HyperVAE: A Minimum Description Length Variational Hyper-Encoding Network

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Abstract

We propose a framework called HyperVAE for encoding distributions of distributions. When a target distribution is modeled by a VAE, its neural network parameters \( \theta \) is drawn from a distribution \( p(\theta) \) which is modeled by a hyper-level VAE. We propose a variational inference using Gaussian mixture models to implicitly encode the parameters \( \theta \) into a low dimensional Gaussian distribution. Given a target distribution, we predict the posterior distribution of the latent code, then use a matrix-network decoder to generate a posterior distribution \( q(\theta) \). HyperVAE can encode the parameters \( \theta \) in full in contrast to common hyper-networks practices, which generate only the scale and bias vectors as target-network parameters. Thus HyperVAE preserves much more information about the model for each task in the latent space. We discuss HyperVAE using the minimum description length (MDL) principle and show that it helps HyperVAE to generalize. We evaluate HyperVAE in density estimation tasks, outlier detection and discovery of novel design classes, demonstrating its efficacy.

1 Introduction

Humans can extract meta knowledge across tasks such that when presented with an unseen task they can use this meta knowledge, adapt it to the new context and quickly solve the new task. Recent advance in meta-learning [Finn et al., 2017; Finn and Levine, 2018; Finn et al., 2018; Grant et al., 2018; Finn et al., 2019] shows that it is possible to learn a single model such that when presented with a new task, it can quickly adapt to the new distribution and accurately classify unseen test points. Since meta-learning algorithms are designed for few-shot or one-shot learning where labeled data exists, it faces challenges when there is none¹ to assist backpropagation when training.

Hyper-networks [Ha et al., 2016] can generate the weights for a target network given a set of embedding vectors of those weights. Due to its generative advantage, it can be used to generate a distribution of parameters for a target network [Ha et al., 2016; Krueger et al., 2017]. In practice, due to the high dimensional parameter space, it only generates scaling factors and biases for the target network. This poses a problem that the weight embedding vectors only encode partial information about the target task, and thus are not guaranteed to perform well on unseen tasks.

On the other hand, variational autoencoders (VAEs) [Kingma and Welling, 2013; Rezende et al., 2014] is a class of deep generative models that can model complex distributions. A major attractive feature of VAEs is that we can draw from simple, low-dimensional distributions (such as isotropic Gaussians), and the model will generate high-dimensional data instantly without going through expensive procedures like those in the classic MCMC. This suggests VAEs can be highly useful for high dimensional design exploration [Gomez-Bombarelli et al., 2018]. In this work, we lift this idea to one more abstraction level, that is, using a hyper-VAE to generate VAE models. While the VAEs work at the individual design level, the hyper-VAE works at the class level. This permits far more flexibility in exploration, because not only we can explore designs within a class, we can explore multiple classes.

We propose HyperVAE, a novel class of VAEs, as a powerful deep generative model to learn to generate the parameters of VAE networks for modeling the distribution of different tasks. HyperVAEs are regularized by using minimum description length (MDL) principle, in that we restrict the total description length of the model family and the tasks. In particular we use MDL with bits-back coding [Hinton and Van Camp, 1993; Hinton and Zemel, 1994] as our training objective for the HyperVAE, minimizing the total description length.

The versatility of the HyperVAE to produce VAE models allows it to be applied for a variety of problems where model flexibility is required, including density estimation, outlier detection, and novelty seeking. For the latter, since HyperVAE enforces a smooth transition in the model family, interpolating in this space will enable us to extrapolate to models of new tasks which are close to trained tasks. Thus as global search techniques can guide the generation of latent spaces of VAEs, search enables HyperVAE to produce novel classes of discovery. We use Bayesian Optimization (BO) [Shahriari et al., 2016], to search in the low dimensional encoding space of VAE. Once a low dimensional design is suggested, we can decode it to the corresponding high dimensional design.

¹This is not the same as zero-shot learning where label description is available.
Using diverse datasets, we demonstrate the ability of HyperVAE on three tasks: density estimation, robust outlier detection and discovery of unseen design classes. Our main contributions and results are: (i) Development of a hyper-encoding framework, guided through MDL; (ii) Construction of a versatile HyperVAE model that can tackle density estimation tasks and outlier detection; and (iii) Demonstration of novel designs produced from our model coupled with BO.

