because ψ_{MLE} only requires T.

The *sufficiency principle* states that, if $T(\mathbf{x})$ is a sufficient statistic for the likelihood function $p(\psi|\mathbf{x})$, then any inference about ψ should depend on $T(\mathbf{x})$ only.

D Experimental Details

D.1 VAE Architecture and Training

For the architecture and the training of our VAEs, we followed Xiao et al. (2020). In addition, we have trained VAEs of varying latent dimensions, {1, 2, 5, 10, 100, 1000, 2000, 3096, 5000, 10000}, and instead of training for 200 epochs and taking the resulting model checkpoint, we took the checkpoint that had the best validation loss. For LPath-1M, we conducted experiments on VAEs with all latent dimensions and for

LPath-2M, we paired one high-dimensional VAE from the group {3096, 5000, 10000} and one low-dimensional VAE from the group {1, 2, 5}.

In addition to Gaussian VAEs as mentioned in Section D.1, we also empirically experimented with a categorical decoder, in the sense the decoder output is between the discrete pixel ranges, as in Xiao et al. (2020). Strictly speaking, this no longer satisfies the Gaussian distribution anymore, which may in turn violate our sufficient statistics perspective. However, we still experimented with it to test whether LPath principles can be interpreted as a heuristic to inspire methods that approximate sufficient statistics that can work reasonably well, and we observed that categorical decoders work similarly with Guassian decoders.

Constant Decoder Covariance In typical VAE learning, the decoder's variance is fixed Dai et al., so it cannot be used as an inferential parameter. We initially treated the decoder as an isotropic Gaussian with a learnable scalar covariance matrix $\sigma_{\mathbf{x}}(\mathbf{z})^2 I$, where I is the identity matrix and $\sigma_{\mathbf{x}}(\mathbf{z})^2$ is a learnable scalar. We later observed that the scalar $\sigma_{\mathbf{x}}(\mathbf{z})$ always converge to a small value and remains fixed for any ID or OOD data. And given that in typical VAE learning, the decoder's variance is fixed Dai et al.. We decided to use a fixed scalar as well and exclude this term from our algorithm.

This reduces the minimal sufficient statistics for encoder and decoder pair:

$$(\mu_{\mathbf{z}}(\mathbf{x}), \sigma_{\mathbf{z}}(\mathbf{x}), \mu_{\mathbf{x}}(\mathbf{z}), \sigma_{\mathbf{x}}(\mathbf{z})) \longrightarrow (\mu_{\mathbf{z}}(\mathbf{x}), \sigma_{\mathbf{z}}(\mathbf{x}), \mu_{\mathbf{x}}(\mathbf{z})) \tag{24}$$

D.2 Feature Processing To Boost COPOD Performances

Like most statistical algorithms, COPOD/MD is not scale invariant, and may prefer more dependency structures closer to the linear ones. When we plot the distributions of $u(\mathbf{x})$ and $v(\mathbf{x})$, we find that they exhibit extreme skewness. To make COPOD's statistical estimation easier, we process them by quantile transform. That is, for ID data, we map the the tuple of statistics' marginal distributions to $\mathcal{N}(0, 1)$. To ease the low dimensional empirical copula, we also de-correlate the joint distribution of $(u(\mathbf{x}), v(\mathbf{x})), w(\mathbf{x}))$. We do so using Kessy et al. (2018)'s de-correlation method, similar to Morningstar et al. (2021).

D.3 Width and Height of a Vector Instead of Its l^2 Norm To Extract Complementary Information

In our visual inspection, we find that the distribution of the scalar components of $(u(\mathbf{x}), v(\mathbf{x}), w(\mathbf{x}))$ can be rather uneven. For example, the visible space reconstruction $\mathbf{x} - \widehat{\mathbf{x}}$ error can be mostly low for many pixels, but very high at certain locations. These information can be washed away by the l^2 norm. Instead, we propose to track both l^p norm and l^q norm for small p and large q.

For small p, l^p measures the width of a vector, while l^q measures the height of a vector for big q. To get a sense of how they capture complementary information, we can borrow intuition from $l^p \approx l^0$, for small p and $l^q \approx l^\infty$, for large q. $\|\mathbf{x}\|_0$ counts the number of nonzero entries, while $\|\mathbf{x}\|_\infty$ measures the height of $\mathbf{x}$. For $\mathbf{x}$ with continuous values, however, l^0 norm is not useful because it always returns the dimension of $\mathbf{x}$, while l^∞ norm just measures the maximum component.

Extreme measures help screen extreme data. We therefore use l^p norm and l^q norm as a continuous relaxation to capture this idea: l^p norm will "count" the number of components in $\mathbf{x}$ that are unusually small, and l^q norm "measures" the average height of the few biggest components. These can be more discriminitive against OOD than l^2 norm alone, due to the extreme (proxy for OOD) conditions they measure. We observe some minor improvements, detailed in Table 3's ablation study.

ID: CIFAR10	OOD			
OOD Dataset	SVHN	CIFAR100	Hflip	Vflip
l^2 norm	0.96	0.60	**0.53**	**0.61**
(l^p, l^q)	**0.99**	**0.62**	**0.53**	**0.61**

Table 3: Comparing the AUC of l^2 norm versus our (l^p, l^q) measures.

