Evaluating Combinatorial Generalization in Variational Autoencoders

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Abstract
We evaluate the ability of variational autoencoders to generalize to unseen examples in domains with a large combinatorial space of feature values. Our experiments systematically evaluate the effect of network width, depth, regularization, and the typical distance between the training and test examples. Increasing network capacity benefits generalization in easy problems, where test-set examples are similar to training examples. In more difficult problems, increasing capacity deteriorates generalization when optimizing the standard VAE objective, but once again improves generalization when we decrease the KL regularization. Our results establish that interplay between model capacity and KL regularization is not clear cut; we need to take the typical distance between train and test examples into account when evaluating generalization.

1 Introduction
Variational autoencoders (VAEs) [Kingma and Welling, 2013; Rezende and Mohamed, 2015] and other deep generative models (DGMs) are used for three related yet distinct tasks. One use emphasizes generation, another emphasizes density estimation, and the third emphasizes learning of representations in an unsupervised or semi-supervised manner. While DGMs are often evaluated in the context of the first two tasks, it is arguably the third use case that ultimately motivates work on these model classes to begin with; we would like to be able to extract features with high predictive power from complex data such as natural images (Gulrajani et al., 2017), audio (van den Oord et al., 2016), 3d scenes (Eslami et al., 2018), or natural language (Liang et al., 2018), with little or no supervision. In this paper we ask to what extent VAEs generalize in domains where the data distribution is characterized by a large combinatorial space of (possibly unknown) generative factors. This question is particularly relevant when the underlying generative process is some form of grammar that gives rise to a combinatorial explosion of possible scenes, pieces of text, molecular configurations, or programs. However, even when the underlying feature space is a simple Cartesian product over generative factors, the set of possible combinations of features grows exponentially with the dimensionality of the feature space. Therefore it is not realistic to expect the training data to contain samples for all possible combinations of features. Any useful generative model operating on similar data must be able overcome this problem and generalize to novel data with unseen combinations of features.

Much of the recent work on generalization of neural architectures has considered discriminative models. In this context, there is evidence that overparameterization aids generalization, which runs contrary to the classic intuition that increasing model capacity beyond a certain point leads to overfitting (Belkin et al., 2019; Zhang et al., 2016; Neyshabur et al., 2014). These results have given rise to the hypothesis that the classically observed deterioration of generalization performance is in fact a local minimum, and that increasing capacity further can lead to a “modern interpolation” regime in which generalization performance again ben-
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It is as yet unclear to what extent this modern interpolation regime can also be observed in VAEs and other DGMs. When training a discriminative model, we typically define a notion of utility (e.g. the classification loss) that allows us to map high-dimensional data onto low-dimensional manifolds (e.g. position relative to a classification boundary). When training generative models, we necessarily need to account for all factors of variation in the data. However, even for feature spaces of intermediate dimensionality, the training data will not contain exemplars for all possible combinations of features. This means that the generalization characteristics of generative models could be qualitatively different from those of discriminative models. To understand the generalization characteristics of VAEs, we therefore need to consider the interplay between the model capacity, the coverage of training data (i.e. how much of the feature space is covered by training examples), and the dimensionality of underlying generative factors.

In this paper, we carry out a systematic empirical study to evaluate the extent to which learned representations and density estimation in VAEs generalize across large combinatorial feature spaces. Our experiments probe the role of the network width, depth, the amount of training data, and the difficulty of the generalization problem. We increase the difficulty of the generalization problem in two ways: 1) decreasing the amount of training data, 2) splitting the data into training and test sets in a structured manner (as illustrated in Figure 1). To establish a baseline understanding that can inform future work, these experiments focus on comparatively simple base cases. We consider fully-connected encoder and decoder architectures with ReLU activations, and evaluate performance on a dataset of simulated tetrominoes, which has been designed to control the difficulty of the generalization problem. We evaluate the models using the log marginal likelihood of the data (LM), and the rate-distortion (RD) curve which we estimate by training each model with a $\beta$-VAE objective for a wide range of $\beta$ values.

