Out-of-Distribution Detection using BiGAN and MDL

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Abstract

We consider the following problem: we have a large dataset of normal data available. We are now given a new, possibly quite small, set of data, and we are to decide if these are normal data, or if they are indicating a new phenomenon. This is a novelty detection or out-of-distribution detection problem. An example is in medicine, where the normal data is for people with no known disease, and the new dataset people with symptoms. Other examples could be in security. We solve this problem by training a bidirectional generative adversarial network (BiGAN) on the normal data and using a Gaussian graphical model to model the output. We then use universal source coding, or minimum description length (MDL) on the output to decide if it is a new distribution, in an implementation of Kolmogorov and Martin-Löf randomness. We apply the methodology to both MNIST data and a real-world electrocardiogram (ECG) dataset of healthy and patients with Kawasaki disease, and show better performance in terms of the ROC curve than similar methods.

1 Introduction

The basic problem we consider is the following: we have a large dataset \( x_i, i = 1 \ldots N \) of ‘normal’ data available for training. For example, this could be ECG data for people with no known heart disease. We are then given a test set \( x'_i, i = 1 \ldots M \) with \( M \ll N \) and wants to determine if this belongs to the class of normal data, or if this should be considered a new class of data. If \( M = 1 \) this is anomaly detection or outlier detection; if \( M > 1 \) this can be called novelty detection, based on the terminology in Pimentel et al. (2014) or group anomaly detection, as in Chalapathy et al. (2018).

Alternatively, if we consider class identity to be solely based on the data distribution, then we can view novelty detection as an out-of-distribution (OOD) or distribution shift test based on Nalisnick et al. (2019); Rabanser et al. (2019).

When \( M = 1 \), the only real possibility of detecting anomalous data is to check if it fits with normal data, i.e., if it was likely to have been generated by the distribution underlying the normal data. When \( M > 1 \), more approaches to analysis open up. One can still check the likelihood of the test data under the distribution of the normal data. But since we have more test data samples available, one
can try to find new patterns in data that could be an expression of a new underlying model. This can be expressed as finding an alternative distribution for the test data.

The goal of our paper is to perform OOD detection on high-dimensional data, \( x'_i, i = 1 \ldots M > 1 \), particularly when there are only subtle differences between the test and training data. Our method uses Rissanen’s minimum description length (MDL) [Rissanen (1978, 1983)], which explicitly accounts for the complexity of the probabilistic model to avoid overfitting.

We focus on subtle changes as these are typical of for example adversarial attacks or medical data. Adversarial attackers want to mimic normal data to go undetected. And in for example ECG data, many heart conditions are difficult to detect in a standard 12-lead electrocardiogram (ECG). The indications is in subtle changes of relationship between multiple variables.

2 Related Work

The problem of novelty or OOD detection using deep generative models has attracted much attention in recent years due to the ability of these networks to estimate the distribution of training data. The central approach to this problem is that these models give lower likelihood to OOD data than in-distribution data. This approach was initially suggested in Bishop (1994). However, further investigations in recent years show that generative models may give higher likelihood to OOD data than in-distribution data in high dimensional cases [Choi et al. (2018); Nalisnick et al. (2018)]. This phenomenon makes their applicability for novelty or OOD detection limited. Choi et al. (2018) use an ensembles of generative models to tackle this issue. In Nalisnick et al. (2019), a method based on typicality set in information theory was suggested to detect OOD data based on the closeness of the information content to the empirical entropy of training data. In a similar work Morningstar et al. (2021), multiple statistics from in-distribution data are extracted to differentiate between in-distribution and OOD data. A parameter-free OOD score similar to likelihood-ratio was proposed in Serra et al. (2019). A combination of Rao’s score test [Rao (1948)] and typicality test [Nalisnick et al. (2019)] was suggested in Bergamin et al. (2022). Chalapathy et al. (2018) proposed an approach based on measuring the deviation from in-distribution data.

All these approaches more or less are based on how well data fits with the default distribution, that is essentially based on the likelihood, eq. (1) below. As explained after (1) this has an inherent limitation. Our approach is based on finding an alternative model for the OOD data through MDL.

3 Problem Statement

Let the data be \( x \in \mathbb{R}^n \). We model the normal data through a probability distribution \( P(x) \). In an ideal setting, this model is given; but in practical scenarios, the model is learned from training data. How this is done is the main topic of the paper. We will start by discussing the problem for known \( P(x) \) and then generalize to unknown \( P(x) \).