2 Preliminaries

We briefly review variational autoencoder (VAE) technique and MDL as a regularization principle. Let \( x \) denote an \( X \)-value random variable associated with a \( Z \)-value random variable \( z \) through a joint distribution \( p(x, z) \). We consider a parametric family \( \mathcal{P} \) of generative models \( p(x, z; \theta) \) factorized as a conditional \( p(x|z; \theta) \) and a simple prior \( p(z) \), usually chosen as \( \mathcal{N}(0, I) \). Maximum likelihood estimate (MLE) of \( \theta \) is the parameter space, over the marginal

\[
\log p(x; \theta) = \log \int p(x, z; \theta) dz \quad \text{is intractable and requires alternatives such as expectation-maximization and variational inference. VAE is an amortized variational inference approach that jointly learns the generative model \( p(x|z; \theta) \) and a variational inference model \( q(z|x; \theta)^2 \). Its ELBO objective defined as

\[
\mathcal{L}(x, p, q; \theta) = \mathbb{E}_{q(z|x; \theta)} \log p(x|z; \theta) - KL(q(z|x; \theta)\|p(z))
\]

(1)

lower-bounds the marginal log-likelihood \( \log p(x; \theta) \). In practice, Monte Carlo estimator of the ELBO’s gradient is used to update the parameters \( \theta \). The form of \( q \) and \( p \) in Eq. 1 makes an encoder and a decoder, hence the name auto-encoder [Kingma and Welling, 2013]. MLE of a single \( \theta \) maximizing the above objective is susceptible to overfitting, especially when \( \theta \) is high dimensional. This raises the needs for model comparison and selection.

Minimum description length (MDL) is an information-theoretic principle for model selection [Honkela and Valpola, 2004] that minimizes the combined code length of the model and data. Assume an optimal coding scheme\(^2\) where the code length of a random variable \( X \) from a discrete distribution \( P(X) \) is defined as the information content in \( X \),

\[
L(X) \overset{\text{def}}{=} -\log P(X)
\]

(2)

The expected code length achieves the Shannon-coding lower bound \( H(X) = \mathbb{E}[L(X)] \), which is the entropy of \( X \). In MDL, the code length, using a crude 2-part code, of transmitting \( X \) under the encoding distribution \( P(X; \theta) \) is given by

\[
L(X) = L(X; \theta) + L(\theta)
\]

(3)

where \( L(\theta) \) is the code length of model parameters \( \theta \) under a chosen prior distribution \( P(\theta) \). For a univariate continuous probability distribution, with density function \( p(x) \), one can approximate a discrete distribution \( P \) by partitioning the sample space into intervals \( I = \{i\} \) of length \( \epsilon \) and assigning a probability mass to each interval \( P(x \in i) \approx p(x_i)\epsilon \), where \( x_i \) is the center of \( i \). For multivariate density \( p(x) \), we can generalize this discretization to have \( P(x \in i) \approx p(x_i)\epsilon |x| \), where \( |x| \) denotes the dimensions of \( x \). We define the code length of \( x \) using this discretized distribution by

\[
L(x) = -\log P(x \in i) \overset{\text{def}}{=} -\log p(x) - \log \epsilon |x| \quad (4)
\]

3 Variational Hyper-Encoding Networks

3.1 Hyper-auto-encoding problem

Given a set of \( T \) distributions \( D = \{D_t\}_{t=1}^T \) called tasks, each containing samples \( x \sim p_{D_t}(x) \), our problem is first fitting each parametric model \( p(x; \theta_t) \), parameterized by \( \theta_t \in \Theta \), to each \( D_t \):

\[
\hat{\theta}_t = \underset{\theta \in \Theta}{\text{argmax}} \ p(D_t; \theta)
\]

(5)

then fitting a parametric model \( p(\theta; \gamma) \), parameterized by \( \gamma \in \Gamma \) to the set \( \{\theta_t\}_{t=1}^T \). However, there are major drawbacks to this approach. First, the number of tasks may not be sufficient to fit enough number of \( \theta \), for fitting \( p(\theta; \gamma) \). Second, although we may resample \( D_t \) and refit \( \theta_t \) to create more samples, it is computationally expensive. A more practical method is to jointly learn the distribution of \( \theta \) and \( D \).

3.2 Hyper-encoding problem

We focus on latent variable models for \( p(x|\theta) \) and \( p(\theta|\gamma) \) where the joint distributions factorize:

\[
p(x|\theta_t) = \int p(x, z|\theta_t) dz = \int p(x|z, \theta_t)p(z) dz
\]

\[
p(\theta|\gamma) = \int p(\theta, u|\gamma) du = \int p(\theta|u, \gamma)p(u) du
\]

where \( z \) is the latent variable of \( x \), and \( u \) is the latent variable of \( \theta \). We assume Gaussian priors for both \( z \) and \( u \), \( z \sim \mathcal{N}(0, I) \) and \( u \sim \mathcal{N}(0, I) \). We also define \( p(x|\theta_t) = p(x; \theta_t) \), i.e. the conditional distribution \( p(x|\theta_t) \) is the distribution \( p(x; \theta_t) \) parameterized by neural networks with parameters \( \theta_t \). Similarly \( p(\theta|\gamma) = p(\theta; \gamma) \). We assume a Dirac delta distribution for \( \gamma \) in this study, i.e. a point estimate \( \gamma \), therefore we will use the parametric notation for \( \gamma \) from now on. Note that \( x \) is observed, and \( \theta \) is observed only if we train \( \theta \) on the dataset \( D \).

