UNCERTAINTY AND THE MEDICAL INTERVIEW

TOWARDS SELF-ASSESSMENT IN MACHINE LEARNING MODELS

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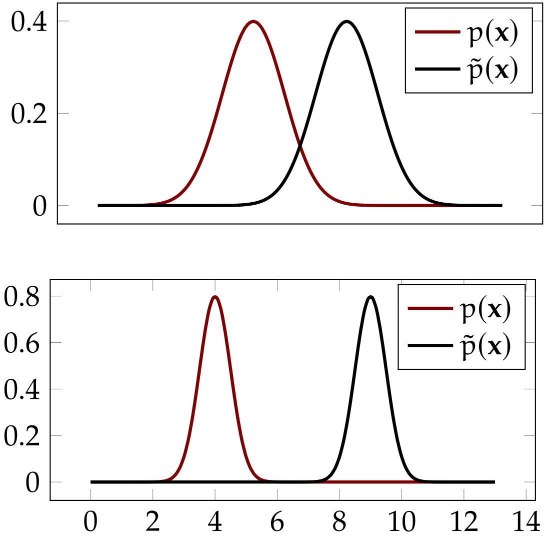
Defining OOD detection

Out-of-distribution (OOD) detection is about enabling models to distinguish the training data distribution $p(\mathbf{x})$ from any other distribution $\tilde{p}(\mathbf{x})$.

We are concerned with doing this on a per-observation basis, i.e. answering the question:

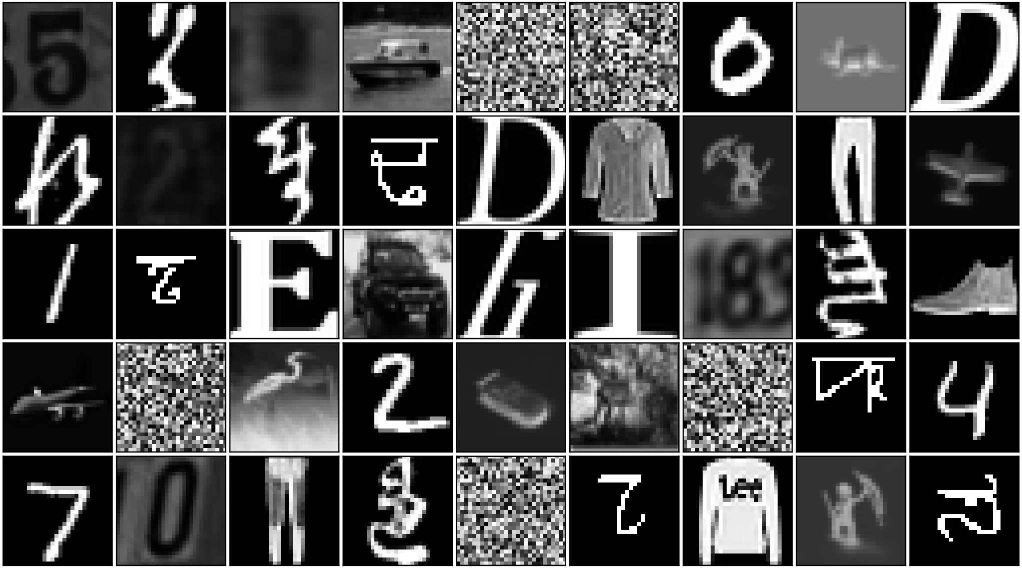
"Was $\mathbf{x}$ sampled from $p(\mathbf{x})$ or not?"