Our extensive experiments, spanning over a large grid over the aforementioned factors concerning generalization, resulted in over 3000 trained models. A known property of VAEs is that the learned generative model can memorize training data in the limit of infinite capacity (Belkin et al. 2019). We find that this memorization is clearly observable in practice. The degree of memorization is primarily dependent on network depth, and to a much lesser extent on the total number of neurons. This result is consistent with recent predictions and empirical results for non-variational autoencoders (Radhakrishnan et al. 2019).

Whereas memorization occurs reliably when we increase model capacity, we find that it can coincide with either improvement or deterioration of generalization performance, depending on how well the training data represent the full combinatorial complexity of the test set. When we have a sufficiently large amount of training data, test examples are well-approximated by convex combinations of training samples. In this regime, generalization performance improves with capacity. In the cases when linear interpolation between training data does not adequately capture the variation in test data, the results are mixed. If we evaluate based on the LM, we find that increasing model capacity can strongly deteriorate generalization perfor-
mance. In this regime, the effect of model capacity is more in line with classical intuitions about overfitt-
ing. If we evaluate based on the RD diagram, we find that decreasing the amount of KL regularization in higher capacity models can improve generalization (if we view the VAE objective as minimizing distortion with the KL acting as a regularizer), where the generalization behaviour is more similar to modern inter-
polation regime. These results hold both when we de-
crease the amount of training data (Figure 1 bottom right) and when we evaluate generalization to combi-
 nations of features that are masked out of the training data (Figure 1 top right).

The rest of the paper is structured as follows: in Section 2 we discuss the relevant prior work. In Section 3 we discuss memorization in VAEs, and provide a moti-
vating example by considering generalization to unseen digits in MNIST (LeCun et al. 1998). We then intro-
duce the Tetrominoes dataset, which is well-calibrated for controlling the difficulty of the generalization prob-
lem, and consider various ways of creating training and test sets with different levels of difficulty (Figure 1). In Section 4 we report experimental results.

2 Related work

There is a body of existing work that applies VAEs to the task of learning representations for datasets in which there is a large combinatorial space of gener-
ative factors. Commonly considered datasets include dSprites (Matthey et al. 2017), 3dShapes (Burgess and Kim 2018), and Chairs (Aubry et al. 2014). These datasets often considered in the context of work that aims to learn disentangled representations [Narayanaswamy et al. 2017; Kim and Mnih 2018; Esmaili et al. 2019; Chen et al. 2018; Locatello et al. 2019], which explicitly separate factors of variation in a fully unsupervised manner. This work has in certain cases been motivated by the desire to learn models that will more readily generalize to unseen combinations of features. While there have been attempts to charac-
terize the generalization performance of disentangled models on held out combinations of features (East-
wood and Williams 2018; Esmaili et al. 2019; Loc-
catello et al. 2019), precisely how disentangling affects generalization, and indeed whether it improves general-
ization, is currently not well-understood.

This paper has a somewhat different focus. Rather than asking the question whether a VAE can explicitly disentangle each factor of variation, we are interested in determining whether a learned (entangled or disentangled) representation can facilitate generalization to unseen combinations of features. There have been a number of attempts for evaluating generalization in DGMs. Work by Zhao et al. (2018) is similar in spirit to our work, but evaluate generalization in a feature-focused manner, drawing similarities to con-
cepts in cognitive psychology. Whereas in this paper, we evaluate models using RD-curves and LM, which are both feature-agnostic. The experimental design of Zhao et al. is based on fixing the architecture (for a given generative model, e.g. a VAE and a GAN) and varying the datasets, whereas in this paper, we use differ-
ent splits of a single dataset, and study how model capacity affects generalization. Our findings are con-
istent with their finding that DGMs can generalize to the immediate neighbourhood of their training data.

In this context, recent work on memorization [Rad-
akrishnan et al. 2019] and generalization (Zhang et al. 2019) in deterministic autoencoders is relevant, which predicts that overparameterized autoencoders will return convex combinations of memorized training data. A similar prediction has been made in work that analyzes the properties of optimal infinite-
capacity VAEs [Bousquet et al. 2017; Rezende and Viola 2018; Alemi et al. 2018; Shin et al. 2018].