We aim to maximize the joint log-likelihood \( \log p(\theta, D; \gamma) \), marginalized over the latent representation \( u \),

\[
\log p(\theta, D; \gamma) = \log \mathbb{E}_{p(u)} p(\theta, D|u; \gamma)
\]

\[
= \log \mathbb{E}_{q(u|\theta, D; \gamma)} \frac{p(\theta, D|u; \gamma)p(u)}{q(u|\theta, D; \gamma)}
\]

(6)

where \( q(u|\theta, D; \gamma) \) is a tractable variational posterior distribution of \( u \).

We use a Monte-Carlo integration to approximate the expectation in Eq. 6 as the sum of \( K \) samples from \( q(u|\theta, D; \gamma) \):

\[
\log p(\theta, D; \gamma) \approx \mathcal{L}(D, \theta; \gamma) \overset{\text{def}}{=} \log \frac{1}{K} \sum_{k=1}^K \frac{p(\theta, D|u_k; \gamma)p(u_k)}{q(u_k|\theta, D; \gamma)}
\]

(7)
where θ we can bypass the optimizing step of η and minimize θ served, we sample α q distribution for q diag µ is a Gaussian with mean D it is dependent on D is updated using gradient ascent, W training objective for unobserved θ: Since θ is unobserved, we sample θ using ancestral sampling:

\[ \theta \sim q(\theta|D) \approx \frac{1}{K} \sum_{k} p(\theta|u; \gamma) q_k(u|D; \gamma) \]

where q_k(u|D; \gamma) is the k-th Gaussian of the mixture in Eq. 11 and minimize \( \mathcal{L}(\theta, D; \gamma) \) in Eq. 7.

Maximizing (7) w.r.t. to the parameter γ using stochastic gradient ascent requires computing the following gradient:

\[
\frac{\partial}{\partial \gamma} \mathcal{L}(D, \theta; \gamma) = \frac{\partial}{\partial \gamma} \log \frac{1}{K} \sum_{k} p(\theta, D|u_k; \gamma) p(u_k) \tag{8}
\]

\[
= \sum_{k} \frac{\partial}{\partial \gamma} \log \frac{p(\theta, D|u_k; \gamma)}{q(u_k|\theta, D; \gamma)} \tag{9}
\]

where \( \frac{\partial}{\partial \gamma} \frac{p(\theta, D|u_k; \gamma)}{q(u_k|\theta, D; \gamma)} \) is a normalizing factor. γ is then updated using gradient ascent,

\[
\gamma = \gamma + \eta \frac{\partial}{\partial \gamma} \mathcal{L}(D, \theta; \gamma) \tag{10}
\]

where η is the learning rate. However, since θ is trained on D, it is dependent on D, the approximate posterior \( q(u|\theta, D; \gamma) \) depends on D through θ. We will use neural networks to approximate this posterior, therefore we can take this advantage to make the dependency explicit, i.e. \( q(u|\theta, D; \gamma) = q(u|D; \gamma) = \mathcal{N}(u; \mu_{\gamma}(D), \text{diag}(\sigma_{\gamma}^2(D))) \) (in this case q is a Gaussian with mean \( \mu_{\gamma}(D) \) and diagonal covariance \( \sigma_{\gamma}^2(D) \), and \( \mu_{\gamma} \) and \( \sigma_{\gamma}^2 \) are neural networks). Thus we can bypass the optimizing step of θ.

In practice, the posterior distribution \( q(u|D; \gamma) \) is usually complex, therefore we propose to use a Gaussian mixture distribution for q:

\[
q(u|D; \gamma) = \sum_{k=1}^{K} \alpha_k(D) q_k(u|D; \gamma) = \sum_{k=1}^{K} \alpha(x_k) q_k(u|x_k; \gamma) \tag{11}
\]

\[
= \sum_{k=1}^{K} \alpha(x_k) \mathcal{N}(u; \mu_{\gamma}(x_k), \text{diag}(\sigma_{\gamma}^2(x_k))) \tag{12}
\]

where \( \alpha, \mu_{\gamma}, \text{and } \sigma_{\gamma}^2 \) are neural networks predicting the parameters for each \( q_k \), and \( x_k \) is a random sample from D. For simplicity we assume a uniform mixing distribution and set \( \alpha(x_k) = 1/K \).