3.1 \( P(x) \) Known

Given a set of test data \( x'_i, i = 1 \ldots M \), the OOD problem can be stated as the hypothesis test

\[
H_0 : \{x'_i\} \sim P \\
H_1 : \{x'_i\} \sim \hat{P}
\]

with \( \hat{P} \neq P \), with \( \hat{P} \) not known. One approach is to check how well the data fits \( P \) through the log-likelihood of \( \{x'_i\} \) under the (known) distribution \( P \),

\[
\ell(\{x'_i\}) = -\sum_{i=1}^{M} \log_2 P(x'_i), \tag{1}
\]

as was done in Nalisnick et al. (2019). We consider base-2 logarithm instead of natural logarithm so that we can interpret the log-likelihood as binary codelength via Kraft’s Inequality.

However, it is possible that \( \{x'_i\} \sim \hat{P} \) and \( \hat{P} \neq P \), but \( \{x'_i\} \) fits perfectly with \( P \). One example is that \( P \) is iid across the \( n \)-components of \( x \), and \( \hat{P} \) has the same marginals as \( P \) but a different joint...
distribution. It is therefore necessary to have an alternative distribution \( \hat{P} \), and since it is unknown, it has to be estimated from data. One such test in one dimension is the Kolmogorov-Smirnov test Corder & Foreman (2014), which compares the CDF \( F \) and the empirical CDF of \( \{ x_i \} \). However, this is difficult to generalize to large dimensions. Instead a probability density \( \hat{P} \) can be estimated from the test data. It could be a parametric or non-parametric estimation (Vapnik, 1998; Chapter 7), Rissanen et al. (1992). For a parametric estimation, \( \hat{P}_\theta \), we can choose the best hypothesis based on the (generalized) log-likelihood test (GLRT). We choose \( H_0 \) if

\[
\min_{P_b} \sum_{i=1}^{M} \log_2 \hat{P}_b(x'_i) + \tau
\]

otherwise, we choose \( H_1 \). Here \( \tau \) is the threshold in the hypothesis test that can adjusted to obtain a desired false alarm probability. If hypothesis \( H_1 \) is chosen, then the test data, \( x'_i \), is considered to be from a different distribution than the training data \( x \). However, if a complicated model \( \hat{P}_\theta \) with many parameters is used, it can easily lead to overfitting, which results in a poor ROC (receiver operating characteristic) curve. Our solution is to instead consider a large class of alternative models \( \{ \hat{P}_\theta \} \), which includes both simple models and very complex models such as non-parametric models like empirical pdfs Rissanen et al. (1992). The complexity of the model is also accounted for through MDL principle Rissanen (1983). This leads to the MDL criterion where we choose \( H_0 \) if

\[
\ell(\{ x'_i \}) > \min_{P_b} \sum_{i=1}^{M} \log_2 \hat{P}_b(x'_i) + L(\hat{P}_\theta) + \tau. \tag{2}
\]

Otherwise, we choose \( H_1 \). The term \( L(\hat{P}_\theta) \) is the description length of the model \( \hat{P}_\theta \) within the class \( \{ \hat{P}_\theta \} \). We can interpret the LHS and RHS of (2) as code lengths. This criterion is a special case of atypicality as defined in Høst-Madsen et al. (2019); Sabeti & Høst-Madsen (2019).

**Definition 3.1.** A test set, \( x'_i \) is (atypical) out of distribution if it can be described (coded) with fewer bits in itself rather than using the (optimum) code for (typical) training set, \( x_i \).

A downside to using (2) is that it is difficult to use the method on complex data which do not have "nice" distributions. An equivalent, but more practical, approach to (atypical) out of distribution detection is based on the observation that if data is encoded by an optimum coder, the resulting bitstream is iid uniform, i.e., totally random (Cover & Thomas 2006). In other words, the output of an optimum coder can not be compressed any further. If it can be further compressed, it is therefore OOD. From a theoretical point of view, this approach is directly an application of the theory of randomness developed by Kolmogorov and Martin-Löf (Li & Vitányi 2008; Nies 2009; Cover & Thomas 2006). Random sequences can be characterized through Kolmogorov complexity. A sequence of bits \( \{ x_n, n = 1, \ldots, \infty \} \) is random (i.e, iid uniform) if the Kolmogorov complexity of the sequence satisfies \( K(x_1, \ldots, x_n) \geq n - c \) for some constant \( c \) and for all \( n \) (Li & Vitányi 2008). The sequence is incompressible if \( K(x_1, \ldots, x_n) \geq n \) for all \( n \), and a finite sequence is algorithmically random if \( K(x_1, \ldots, x_n) \geq n \) (Cover & Thomas 2006). Thus, we characterize a set of data as OOD if the output of the optimum coder is not random according to Martin-Löf’s definition.