There have been a number of works that study the commonly used metrics for evaluating generalization in unsupervised settings. [Theis et al. 2016] review metrics for evaluating generative models and argue that they should be evaluated with respect to the ap-
lications they were intended for; a model with a high test log-likelihood is not necessarily able to generate sharp samples or extract features with high predictive power, and vice versa. Therefore, in this work we study combinatorial generalization for both density estimation and representation learning separately. For density estimation, we consider the LM on the test set. Evaluating the quality of the latent representation is a more challenging task. One possible way is to take the rate-distortion view [Berger 2003]. Rate-distortion theory provides a theoretical framework for lossy data compression through a noisy channel. The framework describes the trade-off between the amount of information that is allowed to be transmitted through the noisy channel (“rate” $R$), against the difference be-
tween the original data and the decoder output (“dis-
tortion” $D$). One way to formulate this problem is minimizing $D$ for a given $R$

$$\text{minimize } D \quad \text{s.t. } R \leq \epsilon. \quad (1)$$

[Alemi et al. 2018] analyze VAEs from the same perspective. They define “distortion” and “rate” as the training log-likelihood and the KL term of the VAE objective, respectively, and analyze model performance by characterizing the trade-off between these two terms in a $RD$ curve. We make use of this type of analysis further on in this work.
Proposition 1 (Shu et al. (2018)) Assume a likelihood \( p(x | z) \) in an exponential family with mean parameters \( \mu \) and sufficient statistics \( T(\cdot) \), a fixed encoder \( q(z | x) \), and training data \( \{x_1, \ldots, x_{N_{\text{train}}}\} \). In the limit of infinite capacity, the optimal decoder \( \mu(z) \) is

\[
\mu(z) = \sum_{n=1}^{N_{\text{train}}} w_n(z) T(x_n),
\]

where

\[
w_n(z) = \frac{q_\phi(z | x_n)}{\sum_m q_\phi(z | x_m)}.
\]

3 Background

VAEs jointly train a generative model \( p_\theta(x, z) \) and an inference model \( q_\phi(z | x) \). The generative model is defined in terms of a prior \( p(z) \) and a likelihood \( p_\theta(x | z) \), which is parameterized using a neural network known as the decoder. The prior is typically a spherical Gaussian. The inference model is defined in terms of an empirical distribution over training data \( \hat{p}(x) = \frac{1}{N} \sum_n \delta_{x_n}(x) \), and a conditional \( q_\phi(z | x) \) that is parameterized by an encoder network. The two models are jointly trained by maximizing a lower bound (ELBO) on the log marginal likelihood

\[
\mathcal{L}(\theta, \phi) = \mathbb{E}_{\hat{p}(x)} \left[ \mathbb{E}_{q_\phi(z|x)} \left[ \log \frac{p_\theta(x, z)}{q_\phi(z|x)} \right] \right],
\]

(2)

Because VAEs maximize log likelihood of the training data, they are at risk of overfitting. Several researchers (Bousquet et al., 2017; Rezende and Viola, 2018; Alemi et al., 2018; Shu et al., 2018) have pointed out that the reconstruction obtained from an infinite capacity optimal decoder of a VAE is a convex combination of examples in the training data. This phenomenon is summarized in the following proposition.

As Proposition 1 predicts, the deep VAE reconstructions closely resemble the nearest neighbors in the training data in latent space. In most cases, a single sample dominates the weighted average. This is evident from the histogram of weight perplexities, which is strongly peaked at 1. This, combined with decoder outputs and neighbours with largest weights, suggests that VAEs can memorize training data even for simple encoder/decoder architectures with moderate capacity, and reconstructions are well-approximated by nearest neighbors in the training set when they do so.

However, it is not the case that VAEs always memorize training data. A surprising finding is that shallow VAEs show comparatively good generalization to out-of-domain samples; reconstructions of 9s are passable, even though this digit class was not seen during training. The same trend is also visible when we compare the binary cross entropy (BCE) between reconstructions and samples from the withheld class, to the BCE between the reconstructions and the weighted averages (see Figure A6). This suggests that the assumption of infinite capacity in Proposition 1 clearly matters, and that layer depth significantly affects the effective capacity of the network.