Training objective for unobserved θ: Since θ is unobserved, we sample θ using ancestral sampling:

\[
\theta \sim q(\theta|D) \approx \frac{1}{K} \sum_{k} p(\theta|u; \gamma) q_k(u|D; \gamma)
\]

Calculating \( p(\theta, D|u_k; \gamma) \): We choose a Dirac delta distribution for the posterior of θ, \( q(\theta|u) = \delta(\theta(u)) \) and define the log-likelihood \( \log p(\theta, D|u_k; \gamma) = \log p(D|\theta(u_k); \gamma) \). Under the VAE model with parameter \( \theta \) we have the standard lower bound of the log-likelihood (ELBO) as:

\[
\log p(D|\theta) = \sum_{x} \log p(x; \theta) \geq \sum_{x} \text{elbo}(\theta, x) \tag{13}
\]

where

\[
\text{elbo}(\theta, x) = \mathbb{E}_{q(z|x; \theta)} \log p(x|z; \theta) - \text{KL}(q(z|x; \theta) || p(z))
\]

We use \( \sum_{x} \text{elbo}(\theta, x) \) in Eq. 13 in place of \( \log p(D|\theta, u_k; \gamma) \), thus optimizing a lower bound of the original objective. Fig. 1 shows the overall graphical models of the HyperVAE.

3.3 HyperVAE and MDL

We assume a setting where there is a sequence of datasets (or tasks) and model parameters \( \{(D_t, \theta_t)\} \), a sender wish to transmit to a receiver using a minimal combined code length. Let also assume we are working with discretized distributions each with its own precision. Under the crude MDL, the expected code length for transmitting a dataset D and the model parameters \( \theta \) for Eq. 5 is:

\[
L(D) = L(D|\theta) + L(\theta) \tag{14}
\]

Therefore, model selection by minimizing this code length is equivalent to minimizing the negative of a regularized MLE objective:

\[
\hat{\theta} = \arg\min_{\theta \in \Theta} L(D|\theta) + L(\theta)
\]

\[
= \arg\min_{\theta \in \Theta} - \log P(D; \theta) - \log P(\theta)
\]

where we used \( P \) to denote the discretized distribution of the corresponding density \( p \) with a chosen precision. However this coding is inefficient. We will describe a more efficient coding scheme using HyperVAE with bits-back coding[Hinton and Van Camp, 1993; Hinton and Zemel, 1994] next.

Under the HyperVAE the code length of D is:

\[
L(D) = L(D|\theta) + L(\theta|u) + L(u) \tag{15}
\]

We choose a Dirac delta distribution for \( \theta, p(\theta|u) = \delta(\theta(u)) \), and make \( \theta \) deterministic from \( u \). Therefore the total code length becomes:

\[
L(D) = L(D|\theta(u)) + L(u)
\]
Using bits-back coding, this code length should be shorter by exploiting the fact that the choice of \( u \) can carry additional information up to the entropy of \( q(u|D) \).

We will briefly describe bits-back coding, where we use \( \log_2 \) for simplicity, more details can be found in [Townsend et al., 2019]. Let assume the sender has some extra bits to transmit in addition to \( D \) and \( u \). Let also assume that both the sender and receiver can compute \( p(u) \) and \( p(D|u) \), and given all \( u \) and \( D \), they can both learn \( q(u|D) \). The sender first use the extra bits to generate a sample \( u \sim q(u|D) \), then encode \( u \) by \( p(u) \) and encode \( D \) by \( p(D|u) \). At the receiver end, all \( u \) and \( D \) received are decoded using the agreed priors \( p(u) \) and \( p(D|u) \). The receiver then learns \( q(u|D) \) and can decode the extra bits from \( u \) using this \( q(u|D) \). Therefore we should subtract the extra bits, \(- \log q(u|D)\), from the total description length.

The expected code length for \( u \) over \( q(u|D) \) is then:

\[
L(u) = \mathbb{E} [- \log P(u) + \log Q(u|D)]
\]

where we omit the discretization formulae of \( P \) and \( Q \) (Eq. 4) in Eq. 17, and we choose the same precision \( \epsilon[u] \) for the prior and posterior of \( u \). Note that the precision \( \epsilon[u] \) in Eq. 17 is canceled out, thus \( u \) can be discretized with arbitrary precision.

The final expected code length of \( D \) in HyperVAE is then:

\[
L(D) = \mathbb{E}_{q(u|D)} [L(D|\theta(u))] + \text{KL}(q(u|D)\|p(u))
\]

which is equivalent to the negative of (7) when \( K = 1 \):

\[
L_1(D, \theta) = \mathbb{E}_{q(u|\theta, D)} \left[ \frac{p(\theta, D|u)p(u)}{q(u|\theta, D)} \right]
\]

where we omit \( \gamma \) for clarity and use the fact that \( p(\theta, D|u) = p(D|u) \) when \( \theta = \delta(\theta(u)) \), and the assumption \( q(u|\theta, D) = q(u|D) \). Therefore, we have designed HyperVAE to minimize the description length (18).