For real-valued data, coding into a bitstream is not feasible or useful. A better approach is to transform data into an iid Gaussian random variables (i.e., \( \mathcal{N}(0, \Sigma) \)), and then use a coder for the Gaussian distribution. The transformation is always possible for continuous random variables Sabeti & Høst-Madsen (2019).

**Proposition 3.2.** For any continuous random variable \( X \) there exists an \( n \)-dimensional iid uniform random variable \( U \) and an invertible \( F \) so that \( X = F^{-1}(U) \).

IID uniform random variables can be converted into an iid Gaussian distribution by using the normal CDF \( F \) on each \( U_i \). We will call the combined invertible map \( F : \mathbb{R}^n \rightarrow \mathbb{R}^n \). Unlike (2), this approach leads to an algorithm that can be applied to complex high-dimensional data: Algorithm 1.

How to code multivariate Gaussian data will be discussed in Section 4. A limitation is that the universal coder (a coder that does not know the underlying data distribution apriori) is also Gaussian. This is because really the only "nice" multivariate distribution is Gaussian. However, one could easily combine this with a coder that codes each component of \( x'_i \) with an MDL based histogram as
Algorithm 1 Known $P(x)$

1: Input: $\{x_i', i = 1 \ldots M\}$
2: Calculate $z_i' = \mathcal{E}(x_i)$. 
3: Code the sequence $\{z_i', i = 1 \ldots M\}$ with an iid Gaussian coder with length $L_1$.
4: Code the sequence $\{x_i', i = 1 \ldots M\}$ with a universal vector Gaussian coder with length $L_2$.
5: if $L_2 + \tau < L_1$ then
6: $\{x_i', i = 1 \ldots M\}$ is OOD.
7: end if

In practice, we generally do not know $P(x)$, and in the following we will therefore generalize Algorithm 1 to this case.

3.2 $P(x)$ Unknown

When $P(x)$ is not known a priori, it first has to be estimated from a set of training data $x_i$, $i = 1 \ldots N$. Then to use Algorithm 1 we need the (invertible) map $\mathcal{E}$. In one dimension one can simply use the empirical CDF, but when the data is high-dimensional, we need a more sophisticated approach. In this paper we choose to use BiGAN [Donahue et al. 2016; Dumoulin et al. 2016]. We will discuss alternatives below.

Shown in Figure 1, BiGAN has a generator map $G : \mathbb{R}^m \to \mathbb{R}^n$ and an encoder map $\mathcal{E} : \mathbb{R}^n \to \mathbb{R}^m$. Here $\mathbb{R}^m$, $m \leq n$, is the feature or latent space, on which the distribution is specified to be $\mathcal{N}(0, I)$, as is usual in GAN. Extending the usual GAN architecture, the discriminator now trains to jointly discriminate in data and latent space (tuples $(x, \mathcal{E}(x))$ versus $(G(z), z)$).

If the training of the BiGAN is perfect, the mappings $G$ and $\mathcal{E}$ are each others inverses according to [Donahue et al. 2016]. However, in practical training scenarios, the solutions for $G$ and $\mathcal{E}$ do not necessarily converge to the global optimum. That means $x \neq G(\mathcal{E}(x))$. Since MDL is based on lossless coding, that is, reproducing data exactly from the encoding, this is an issue.

Our solution is that we first encode $z = \mathcal{E}(x)$, as in Algorithm 1 and subsequently also encode the residual, $x - G(z)$. We will detail how this joint coding is done. Notice that MDL [Rissanen 1983] is based on quantizing the real-valued data and then letting the quantization step converge to zero. We need to carefully derive how this works for the joint coding.