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**Figure 2**: MNIST 9-removal experiment: Reconstruction of out-of-domain samples by shallow and deep VAEs, alongside weighted average, and neighbours in training data with largest weights. Reconstructions in a deep VAE closely match the weighted average, which in turn are often just the nearest neighbour in training data. Shallow VAE does not exhibit this behaviour and can reconstruct samples cannot be represented by the convex combination of its training data.

| Agent                     | Weighted Average | Neighbours with Largest Weight | Weight Perplexity |
|---------------------------|------------------|--------------------------------|-------------------|
| **Original**              |                  |                                |                   |
| **Recon**                 |                  |                                |                   |
| **Shallow (1 Layer)**     | 4.44             | 4.44                           | 0.17              |
| **Deep (3 Layers)**       | 4.44             | 4.44                           | 0.17              |

For expedience, we use “deep” throughout the paper for architectures with 3 hidden layers, although such networks are of course not deep by modern standards.
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Figure 3: Samples from the Tetrominoes dataset, which comprises 164k images of a J-shaped tetromino that varies in position, orientation, size, and color.

4 Experiments

We evaluate generalization to novel examples in a series of experiments that systematically vary network width, depth, and the difficulty of the generalization problem. We begin by evaluating generalization as a function of model capacity in standard VAEs. We then perform RD analysis to characterize the trade-offs between reconstruction loss (distortion) and the KL regularization (rate). The factors that most strongly determine generalization performance are layer depth and the typical distance between training and test data. Layer width and the amount of training data have much weaker effects. We find that increasing capacity can improve generalization in some cases and deteriorate generalization in others, depending on both the difficulty of the generalization problem, and the degree of KL regularization.

4.1 Tetrominoes Dataset

To assess the ability of a VAE to generalize to unseen combinations of features, we not only require a dataset with known ground truth features, but also one in which we can control the typical distance in pixel space between the training and test examples. There are existing datasets one might use for this purpose; an obvious candidate is the dSprites dataset (Matthey et al., 2017). Unfortunately the shapes in this dataset are close to convex, resulting in an imperceptible deviation in pixel space as we vary rotation. To overcome this limitation, we created the Tetrominoes dataset. Our dataset comprises 32×32 color images of a J-shaped tetromino, which is concave and lacks rotational symmetry. We have procedurally generated 163,840 images based on five i.i.d. continuous generative factors: rotation (sampled from the [0.0, 360.0] range), color (hue, sampled from [0.0, 0.875] range), scale (sampled from [2.0, 5.0] range), and horizontal and vertical position (sampled from an adaptive range to ensure no shape is placed out of bounds). In order to generate uniformly distributed values for all features, we provide code to generate all 7 tetrominoes (I-, O-, T-, S-, Z-, J-, and L-shaped), but use only the J-shaped tetromino in this work due to its concavity and lack of rotational symmetry.

4.2 Train/Test Splits

In our experiments, we compare 4 train/test splits that are designed to vary both the amount of training data and the typical distance between training and test examples.

1. 50/50 random split (Default). The base case in our analysis (Figure 1, top left) is a 82k/82k random train/test split of the full dataset. This case is designed to define an “easy” generalization problem, in the sense that similar training examples will exist for most test examples.

2. Small data, constant density (CD). We create train/test splits for datasets of \{8k, 16k, 25k, 33k, 41k, 49k, 57k, 65k\} examples by applying a mask that constrains the range of feature values (Figure 1, bottom left), ensuring that the density in the feature space remains constant as we reduce the amount of training data.

3. Large data, checkerboard split (Checkerboard). We create a 82k/82k split in which a 5-dimensional “checkerboard” mask partitions the training and test set (Figure 1, top right). This split has the same amount of training data as the base case, as well as the same (uniform) marginal distribution with respect to each of the feature values. This design ensures that for any given test example, we will have 5 training examples that differ in terms of one feature (e.g. color) but are similar with respect to all other features (e.g. position, size, and rotation). In this manner, we pose an out-of-domain generalization task, whilst at the same time ensuring that the model does not need to extrapolate to unseen feature values.

4. Small data for constant volume (CV). Finally, we create train/test splits by selecting \{8k, 16k, 25k, 33k, 41k, 49k, 57k, 65k\} training examples at random without replacement (Figure 1, bottom right). This reduces the amount of training data whilst keeping the volume fixed, which increases the typical distance between training and test examples.