3.4 Compact hyper-decoder architecture

Since neural networks weights are matrices that are highly structured and often overparameterized, we discover that a more powerful but compact method is to use a matrix encoding for network weights. More concretely, a matrix hyper-layer receives an input matrix \( H \) and computes a weight matrix \( W \) as \( W = \sigma(UHV + B) \), where \( U, V, B \) are parameters. As an example, if \( H \) is a 1D matrix of size 400 \( \times \) 1 and a target weight \( W \) of size 400 \( \times \) 400, a matrix-layer will require 176 thousand parameters, a 3 order of magnitude reduction from 64.16 million parameters of the standard fully-connected hyper-layer. This compactness allows for complex decoder architecture for generating the target network, unlike hyper-networks methods which rely on a linear layer of an embedding vector for each target-network layer.

3.5 Novel discovery

HyperVAE provides an extra dimension for exploring the model space \( \Theta \) in addition to exploring the design space \( \mathcal{X} \). Once trained, the network can guide exploration of new VAE models for new tasks with certain similarity to the trained tasks.

Given no prior information, we can freely draw models \( \theta(u) \) from \( u \sim p(u) \) and designs \( x \sim p_0(x|z) \) with \( z \sim p_0(u)(z) \) and search for the desired \( x^* \) satisfying some property \( F(x^*) \).

An intuitive approach is to employ a global search technique such as Bayesian Optimization (BO) in both the model latent space of \( u \) and in the data latent space of \( z \). However searching for both \( u \in \mathcal{U} \) and \( z \in \mathcal{Z} \) is expensive due to the combined number of dimensions can be very high. Furthermore, reducing the latent dimension would affect the capacity of VAE. To overcome this major challenge, we use BO for optimizing the \( z \) space and replace the search in \( u \) space by an iterative search heuristic. The workflow starts with an initial exemplar \( x_0^* \) which can be completely uninformative (e.g., an empty image for digits or a random design), or properly guided (e.g., from the best choice thus far in the database, or from what is found by VAE+BO itself). The search process for the optimal design at step \( t \) as follows:

\[
\begin{align*}
\theta_t &= g_{\gamma}(u_t); \\
\theta_t &= \text{BO}(g_{\gamma}(z^*_t)); \\
z^*_t &\leftarrow g(z^*_t).
\end{align*}
\]

where \( d_{t-1} \leftarrow x_{t-1}^* \).

The optimization step in the \( z \) space maximizes a function \( \max_x F(x) = \max_z F \circ g_{\gamma}(z) \) for a fixed generator \( \theta_t \). Let \( z_t^* \) and thus \( x_t^* = g_{\gamma}(z_t^*) \) be the solution found at step \( t \). The generator parameter in the subsequent step is set as \( \theta_{t+1} = \theta(\mu_t(x_t^*)) \) where \( \mu_t \) is the posterior mean. Thus the HyperVAE step transforms the objective function with respect to \( z \) by shifting \( \theta_t \).

4 Experiments

We evaluate HyperVAE on three tasks: density estimation, robust outlier detection, and novel discovery.

4.1 Data sets

We use three datasets: MNIST handwritten digits, Omniglot handwritten characters, and Aluminium Alloys dataset. The MNIST contains 60,000 training and 10,000 test examples of 10 classes ranging from 0 to 9. The Omniglot contains 24,345 training and 8,070 test examples. In both datasets, the images are binarized to have pixel values in \{0, 1\}.

The Alloys dataset (https://tinyurl.com/tmah538), previously studied in [Nguyen et al., 2019], consists of 15,000 aluminium alloys. Aluminium alloy is a combination of about 85% aluminium and other elements.

Phase diagram contains important characteristics of alloys, representing variations between the states of compounds at different temperatures and pressures. They also contain thermodynamic properties of the phases. In this experiment, a phase diagram is coded as a 2D matrix, in which each cell is the prevalence of a phase at a particular temperature.

4.2 Model setting

We use a similar architecture for VAE in all datasets. The encoder has 2 convolution layers with 32 and 64 filters of
size $3 \times 3$, stride 2, followed by one dense layer with 400 hidden units, then two parallel dense layers to output the mean and log variance of $q(z|x; \theta)$. The decoder architecture exactly reverses that of the encoder to map from $z$ to $x$, with transposed convolution layers in place of convolution layers, and outputs the Bernoulli mean of $p(x|z; \theta)$. For the alloys dataset, the convolution layers are replaced by matrix layers with size $200 \times 200$, as in [Do et al., 2018]. We also use a similar architecture for HyperVAE in all datasets. The encoder uses the same architecture as the VAE’s encoder. The decoder uses a dense layer with 400 hidden units, followed by $L$ parallel matrix layers generating the weights, biases, and filters of the target VAE network, resembling the parameter $\theta$. The input to the matrix layer is reshaped into size $20 \times 20$. All layers except the last layer use RELU activation. The $z$-dimension is: 50 (MNIST&Omniglot), 10 (Alloys), and the $u$-dimension is: 50 (MNIST&Omniglot), and 10 (Alloys).