Consider coding of a single data $x$. We represent each component of $z = \mathcal{E}(x)$ in fixed point with $r_z$ digits after `.' and unlimited number of digits prior as in [Rissanen 1983]. The number of bits required to encode $z$ is then

$$L_z(z) = -\log_2 \int_{x}^{x + 2^{-r_z}} P_z(t) dt \approx -\log_2 (P_z(z) 2^{-mr_z})$$

$$= -\log_2 P_z(z) + mr_z. \quad (3)$$

Next the coder encodes $x - G(\hat{z})$ with $r$ bits precision, where $\hat{z}$ is the quantized version of $\mathcal{E}(x)$. The number of bits required is

$$L(x) = -\log_2 \int_{x}^{x + 2^{-r}} P(t - G(\hat{z})) dt$$

$$\approx -\log_2 (P(x - G(\hat{z})) 2^{-nr})$$

$$= -\log_2 P(x - G(\hat{z})) + nr. \quad (4)$$
we have here assumed that \( \hat{z} \) does not change inside the quantization cube \([x, x + 2^{-r}]\). This is true if the number of digits \( r \) is large relative to \( r_z \), which is reasonable as even if let \( r_z \to \infty \), we do not get lossless coding due the non-invertibility of \( \mathcal{E} \), but \( r \to \infty \) gives lossless coding. Here \( mr_z \) and \( nr \) do not depend on which coder is used, and therefore cancels out: In the criterion (2) we always compare two codelengths and the \( mr_z + nr \) in both sides cancel out. We can therefore let \( r, r_z \to \infty \) and we end up with the codelength

\[
- \log_2 P_z(x) - \log_2 P(x - G(z))
\]

as codelength \( L_1 \). The remaining question is what to use for the distribution \( P(x - G(z)) \). Since the idea is that \( \mathcal{E} \) should capture all structure in the data, we suggest to simply use an iid Gaussian distribution, \( x - G(z) \sim N(\mu, \sigma^2 I) \), with either estimated \( \mu, \sigma^2 \) for training coding, or using MDL for \( \mu, \sigma^2 \) in the universal coder.

The method is described in Algorithm 2.

**Algorithm 2 Unknown \( P(x) \)**

**Training phase**

1: **Input:** \( \{x_i, i = 1 \ldots N\} \)
2: Train BiGAN on \( x_i \) with output \( G, \mathcal{E} \).
3: Estimate the covariance matrix of \( \{\mathcal{E}(x_i), i = 1 \ldots N\} \) as described in Section 4
4: Estimate the scalars \( \mu \) and \( \sigma^2 \) of \( \{x_i - G(\mathcal{E}(x_i)), i = 1 \ldots N\} \)

**Test phase**

5: **Input:** \( \{x'_i, i = 1 \ldots M\} \)
6: Calculate \( z'_i = \mathcal{E}(x'_i) \).
7: Code the data \( \{z'_i, i = 1 \ldots M\} \) with the estimated covariance matrix from training using a multivariate Gaussian coder, and \( \{x'_i - G(\mathcal{E}(x'_i)), i = 1 \ldots M\} \) with \( \mu, \sigma^2 \) from training using a univariate Gaussian coder. Combine using (5) resulting in codelength \( L_1 \).
8: Code the data \( \{z'_i, i = 1 \ldots M\} \) with a universal multivariate Gaussian coder as described in Section 4 and \( \{x'_i - G(\mathcal{E}(x'_i)), i = 1 \ldots M\} \) with a universal univariate Gaussian coder (Cover & Thomas 2006, Section 13.2). Sum the two codelengths together to obtain \( L_2 \).
9: if \( L_2 + r < L_1 \) then
10: \( \{x'_i, i = 1 \ldots M\} \) is out-of-distribution.
11: end if

The reason we code \( \{z'_i\} \) with an estimated covariance matrix in step 7 is that the distribution of \( \mathcal{E}(x) \) might not be perfectly \( N(0, I) \), and then the universal coder would always be better if we did not encode with the estimated covariance matrix.

The main issue with BiGAN in our context is that the reconstruction error \( x - G(\mathcal{E}(x)) \) can be large with an “ugly” distribution for both in-distribution and OOD data. We did experiment with autoencoders as alternatives. A key feature required of methods in our context is the ability to prescribe the distribution in the latent space, and not all autoencoders have that ability. We tried alternative methods that have that ability: Adversarial AutoEncoder (AAE) (Makhzani et al. 2015), and Variational AutoEncoder (VAE) (Kingma & Welling 2013). Both of these were better at reconstruction, i.e., \( x - G(\mathcal{E}(x)) \) was significantly smaller. However, the distribution of \( \mathcal{E}(x) \) were very far from Gaussian, where BiGAN gives something that is close to Gaussian, and in the end BiGAN therefore had better performance.