D.4 (Attempted) Training Objective Modification for Stronger Concentration

Inspired by the well known concentration of Gaussian probability measures, to encourage stronger concentration of the latent code around the spherical shell with radius $\sqrt{m}$ for better OOD detection, we propose the following modifications to standard VAEs' loss functions:

We replace the initial KL divergence by:

$$\mathcal{D}^{\text{typical}}[Q_\phi(\mathbf{z} \mid \mu_{\mathbf{z}}(\mathbf{x}), \sigma(\mathbf{x}))\|P(\mathbf{z})] \tag{25}$$

$$=\mathcal{D}^{\text{typical}}[\mathcal{N}(\mu_{\mathbf{z}}(\mathbf{x}), \sigma_{\mathbf{z}}(\mathbf{x}))\|\mathcal{N}(0, I)] \tag{26}$$

$$=\frac{1}{2}\left(\text{tr}(\sigma_{\mathbf{z}}(\mathbf{x})) + |(\mu_{\mathbf{z}}(\mathbf{x}))^\top(\mu_{\mathbf{z}}(\mathbf{x})) - m| - m - \log\det(\sigma_{\mathbf{z}}(\mathbf{x}))\right) \tag{27}$$

where m is the latent dimension.

In training, we also use Maximum Mean Discrepancy (MMD) Gretton et al. (2012) as a discriminator since we are not dealing with complex distribution but Gaussian. The MMD is computed with Gaussian kernel. This extra modification is because the above magnitude regularization does not take distribution in to account.

The final objective:

$$\mathbb{E}_{\mathbf{x}\sim P_{\text{ID}}}\mathbb{E}_{\mathbf{z}\sim Q_\phi}\mathbb{E}_{\mathbf{n}\sim\mathcal{N}}[\log P_\theta(\mathbf{x} \mid \mathbf{z})] - \mathcal{D}^{\text{typical}}[Q_\phi(\mathbf{z} \mid \mu_{\mathbf{z}}(\mathbf{x}), \sigma(\mathbf{x}))\|P(\mathbf{z})] - \text{MMD}(\mathbf{n}, \mu_{\mathbf{z}}(\mathbf{x})) \tag{28}$$

The idea is that for P_{ID}, we encourage the latent codes to concentrate around the prior's *typical sets*. That way, P_{OOD} may deviate further from P_{ID} in a controllable manner. In experiments, we tried the combinations of the metric regularizer, $\mathcal{D}^{\text{typical}}$, and the distribution regularizer, MMD. This leads to two other objectives:

$$\mathbb{E}_{\mathbf{x}\sim P_{\text{ID}}}\mathbb{E}_{\mathbf{z}\sim Q_\phi}[\log P_\theta(\mathbf{x} \mid \mathbf{z})] - \mathcal{D}^{\text{typical}}[Q_\phi(\mathbf{z} \mid \mu_{\mathbf{z}}(\mathbf{x}), \sigma(\mathbf{x}))\|P(\mathbf{z})] \tag{29}$$

$$\mathbb{E}_{\mathbf{x}\sim P_{\text{ID}}}\mathbb{E}_{\mathbf{z}\sim Q_\phi}\mathbb{E}_{\mathbf{n}\sim\mathcal{N}}[\log P_\theta(\mathbf{x} \mid \mathbf{z})] - \mathcal{D}[Q_\phi(\mathbf{z} \mid \mu_{\mathbf{z}}(\mathbf{x}), \sigma(\mathbf{x}))\|P(\mathbf{z})] - \text{MMD}(\mathbf{n}, \mu_{\mathbf{z}}(\mathbf{x})) \tag{30}$$

where $\mathcal{D}$ is the standard KL divergence.

But we **did not** observe a significant difference in the final AUROC different variations. We still include those attempted modifications for future work.

E Ablation Studies

E.1 Individual statistics

To empirically validate how $(u(\mathbf{x}), v(\mathbf{x}), w(\mathbf{x}))$ complement each other, we use individual component alone in first stage and fit the second stage COPOD as usual. We notice signigicant drops in performances. We fit COPOD on individual statistics $u(\mathbf{x})$, $v(\mathbf{x})$, $w(\mathbf{x})$ and show the results in Table 4. We can see that our original combination in Table 1 is better overall.

E.2 MD

To test the efficacy of $(u(\mathbf{x}), v(\mathbf{x}), w(\mathbf{x}))$ without COPOD, we replace COPOD by a popular algorithm in OOD detection, the MD algorithm Lee et al. (2018) and report such scores in Table 1. The scores are comparable to COPOD, suggesting $(u(\mathbf{x}), v(\mathbf{x}), w(\mathbf{x}))$ is the primary contributor to our performances.

E.3 Latent dimensions

One hypothesis on the relationship between latent code dimension and OOD detection performance is that lowering dimension incentivizes high level semantics learning, and higher level feature learning can help discriminate OOD v.s. ID. We conducted experiments on the below latent dimensions and report their AUC based on $v(\mathbf{x})$ (norm of the latent code) in Table 5

Clearly, lowering the dimension isn't sufficient to increase OOD performances.

	OOD Dataset			
Statistic	SVHN	CIFAR100	Hflip	Vflip
$u(\mathbf{x})$	0.96	0.59	0.54	0.59
$v(\mathbf{x})$	0.94	0.56	0.54	0.59
$w(\mathbf{x})$	0.93	0.58	0.54	0.61
$v(\mathbf{x})$ & $w(\mathbf{x})$	0.94	0.58	0.54	0.60
$u(\mathbf{x})$ & $v(\mathbf{x})$	0.97	0.61	0.53	0.61
$u(\mathbf{x})$ & $w(\mathbf{x})$	0.98	0.61	0.54	0.61

Table 4: COPOD on individual statistics. ID dataset is CIFAR10.

Latent dimension	1	2	5	10	100	1000	3096	5000
$v(\mathbf{x})$ AUC	0.39	0.63	0.52	0.45	0.22	0.65	0.76	0.59

Table 5: Lower latent code dimension doesn't help to discriminate in practice.