4.3 Network Architectures and Optimization

All experiments employ fully-connected encoders and decoders. In the generative model, we use a spherical Gaussian prior and a Bernoulli likelihood. Unless otherwise stated, shallow networks have 1 hidden layer with 512 neurons followed by a ReLU activation for both the encoder and the decoder. Deep networks have...
3 hidden layers with 512 neurons per layer for both the encoder and the decoder. We use a 10-dimensional latent space. All models are trained for 257k iterations with Adam (default parameters, amsgrad enabled) using a batch size of 128.

4.4 Evaluation Metrics

We use RD analysis and log-marginal likelihood (LM) to evaluate generalization. In RD analysis, we compare the distortion (the reconstruction loss) and the rate (the KL term)

\[
D = -\mathbb{E}_{p(x)q_\phi(z|x)} \left[ \log p_\theta(x | z) \right], \\
R = \mathbb{E}_{p(x)} \left[ \text{KL} \left( q_\phi(z | x) \middle| \middle| p(z) \right) \right].
\]

We approximate LM with an IWAE bound (Burda et al., 2016) that we compute using 1000 samples.

4.5 Effect of Network Capacity

To probe the role of the model capacity in generalization, we compare 9 architectures that are trained using a standard VAE objective on the Default, CV (16k/147k), and Checkerboard splits. The 16k/147k split is designed have similar typical pixel distance between nearest neighbors in the training and test set to the Checkerboard split (see Appendix B), which enables a fair comparison by controlling for the difficulty of the generalization problem. We vary model capacity by using architectures with \{1, 2, 3\} layers that each have \{256, 512, 1024\} neurons.

Figure 4 (left) shows the test-set rate and distortion for all 27 models. Dashed lines indicate contours of equal ELBO = \( D + R \). In Figure 4 (right) we compare the LM for the training and test set. Here the dashed line marks the boundary where the test LM equals the training LM. For the Default split, increasing the model capacity uniformly improves generalization. Conversely, for the CV (16k/147k) and Checkerboard splits, we observe a strong deterioration in generalization performance in all 3-layer architectures.

Figure 4 suggests that increasing model capacity can either improve or hurt generalization, depending on the difficulty of the generalization problem. In the Default split, which poses a comparatively easy generalization task, we observe that increasing model capacity improves generalization, whereas for more difficult tasks (as classically predicted in terms of a bias-variance trade-off), increasing model capacity deteriorates generalization. We note here that the discrepancy between generalization performance on the CV and Checkerboard splits is relatively small, which suggests that these in-domain and out-of-domain tasks are indeed comparable in terms of their difficulty.

4.6 Memorization and Generalization

We qualitatively evaluate the extent to which VAEs memorize the training data (as predicted by Proposition 1). Figure 4 compares the reconstructions of test examples in the Default and Checkerboard splits, by shallow and deep architectures. For each architecture, we show 3 examples from the test set along with reconstructions and nearest training neighbours (with respect to \( w_n \)) for both models. The 3 examples are representatives of easy (<10th percentile), typical (45th-55th percentile), or difficult (>90th percentile) samples in terms of pixel-wise nearest-neighbor distance to the training data. In the case of the Checkerboard split, we see that the 1-layer VAE can reconstruct unseen examples even when the nearest neighbour in the latent space is quite different, while reconstructions for the deep VAE are consistent with the memorization behavior described by Proposition 1. In the Default split, we observe that reconstructions are similar for shallow and deep architectures, and are of-
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Shallow (1 Layer) Deep (3 Layers)

Original $x$ Recons. $\hat{x}$ Nearest Neighbour $x - \hat{x}$ $\hat{x} - \tilde{x}_{nn}$

Original $x$ Recons. $\hat{x}$ Nearest Neighbour $x - \hat{x}$ $\hat{x} - \tilde{x}_{nn}$

Figure 5: Reconstruction of test examples from the Default and Checkerboard splits, along with the nearest neighbour (training example with the largest $w_n$). We compare a shallow and a deep VAE. Rows show examples with increasing reconstruction loss, randomly selected from the 10th (top), 45th to 55th (middle), and 90th (bottom) percentiles.

ten well-approximated by their nearest-neighbors in the training data. Figure A9 shows additional examples for the CV (16k/147k) split.