**4 Universal Multivariate Gaussian Coder**

A multivariate Gaussian distribution with zero mean is completely characterized by its covariance matrix \( \Sigma \). When the covariance matrix is not known, it has to be estimated from data. A simple solution to estimate \( \Sigma \) is the maximum likelihood, which is empirical covariance matrix \( \hat{\Sigma} \). However, the empirical covariance matrix is an overparametrized solution especially when the data is generated under a sparse Gaussian graphical model; that is \( \Sigma^{-1} \) is sparse (Dempster 1972). An efficient method
We used the ImageDataGenerator.

As it can be seen in Figure 2, it is hard to distinguish between in-distribution (unperturbed) and OOD (perturbed) data by visual inspection. In fact, each of samples in the OOD test set individually can be considered as a normal sample but their collective behavior is OOD. Our goal is exactly to detect such subtle changes.
Table 1: Scenarios for OOD detection. Rotation and shearing values are in degree, width and height shift in fraction, zoom and brightness in range.

| Perturbation type | Value/Range value |
|-------------------|-------------------|
| CASE–1 Rotation   | 5                 |
| CASE–2 Shearing   | 20                |
| CASE–3 Width shift, Height shift | [0.02, 0.02] |
| CASE–4 Zooming    | [0.8, 1.2]        |
| CASE–5 Zooming    | [1, 1.1]          |
| CASE–6 Zooming    | [0.9, 1]          |
| CASE–7 Brightness | [0.2, 2]          |
| CASE–8 Brightness | [1, 2]            |
| CASE–9 Brightness | [0.2, 1]          |
| CASE–10 Gaussian noise | \( \mu = 0, \sigma = 0.05 \) |

In our experiment, 60,000 examples in the original MNIST dataset were used for training and validation, and 10,000 original test images were used as in-distribution test data. All the modified datasets were considered as OOD in testing.

Figure 2: Sample plot for original test images and corresponding images in OOD test cases. Note that the differences between the normal data and the OOD data is very subtle.

After training BiGAN, we transfer both training and test datasets into the latent space of size 20. For the comparison scenarios, the AAE and VAE autoencoders as described in Chalapathy et al. (2018) were used to transfer the data into the latent space of the same dimension. Table 2 provides the details of the employed BiGAN, AAE, and VAE hyperparameters in this experiment. For the sake of fairness, we employ two fully connected hidden layers of size 512, each followed by a Leaky Relu and Batch normalization layers for the encoder and decoder/generator networks in all three BiGAN, AAE, and VAE schemes. The same architecture is used for the discrimination network in BiGAN and AAE. The sigmoid activation function in the last layer is used for the decoder/generator networks in all three schemes and in the discriminator network for BiGAN and AAE.

Afterward, we encode the data using Algorithm 2, which entails the coding of data in latent space and encoding of reconstruction error.
we can obtain ROC curve by plotting Algorithm 2 denotes our approach, and \( \ell_2 \) to refer to method in Chalapathy et al. (2018) under different architectures. To perform the experiments, we split the data into batches of size \( M \) for each of the OOD test cases and also the original in-distribution test data and compute \( L_2 - L_1 \) based on each batch. Next, we can obtain ROC curve by plotting \( L_2 - L_1 \) of the OOD data versus \( L_2 - L_1 \) of the in-distribution test data. Table 3 shows the area under ROC curve (AUROC) for each test case across different values of test set size \( M \) for Algorithm 2 versus the distance-based \( \ell_2 \) approach by “flipping-the-output,” i.e., decide the opposite of what the test says, since this does not apply to all the test cases such as CASE–2, 4, 8, 10, and in real world we don’t know what is the type of OOD data.

Table 2: BiGAN, AAE, and VAE networks and training hyperparameters

| Hyperparameter             | Value |
|---------------------------|-------|
| Number of epochs          | 50,000|
| Batch size                | 128   |
| Initial learning rate     | 0.002 |
| Learning rate decay       | 0.01 after 25,000 epochs |
| \( \ell_2 \)-regulizer     | \( 2.5 \times 10^{-4} \) |
| Initializing network weight| \( \mathcal{N}(0, 0.2) \) |
| Bath normalization momentum| 0.8   |
| LeakyRelu                 | \( \alpha = 0.2 \) |

Table 3: AUROC for different test cases and testset size \( M \). The best value for each case is boldfaced. Algorithm 2 denotes our approach, and \( \ell_2 \) to refer to method in Chalapathy et al. (2018) under different architectures.