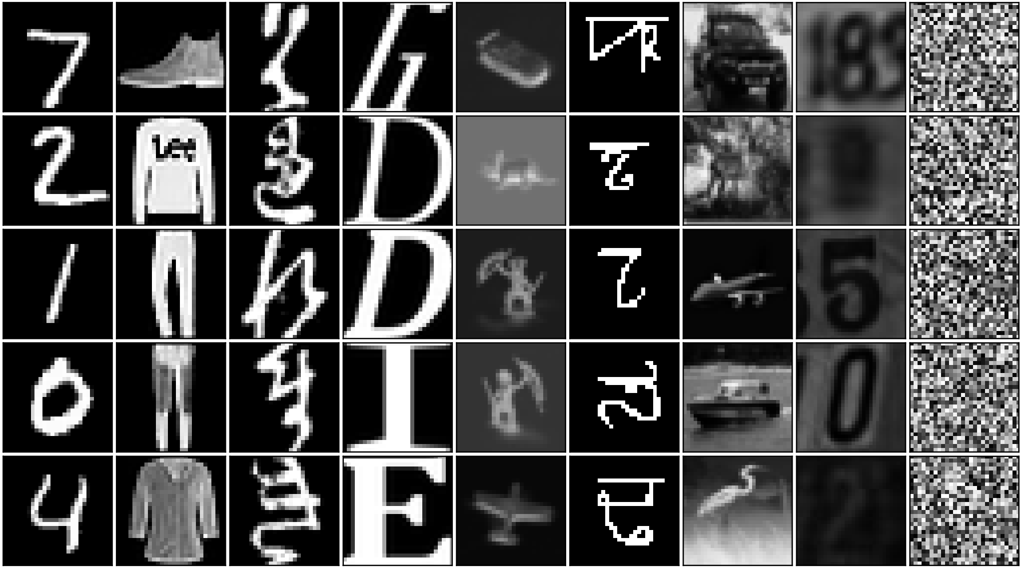
Problem and Contributions

- Deep generative models often fail at OOD detection task when using their likelihood estimate as the score function [6] by, perhaps surprisingly, assigning **higher likelihoods** to the OOD data.
- Contributions:
  - We present a fast and fully unsupervised method for OOD detection competitive with the state-of-the-art
  - We provide evidence that out-of-distribution detection fails due to learned low-level features that generalize across datasets.

In distribution?



Out of distribution?



Hierarchical VAE

We choose the hierarchical VAE as our model [2, 3].

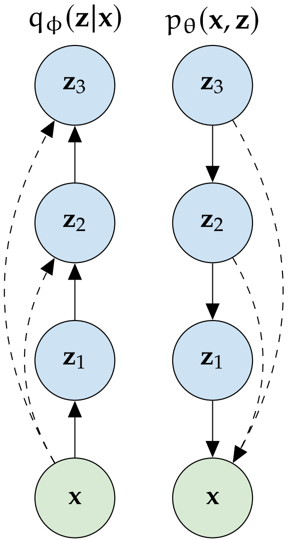
$$p_\theta(\mathbf{x}) = \int p_\theta(\mathbf{x}, \mathbf{z})d\mathbf{z} = \int p_\theta(\mathbf{x}|\mathbf{z})p_\theta(\mathbf{z})d\mathbf{z}$$

Specifically we use

1. a three-layered hierarchical VAE with bottom-up inference and deterministic skip-connections for both inference and generation.

$$\begin{aligned} \text{Generative model:} \quad & p_\theta(\mathbf{x}|\mathbf{z}) = p_\theta(\mathbf{x}|\mathbf{z}_1)p_\theta(\mathbf{z}_1|\mathbf{z}_2)p(\mathbf{z}_3), \\ \text{Inference model:} \quad & q_\phi(\mathbf{z}|\mathbf{x}) = q_\phi(\mathbf{z}_1|\mathbf{x})q_\phi(\mathbf{z}_2|\mathbf{z}_1)q_\phi(\mathbf{z}_3|\mathbf{z}_2). \end{aligned}$$

2. a ten-layered layered Bidirectional-Inference Variational Autoencoder (BIVA) [5].



What is wrong with the ELBO for OOD detection?

We can split the ELBO into two terms

$$\mathcal{L}(\mathbf{x};\theta,\phi) = \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[\log \frac{p_\theta(\mathbf{x},\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}\right] = \underbrace{\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x}|\mathbf{z})]}_{\text{reconstruction likelihood}} - \underbrace{D_{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p(\mathbf{z}))}_{\text{regularization penalty}} \ . \tag{1}$$

The first term is high if the data is well-explained by $\mathbf{z}$.