We used Adam optimizer with parameters $\beta_1 = 0.9$, $\beta_2 = 0.999$, learning rate $\eta = 0.0003$, minibatches of size 30, and ran for 100000 iterations or when the models converge.

### 4.3 Model behavior

We study whether the HyperVAE learns a meaningful latent representation and data distribution for the MNIST and Omniglot datasets. We use negative log-likelihood (NLL) and $KL(q(z|x)||p(z))$ as measures. NLL is calculated using importance sampling with 1024 samples. We compare VAE and HyperVAE in Table 1, and as seen the HyperVAE outperforms the VAE on NLL on MNIST dataset and on NLL and KL on Omniglot dataset.

|       | MNIST | Omniglot |
|-------|-------|----------|
|       | NLL   | KL       | NLL   | KL     |
| 1     | 80.7 ± 0.6 | 30.0 ± 0.1 | 120.4 ± 0.6 | 28.9 ± 0.1 |
| 2     | 76.5 ± 0.3 | 30.7 ± 0.2 | 117.7 ± 0.1 | 28.0 ± 0.3 |

Table 1: Model behavior of VAE (1) vs HyperVAE(2): Negative Log-likelihood (NLL) and $KL(q(z|x)||p(z))$ (KL) and their standard errors shown. Smaller values are better.

### 4.4 Robust outlier detection

Next, we study HyperVAE model for outlier detection tasks. We use MNIST dataset to create 10 outlier detection tasks. In each task $t \in \{0, \ldots, 9\}$, we select all digits of class $t$ as normal data and randomly select the digits to create 5% outliers. We use MNIST training set for training tasks and its test set for test tasks. Both VAE and HyperVAE models are trained on only normal data. The negative ELBO is used for outlier scoring. Table 2 shows that HyperVAE has better AUC compared to VAE. While the false negative rate of both models is similar, the false positive rate for HyperVAE is one third of that of VAE. This is because HyperVAE was trained across tasks and can have better support between tasks.

|       | VAE  | HyperVAE |
|-------|------|----------|
| AUC   | 0.88 | 0.96     |
| FPR   | 0.015| 0.005    |
| FNR   | 0.055| 0.04     |
| Precision | 0.75 | 0.92 |

Table 2: Outlier detection on MNIST. AUC (Area under curve), False positive Rate (FPR), False Negative Rate (FNR), and Precision.

This experiment illustrates the capability of HyperVAE+BO in novel exploration on MNIST. For each experiment, one digit is held out. We used nine digit classes for training and tested the model ability to search for high quality digits of the remaining unseen digit class. BO is applied to search for new digits that are similar to a given new exemplar in the $z$-space.

In the iterative process, an empty image $d_t = 0$ is given at the first step, and subsequently updated as $d_t = x_t^*$. After each step $t$ we set $u_t = \mu(x_t^*)$. The quality curves are
presented Fig. 3. Examples of discovery process are listed in Fig. 2. The figures show that VAE has a very limited capability to support exploration outside the known regions, while Hyper-VAE is much more flexible, even without the iterative process (#Step = 1). With more iterative refinements, the quality of the explored samples improves.

**Alloy discovery**

We now use the framework to search for a new class of alloys. For each experiment, one alloy is held out. Models are trained on the remaining 29 alloys. We work on the phase space as a representation of the material composition space, to take advantage of the closeness of phase space to the target performance. We treat the phase diagrams as matrices whose values are proportions of phases at different temperatures. The goal is to search for a new class of alloys that is similar to the “ideal” alloy that has not been seen in any previous alloy classes. BO is applied to search for new alloys that are similar to a given new ideal alloy in the space of z. In the iterative process, we can initialize the search by an uninformative model \( u_1 = 0 \) or the one found by VAE+BO (the “Iterative + VAE init”). Subsequently the model is updated by setting \( d_t = x^∗_{t-1} \). The \( u \) variable is set to \( u_t = \mu(x^∗_t) \) after each step \( t \).

We utilize the matrix structure of the phase diagram and avoid overfitting by using matrix representation for the input [Do et al., 2018]. To inversely map the phase diagram back to the element composition, we use the inverse program learned from the phase-composition dataset, as described in [Nguyen et al., 2019]. To verify that the found materials are realistic (to account for the possible error made by the inverse program), we run the Thermo-Calc software to generate the phase diagrams. These computed phase diagrams are compared against the explored samples. The result from Thermo-Calc confirms that the found alloys are in the target class.