| M = 50 | M = 100 | M = 200 |
|--------|---------|---------|
| \( \ell_2 \)-BiGAN | \( \ell_2 \)-AAE | \( \ell_2 \)-VAE | \( \ell_2 \)-BiGAN | \( \ell_2 \)-AAE | \( \ell_2 \)-VAE | \( \ell_2 \)-BiGAN | \( \ell_2 \)-AAE | \( \ell_2 \)-VAE |
| CASE–1 | 0.633 | 0.167 | 0.015 | 0.003 | 0.693 | 0.076 | 0.001 | 0.000 | 0.769 | 0.032 | 0.000 | 0.000 |
| CASE–2 | 0.709 | 0.685 | 0.505 | 0.501 | 0.791 | 0.765 | 0.501 | 0.475 | 0.873 | 0.839 | 0.502 | 0.511 |
| CASE–3 | 0.592 | 0.192 | 0.002 | 0.000 | 0.638 | 0.108 | 0.000 | 0.000 | 0.687 | 0.054 | 0.000 | 0.000 |
| CASE–4 | 0.930 | 0.928 | 0.539 | 0.464 | 0.987 | 0.980 | 0.606 | 0.503 | 1.000 | 1.000 | 0.573 | 0.477 |
| CASE–5 | 0.707 | 0.176 | 0.002 | 0.000 | 0.815 | 0.090 | 0.000 | 0.000 | 0.914 | 0.038 | 0.000 | 0.000 |
| CASE–6 | 0.840 | 0.645 | 0.317 | 0.167 | 0.933 | 0.711 | 0.254 | 0.074 | 0.989 | 0.775 | 0.174 | 0.021 |
| CASE–7 | 0.740 | 0.666 | 0.139 | 0.139 | 0.846 | 0.722 | 0.050 | 0.067 | 0.917 | 0.774 | 0.012 | 0.012 |
| CASE–8 | 0.896 | 0.963 | 0.956 | 0.982 | 0.971 | 0.965 | 0.993 | 0.998 | 0.997 | 0.997 | 1.000 | 1.000 |
| CASE–9 | 0.988 | 0.197 | 0.000 | 0.000 | 1.000 | 0.111 | 0.000 | 0.000 | 1.000 | 0.058 | 0.000 | 0.000 |
| CASE–10 | 0.904 | 0.712 | 0.845 | 0.663 | 0.967 | 0.802 | 0.522 | 0.725 | 0.998 | 0.573 | 0.978 | 0.807 |

We used graphical lasso (Friedman et al., 2008) to solve 6. It is possible to use any regularized estimator of Gaussian graphical models. For regularization hyperparameter \( \lambda \), we consider 20 candidate values within the range \([0.1, 1]\) with logarithmic step size. The results are given for one of the graph coders, i.e., coding with number of common neighbors and degree distribution. For details of coding, an interested reader can refer to Abolfazli et al. (2021b).

To perform the experiments, we split the data into batches of size \( M \) for each of the OOD test cases and also the original in-distribution test data and compute \( L_2 - L_1 \) based on for each batch. Next, we can obtain ROC curve by plotting \( L_2 - L_1 \) of the OOD data versus \( L_2 - L_1 \) of the in-distribution test data. Table 3 shows the area under ROC curve (AUROC) for each test case across different values of test set size \( M \) for Algorithm 2 versus the distance-based \( \ell_2 \) approach proposed in Chalapathy et al. (2018). We implemented the distance-based approach for three different generative networks: BiGAN, AAE, and VAE. The results indicate that our approach performed best in all cases except CASE–8. Even for CASE–8, our approach still had decent detection performance. The performance of Algorithm 2 improves with test set size.

It might seem odd that we get AUROC less than 0.5 (i.e., random guessing) in some cases for \( \ell_2 \)-BiGAN, \( \ell_2 \)-AAE, and \( \ell_2 \)-VAE. The reason is that in these cases, the OOD data somehow has smaller reconstruction error than the in-distribution data even though the generative model has never seen the OOD data before. This phenomenon has also been observed in the literature Chalapathy et al. (2018); Rabanser et al. (2019); Nalisnick et al. (2019).