The second term we can rewrite as,

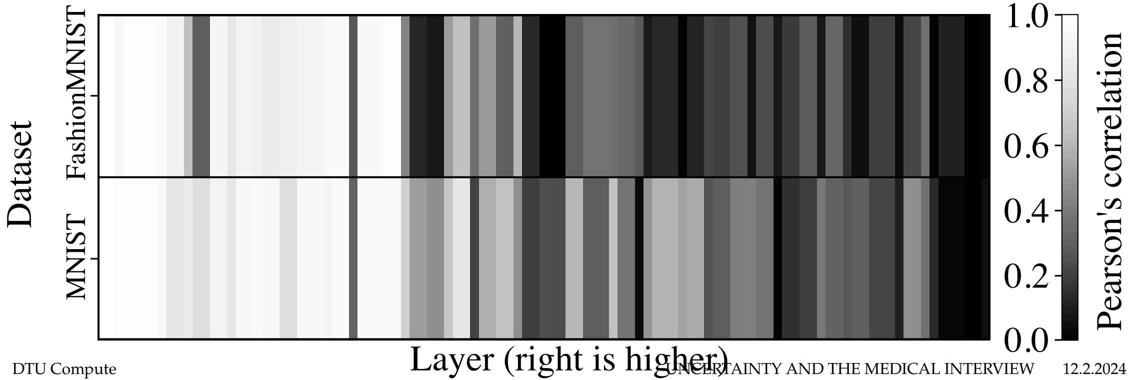
$$D_{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p(\mathbf{z})) = \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[\sum_{i=1}^{L-1} \log \frac{p_\theta(\mathbf{z}_i|\mathbf{z}_{i+1})}{q_\phi(\mathbf{z}_i|\mathbf{z}_{i-1})} + \log \frac{p_\theta(\mathbf{z}_L)}{q_\phi(\mathbf{z}_L|\mathbf{z}_{L-1})}\right] . \tag{2}$$

The absolute log-ratios grow with $\dim(\mathbf{z}_i)$ since the log probability terms are computed by summing over the dimensionality of $\mathbf{z}_i$.

What do the lowest latent variables code for?

Absolute Pearson correlations between data representations in all layers of the inference network of a hierarchical VAE trained on FashionMNIST and of another trained on MNIST.

Correlation computed between the representations of the two different models given the same data, FashionMNIST (top) and MNIST (bottom).



An alternative likelihood bound, $\mathcal{L}^{>k}$

An alternative version of the ELBO that only partially uses the approximate posterior can be written as [5]

$$\mathcal{L}^{>k}(\mathbf{x};\theta,\phi) = \mathbb{E}_{p_\theta(\mathbf{z}_{\leqslant k}|\mathbf{z}_{>k})q_\phi(\mathbf{z}_{>k}|\mathbf{x})}\left[\log \frac{p_\theta(\mathbf{x}|\mathbf{z})p_\theta(\mathbf{z}_{>k})}{q_\phi(\mathbf{z}_{>k}|\mathbf{x})}\right] \tag{3}$$

Here, we have replaced the approximate posterior $q_\phi(\mathbf{z}|\mathbf{x})$ with a different proposal distribution that combines part of the approximate posterior with the conditional prior, namely

$$p_\theta(\mathbf{z}_{\leqslant k}|\mathbf{z}_{>k})q_\phi(\mathbf{z}_{>k}|\mathbf{x})$$

This bound uses the conditional prior for the lowest latent variables in the hierarchy.

Likelihood ratios

We can use our new bound to compute the score used in a standard likelihood ratio test [1].

$$\mathrm{LLR}^{>k}(\mathbf{x}) \equiv \mathcal{L}(\mathbf{x}) - \mathcal{L}^{>k}(\mathbf{x}) \,. \tag{4}$$

We can inspect what this likelihood-ratio measures by considering the exact form of our bounds.

$$\begin{aligned} \mathcal{L} &= \log p_\theta(\mathbf{x}) - D_{\mathrm{KL}}\left(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x})\right), \\ \mathcal{L}^{>k} &= \log p_\theta(\mathbf{x}) - D_{\mathrm{KL}}\left(p_\theta(\mathbf{z}_{\leqslant}|\mathbf{z}_{>k})q_\phi(\mathbf{z}_{>k}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x})\right) \,. \end{aligned} \tag{5}$$

In the likelihood ratio the reconstruction terms cancel out and only the KL-divergences from the approximate to the true posterior remain.

$$\begin{aligned} \mathrm{LLR}^{>k}(\mathbf{x}) = &-D_{\mathrm{KL}}\left(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x})\right) \\ &+ D_{\mathrm{KL}}\left(p_\theta(\mathbf{z}_{\leqslant}|\mathbf{z}_{>k})q_\phi(\mathbf{z}_{>k}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x})\right) \,. \end{aligned} \tag{6}$$

Importance sampling the ELBO

The well-known importance weighted autoencoder (IWAE) bound is tight with the true likelihood in the limit of infinite samples, $S \to \infty$ [4],