To examine the effect of initialization to HyperVAE+BO performance, we initialized it by either uninformative hypothetical alloy (e.g., with hyper prior of zeros), with the alloy found by VAE+BO, or with a chosen known alloy. The performance curves are shown in Fig. 4. “Once” means running HyperVAE for just one step. “Iterative + VAE init” means initialization of \( d_1 = x^∗ \) by VAE. It shows: (a) For a majority of cases, HyperVAE+BO initialized uninformatively could find a better solution than VAE+BO, and (b) initializing HyperVAE+BO with solution found by VAE+BO boosts the performance further, sometimes a lot more. This suggests that care must be taken for initializing HyperVAE+BO.

**5 Related Work**

Our method can be considered as a lossless compression strategy where the HyperVAE compresses a family of networks that parameterizes the parameters of distributions across datasets. The total code length of both the model and data misfits are minimized using HyperVAE, thus help it generalize to unseen data. This is in contrast to the lossy compression strategy [Chen et al., 2016] where local information of images are freely decoded independent of the compressed information.

The HyperVAE shares some insight with the recent MetaVAE [Choi et al., 2019], which models the joint distribution of data \( x \) and task \( D: P(D, x, z) = P(D \mid z)P(x \mid z) \). But this is different from ours in the target and modeling, where the latent \( z \) is factored into data latent variable \( z \) and the task latent variable \( u \). Hyper-VAE is related to Bayesian VAE, where the model is also a random variable generated from some hyper-prior. There has been some work on priors of VAE [Le et al., 2018; Tomczak and Welling, 2017], but using VAE as a prior for VAE is new.

HyperGAN [Ratzlaff and Fuxin, 2019] is a recent attempt to generate the parameters of model for classification. This framework generates all parameters from a single low dimension Gaussian noise vector. Bayesian neural networks (BNN) in [Wang et al., 2018] also use GAN framework for generating network parameters \( \theta \) that looks real similar to one drawn from BNN trained with stochastic gradient Langevin dynamics. However, GAN is not very successful for exploration but more for generating realistic samples.

Continual learning are gaining ground in recent years. Variational continual learning [Nguyen et al., 2018], for example, solves catastrophic forgetting problems in supervised learning, but it still needs a set of prototype points for old tasks. [Rao et al., 2019] tackles this problem in unsupervised tasks and also does task inference as ours, however our settings and approaches are different. Meta-learning frameworks for classification and regression [Finn and Levine, 2018; Finn et al., 2018; Yoon et al., 2018; Grant et al., 2018; Mishra et al., 2018] is another direction where the purpose is to learn agnostic models that can quickly adapt to a new task.

**6 Conclusion**

We propose a new method called HyperVAE for encoding a family of neural network models into a simple distribution of latent representations. By explicitly training the variational hyper-encoder network over a complex distribution of tasks, the hyper-network learns the smooth manifold of the family encoded in the posterior distribution of the family. This enables the model to extrapolate to new tasks close to trained tasks. It can be thought of as expanding the support of the distribution of trained model, thus is useful for downstream tasks such as searching for a data distribution close to existing ones and reducing the false positive error in outlier detection.
References

[Chen et al., 2016] Xi Chen, Diederik P Kingma, Tim Salimans, Yan Duan, Prafulla Dhariwal, John Schulman, Ilya Sutskever, and Pieter Abbeel. Variational lossy autoencoder. arXiv preprint arXiv:1611.02731, 2016.

[Choi et al., 2019] Kristy Choi, Mike Wu, Noah Goodman, and Stefano Ermon. Meta-amortized variational inference and learning. arXiv preprint arXiv:1902.01950, 2019.

[Do et al., 2018] Kien Do, Truyen Tran, and Svetha Venkatesh. Learning deep matrix representations. arXiv preprint arXiv:1703.01454, 2018.

[Finn and Levine, 2018] Chelsea Finn and Sergey Levine. Meta-learning and universality: Deep representations and gradient descent can approximate any learning algorithm. ICLR, 2018.

[Finn et al., 2017] Chelsea Finn, Pieter Abbeel, and Sergey Levine. Model-agnostic meta-learning for fast adaptation of deep networks. In Proceedings of the 34th International Conference on Machine Learning-Volume 70, pages 1126–1135. JMLR. org, 2017.

[Finn et al., 2018] Chelsea Finn, Kelvin Xu, and Sergey Levine. Probabilistic model-agnostic meta-learning. In Advances in Neural Information Processing Systems, pages 9516–9527, 2018.

[Finn et al., 2019] Chelsea Finn, Aravind Rajeswaran, Sham Kakade, and Sergey Levine. Online meta-learning. arXiv preprint arXiv:1902.08438, 2019.