Note that we can not improve the performance of the \( \ell_2 \)-based approach by “flipping-the-output,” i.e., decide the opposite of what the test says, since this does not apply to all the test cases such as CASE–2, 4, 8, 10, and in real world we don’t know what is the type of OOD data.
5.2 ECG dataset

We were provided ECG data of 23522 subjects, 423 subjects were diagnosed with the Kawasaki disease and the rest are considered healthy subjects. Kawasaki disease causes inflammation in blood vessels in children under the age of five years old [McCrindle et al., 2017]. However, it can be very difficult for medical professionals to diagnose using since ECG data between healthy and diseased subjects can be very similar.

For each patient, a total of 176 Heart Rate Variation (HRV) features were automatically extracted from 12 leads ECG signals [Bratincsák et al., 2020]. We used 90% of the healthy (normal data) subjects were used for training. The remaining healthy subjects and diseased subjects were used as test set. A batch of healthy subjects should be detected as an in-distribution data whereas a batch of diseased subjects should be detected as an OOD sample.

To test the performance of Algorithm 2, we randomly pick 50 samples from each of in-distribution test data and OOD data (i.e., Kawasaki data). We repeat this experiment 500 times. We used BiGAN, where the dimension of the latent space is 40. The ROC curve is obtained by changing the threshold $\tau$. Figure 3 represents ROC curve for this experiment. The corresponding AUROC is equal to 0.9996. This shows that our approach can distinguish Kawasaki subjects as OOD data with high performance.

![ROC curve for dim=40](image)

Figure 3: ROC curve of detecting Kawasaki subjects as OOD data.

6 Conclusion, Limitations, and Future work

We have developed a method for out-of-distribution detection based on MDL. We have shown that it performs well on both MNIST and real-world ECG data.

There are two future directions to consider. First, from our experiments, we learned that BiGAN is far from ideal: the reconstruction error $x - G(\mathcal{E}(x))$ is quite large, and has a strange distribution. For future work, we will consider other deep generative models; we did experiment with AAE and VAE but they do resulted in additional issues compared with BiGAN. Second, we only considered multivariate Gaussian distributions as the alternative models in this paper. An advantage of our MDL/coding approach is that we can substitute a single coder with a combination of multiple coders. For future work, we will use such an approach to consider alternative models that are mixtures of multivariate Gaussians, and in more generality non-parametric distributions.

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References

Abolfazli, M., Høst-Madsen, A., Zhang, J., and Bratincsák, A. Graph coding for model selection and anomaly detection in gaussian graphical models. In ISIT’2021, Melbourne, Australia, July 12-20, 2021a.

Abolfazli, M., Host-Madsen, A., Zhang, J., and Bratincsák, A. Graph compression with application to model selection. arXiv preprint arXiv:2110.00701, 2021b.

Bergamin, F., Mattei, P.-A., Havtorn, J. D., Senetaire, H., Schmutz, H., Maaløe, L., Hauberg, S., and Frellsen, J. Model-agnostic out-of-distribution detection using combined statistical tests. In International Conference on Artificial Intelligence and Statistics, pp. 10753–10776. PMLR, 2022.

Bishop, C. M. Novelty detection and neural network validation. IEE Proceedings-Vision, Image and Signal processing, 141(4):217–222, 1994.

Bratincsák, A., Kimata, C., Limm-Chan, B. N., Vincent, K. P., Williams, M. R., and Perry, J. C. Electrocardiogram standards for children and young adults using Z-scores. Circulation: Arrhythmia and Electrophysiology, 13(8):e008253, 2020.

Chalapathy, R., Toth, E., and Chawla, S. Group anomaly detection using deep generative models. In Joint European Conference on Machine Learning and Knowledge Discovery in Databases, pp. 173–189. Springer, 2018.

Choi, H., Jang, E., and Alemi, A. A. Waic, but why? generative ensembles for robust anomaly detection. arXiv preprint arXiv:1810.01392, 2018.

Corder, G. W. and Foreman, D. I. Nonparametric Statistics: A Step-by-Step Approach. John Wiley & Sons, 2014.

Cover, T. and Thomas, J. Information Theory, 2nd Edition. John Wiley, 2006.

Dempster, A. P. Covariance selection. Biometrics, 28(1):157–175, 1972. ISSN 0006341X, 15410420. URL http://www.jstor.org/stable/2528966.

Deng, L. The mnist database of handwritten digit images for machine learning research. IEEE Signal Processing Magazine, 29(6):141–142, 2012.

Donahue, J., Krähenbühl, P., and Darrell, T. Adversarial feature learning. arXiv preprint arXiv:1605.09782, 2016.