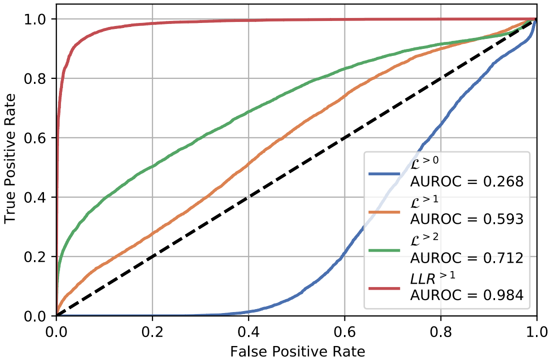
$$\mathcal{L}_S = \mathbb{E}_{q(\mathbf{z}|\mathbf{x})}\left[\log \frac{1}{N} \sum_{s=1}^{S} \frac{p(\mathbf{x}, \mathbf{z}^{(s)})}{q(\mathbf{z}^{(s)}|\mathbf{x})}\right] \leqslant \log p_\theta(\mathbf{x}) \,, \tag{7}$$

Consequently, by importance sampling the ELBO, the associated KL-divergence associated vanishes and our likelihood ratio reduces to the KL-divergence associated with $\mathcal{L}^{>k}$.

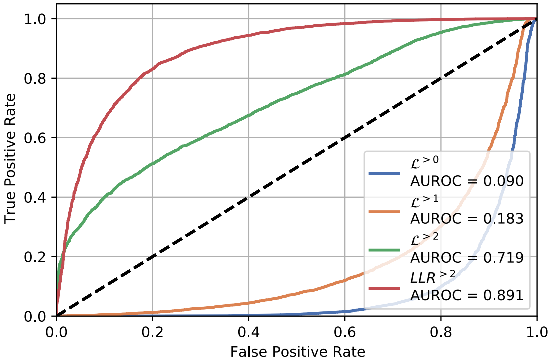
$$\mathrm{LLR}_S^{>k}(\mathbf{x}) \to D_{\mathrm{KL}}(p(\mathbf{z}_{\leqslant}|\mathbf{z}_{>k})q(\mathbf{z}_{>k}|\mathbf{x})||p(\mathbf{z}|\mathbf{x})) \,. \tag{8}$$

We can now see that $\mathrm{LLR}_S^{>k}(\mathbf{x})$ performs OOD detection based on the top-most latent variables.

Results with $\mathrm{LLR}^{>k}$



(a) FashionMNIST HVAE evaluated on MNIST



(b) CIFAR10 BIVA evaluated on SVHN

Results with $\mathrm{LLR}^{>k}$

The score has good performance across many different datasets.

OOD dataset	Metric	AUROC↑	AUPRC↑	FPR80↓
Trained on CIFAR10				
SVHN	$\mathrm{LLR}^{>2}$	0.811	0.837	0.394
CIFAR10	$\mathrm{LLR}^{>1}$	0.469	0.479	0.835
Trained on SVHN				
CIFAR10	$\mathrm{LLR}^{>1}$	0.939	0.950	0.052
SVHN	$\mathrm{LLR}^{>1}$	0.489	0.484	0.799

OOD dataset	Metric	AUROC↑	AUPRC↑	FPR80↓
Trained on FashionMNIST				
MNIST	$\mathrm{LLR}^{>1}$	0.986	0.987	0.011
notMNIST	$\mathrm{LLR}^{>1}$	0.998	0.998	0.000
KMNIST	$\mathrm{LLR}^{>1}$	0.974	0.977	0.017
Omniglot28x28	$\mathrm{LLR}^{>2}$	1.000	1.000	0.000
Omniglot28x28Inverted	$\mathrm{LLR}^{>1}$	0.954	0.954	0.050
SmallNORB28x28	$\mathrm{LLR}^{>2}$	0.999	0.999	0.002
SmallNORB28x28Inverted	$\mathrm{LLR}^{>2}$	0.941	0.946	0.069
FashionMNIST	$\mathrm{LLR}^{>1}$	0.488	0.496	0.811
Trained on MNIST				
FashionMNIST	$\mathrm{LLR}^{>1}$	0.999	0.999	0.000
notMNIST	$\mathrm{LLR}^{>1}$	1.000	0.999	0.000
KMNIST	$\mathrm{LLR}^{>1}$	0.999	0.999	0.000
Omniglot28x28	$\mathrm{LLR}^{>1}$	1.000	1.000	0.000
Omniglot28x28Inverted	$\mathrm{LLR}^{>1}$	0.944	0.953	0.057
SmallNORB28x28	$\mathrm{LLR}^{>1}$	1.000	1.000	0.000
SmallNORB28x28Inverted	$\mathrm{LLR}^{>1}$	0.985	0.987	0.000
MNIST	$\mathrm{LLR}^{>2}$	0.515	0.507	0.792

Thank you for your attention

Bibliography I

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