[Gómez-Bombarelli et al., 2018] Rafael Gómez-Bombarelli, Jennifer N Wei, David Duvenaud, José Miguel Hernández-Lobato, Benjamín Sánchez-Lengeling, Dennis Sheberla, Jorge Aguilera-Iparraguirre, Timothy D Hirzel, Ryan P Adams, and Alán Aspuru-Guzik. Automatic chemical design using a data-driven continuous representation of molecules. ACS central science, 4(2):268–276, 2018.

[Grant et al., 2018] Erin Grant, Chelsea Finn, Sergey Levine, Trevor Darrell, and Thomas Griffiths. Recasting gradient-based meta-learning as hierarchical bayes. arXiv preprint arXiv:1801.08930, 2018.

[Ha et al., 2016] David Ha, Andrew Dai, and Quoc V Le. Hypernetworks. arXiv preprint arXiv:1609.09106, 2016.

[Hinton and Van Camp, 1993] Geoffrey Hinton and Drew Van Camp. Keeping neural networks simple by minimizing the description length of the weights. In In proc. of the 6th Ann. ACM Conf. on Computational Learning Theory. Citeseer, 1993.

[Hinton and Zemel, 1994] Geoffrey E Hinton and Richard S Zemel. Autoencoders, minimum description length and helmholtz free energy. In Advances in neural information processing systems, pages 3–10, 1994.

[Honkela and Valpola, 2004] Antti Honkela and Harri Valpola. Variational learning and bits-back coding: an information-theoretic view to bayesian learning. IEEE Transactions on Neural Networks, 15(4):800–810, 2004.

[Kingma and Welling, 2013] Diederik P Kingma and Max Welling. Auto-encoding variational Bayes. arXiv preprint arXiv:1312.6114, 2013.

[Krueger et al., 2017] David Krueger, Chin-Wei Huang, Riashat Islam, Ryan Turner, Alexandre Lacoste, and Aaron Courville. Bayesian hypernetworks. arXiv preprint arXiv:1710.04759, 2017.

[Le et al., 2018] Hung Le, Truyen Tran, Thin Nguyen, and Svetha Venkatesh. Variational memory encoder-decoder. In NeurIPS, 2018.

[Mishra et al., 2018] Nikhil Mishra, Mostafa Rohaninejad, Xi Chen, and Pieter Abbeel. A simple neural attentive meta-learner. ICLR’18, 2018.

[Nguyen et al., 2018] Cuong V Nguyen, Yingzhen Li, Thang D Bui, and Richard E Turner. Variational continual learning. ICLR, 2018.

[Nguyen et al., 2019] Phuoc Nguyen, Truyen Tran, Sunil Gupta, Santu Rana, Matthew Barnett, and Svetha Venkatesh. Incomplete conditional density estimation for fast materials discovery. In Proceedings of the 2019 SIAM International Conference on Data Mining, pages 549–557. SIAM, 2019.

[Rao et al., 2019] Dushyant Rao, Francesco Visin, Andrei Rusu, Razvan Pascanu, Yee Whye Teh, and Raia Hadsell. Continual unsupervised representation learning. In Advances in Neural Information Processing Systems, pages 7645–7655, 2019.

[Ratzlaff and Fuxin, 2019] Neale Ratzlaff and Li Fuxin. HyperGAN: A Generative Model for Diverse, Performant Neural Networks. ICML, 2019.

[Rezende et al., 2014] Danilo Jimenez Rezende, Shakir Mohamed, and Daan Wierstra. Stochastic backpropagation and approximate inference in deep generative models. arXiv preprint arXiv:1401.4082, 2014.

[Shahriari et al., 2016] Bobak Shahriari, Kevin Swersky, Ziyu Wang, Ryan P Adams, and Nando De Freitas. Taking the human out of the loop: A review of bayesian optimization. Proceedings of the IEEE, 104(1):148–175, 2016.

[Tomczak and Welling, 2017] Jakub M Tomczak and Max Welling. VAE with a VampPrior. arXiv preprint arXiv:1705.07120, 2017.

[Townsend et al., 2019] James Townsend, Tom Bird, and David Barber. Practical lossless compression with latent variables using bits back coding. arXiv preprint arXiv:1901.04866, 2019.

[Wang et al., 2018] Kuan-Chieh Wang, Paul Vicol, James Lucas, Li Gu, Roger Grosse, and Richard Zemel. Adversarial distillation of bayesian neural network posteriors. In International Conference on Machine Learning, pages 5177–5186, 2018.

[Yoon et al., 2018] Jaesik Yoon, Taesup Kim, Ousmane Dia, Sungwoong Kim, Yoshua Bengio, and Sungjin Ahn. Bayesian model-agnostic meta-learning. In Advances in Neural Information Processing Systems, pages 7332–7342, 2018.