Dumoulin, V., Belghazi, I., Poole, B., Mastropietro, O., Lamb, A., Arjovsky, M., and Courville, A. Adversarially learned inference. arXiv preprint arXiv:1606.00704, 2016.

Friedman, J., Hastie, T., and Tibshirani, R. Sparse inverse covariance estimation with the graphical lasso. Biostatistics, 9(3):432–441, 2008.

Høst-Madsen, A., Sabeti, E., and Walton, C. Data discovery and anomaly detection using atypicality. IEEE Transactions on Information Theory, 65(9), September 2019.

Kingma, D. P. and Welling, M. Auto-encoding variational bayes. arXiv preprint arXiv:1312.6114, 2013.

Li, M. and Vitányi, P. An Introduction to Kolmogorov Complexity and Its Applications. Springer, third edition, 2008.

Makhzani, A., Shlens, J., Jaitly, N., Goodfellow, I., and Frey, B. Adversarial autoencoders. arXiv preprint arXiv:1511.05644, 2015.

McCrindle, B. W., Rowley, A. H., Newburger, J. W., Burns, J. C., Bolger, A. F., Gewitz, M., Baker, A. L., Jackson, M. A., Takahashi, M., Shah, P. B., et al. Diagnosis, treatment, and long-term management of kawasaki disease: a scientific statement for health professionals from the american heart association. Circulation, 135(17):e927–e999, 2017.
Morningstar, W., Ham, C., Gallagher, A., Lakshminarayanan, B., Alemi, A., and Dillon, J. Density of states estimation for out of distribution detection. In *International Conference on Artificial Intelligence and Statistics*, pp. 3232–3240. PMLR, 2021.

Nalisnick, E., Matsukawa, A., Teh, Y. W., Gorur, D., and Lakshminarayanan, B. Do deep generative models know what they don’t know? *arXiv preprint arXiv:1810.09136*, 2018.

Nalisnick, E., Matsukawa, A., Teh, Y. W., and Lakshminarayanan, B. Detecting out-of-distribution inputs to deep generative models using typicality, 2019. URL [https://arxiv.org/abs/1906.02994](https://arxiv.org/abs/1906.02994).

Nies, A. *Computability and Randomness*. Oxford University Press, 2009.

Pimentel, M. A., Clifton, D. A., Clifton, L., and Tarassenko, L. A review of novelty detection. *Signal Processing*, 99:215–249, 2014. ISSN 0165-1684. doi: https://doi.org/10.1016/j.sigpro.2013.12.026. URL [https://www.sciencedirect.com/science/article/pii/S016516841300515X](https://www.sciencedirect.com/science/article/pii/S016516841300515X).

Rabanser, S., Günemann, S., and Lipton, Z. Failing loudly: An empirical study of methods for detecting dataset shift. In *Advances in Neural Information Processing Systems*, volume 32. Curran Associates, Inc., 2019. URL [https://proceedings.neurips.cc/paper/2019/file/846c260d715e5b854ffad5f70a516c88-Paper.pdf](https://proceedings.neurips.cc/paper/2019/file/846c260d715e5b854ffad5f70a516c88-Paper.pdf).

Rao, C. R. Large sample tests of statistical hypotheses concerning several parameters with applications to problems of estimation. In *Mathematical Proceedings of the Cambridge Philosophical Society*, volume 44, pp. 50–57. Cambridge University Press, 1948.

Rissanen, J. Modeling by shortest data description. *Automatica*, pp. 465–471, 1978.

Rissanen, J. A universal prior for integers and estimation by minimum description length. *The Annals of Statistics*, (2):416–431, 1983.

Rissanen, J., Speed, T., and Yu, B. Density estimation by stochastic complexity. *IEEE Transactions on Information Theory*, 38(2):315–323, 1992. doi: 10.1109/18.119689.

Sabeti, E. and Høst-Madsen, A. Data discovery and anomaly detection using atypicality for real-valued data. *Entropy*, pp. 219. Feb. 2019. Available at https://doi.org/10.3390/e21030219.

Serrà, J., Álvarez, D., Gómez, V., Slizovskaia, O., Núñez, J. F., and Luque, J. Input complexity and out-of-distribution detection with likelihood-based generative models. In *International Conference on Learning Representations*, 2019.

Vapnik, V. N. *Statistical Learning Theory*. John Wiley, 1998.

Yuan, M. and Lin, Y. Model selection and estimation in the gaussian graphical model. *Biometrika*, 94(1):19–35, 2007.