To provide a more quantitative evaluation, we report distances between $x$, $\mu$ and $\hat{x}$. Figure 6 shows violin plots of the pixel-wise distances between test images and their reconstructions ($\|\hat{x} - x\|$) and the infinite-capacity decoder outputs ($\|\hat{x} - \mu\|$) as defined in Equation (3). We split the test set into 4 bins of equal sizes according to the distance of examples to their nearest training example ($\|x - x_{nn}\|$) and show histogram pairs for each bin. Values in x-axis indicate the limits of each bin.

For splits that are not trivial, we see different behavior across different bins. Looking at the rightmost histogram-pairs (the most difficult 25% of test samples) in each panel, we once again observe qualitatively different behaviors for shallow and deep networks. For the 1-layer networks $\|\hat{x} - x\|$ is smaller than $\|\hat{x} - \mu\|$, which shows that reconstructions cannot be explained by memorization alone. This result holds across all 3 train-test splits. For deep networks, we see that $\|\hat{x} - x\|$ slightly decreases relative to the 1-layer model in the Default split, once again indicating that over-parameterization aids generalization (here in terms of reconstruction loss) in this regime. Conversely for the CV and Checkerboard splits, we see that $\|\hat{x} - x\|$ increases relative to the 1-layer model. Moreover, in the Checkerboard split, we observe that $\|\hat{x} - \mu\|$ is smaller than $\|\hat{x} - x\|$, which shows that reconstructions are closer to memorized data than to the actual test examples.

4.7 Rate-Distortion Analysis

The results we observe in Figure 4 are based on the standard VAE objective. In this objective, there is a trade-off between minimizing the distortion and the rate. To account for this trade-off, we consider the $\beta$-VAE objective, which incorporates a multiplier $\beta$ to control the strength of the KL term

\[
\mathcal{L}(\theta, \phi) = \mathbb{E}_p(x) \left[ \mathbb{E}_{q_\phi(z|x)} \left[ \log p_\theta(x | z) \right] - \beta \text{KL} (q_\phi(z | x) \| p(z)) \right].
\]

Figure 7 shows test-set $RD$ curves for 1-layer, 2-layer, and 3-layer architectures with 512 hidden units in each layer. Each dot constitutes a $\beta$ value averaged over 5 independent restarts. In the Default split, we once again see that increasing model capacity uniformly improves generalization, shifting the curve to the bottom left. However, in the CV and the Checkerboard splits, we see a different pattern. For small $\beta$ values, higher-capacity models are able to achieve a lower distortion, albeit at the expense of a higher rate, shifting the curve to the bottom right.

White stars in Figure 7 indicate the position of the standard VAE ($\beta = 1$) on the $RD$ plane. Normally, we expect the model with $\beta = 1$ to result in the

\[
\beta \in \{0.001, 0.005, 0.01, 0.1, 0.3, 0.5, 0.7, 0.9, 1.0, 2.0, 3.0, 5.0\}
\]
highest ELBO given that it matches the objective exactly. However, as the generalization problem gets more difficult, we observe that increasing the rate (setting $\beta < 1$) in 3-layer networks sharply decreases the distortion and even yields a higher test ELBO.

Figure 6 shows reconstructions for models trained with various $\beta$ values on the CV split. We observe in the low rate regime, both shallow and deep VAEs perform poorly, with shallow VAE performing better. In the high rate regime however, the deep VAE does a better job of reconstructing an unseen example compared the shallow one. More precisely, the $RD$ curve for the 1-layer model shows a small “dip”, which we will discuss in more detail in Section 4.8.

### 4.8 Effect of Dataset Size

As a final experiment, we evaluate the role of the training set size. Our goal is to determine whether a lack of training data in itself hurts generalization, or whether the typical distance between the training and test sets is the main factor that influences the generalization behaviour. To this end, we compute $RD$ curves and LMs for both the CV and the CD splits, in which the training set comprise {8k, 16k, 25k, 33k, 41k, 49k, 57k, 65k} points. In the case of the CV splits, the typical distance between the test examples and their nearest training neighbors increases as we decrease the amount of training data. In the CD splits, this typical distance remains (approximately) constant.

Figure 9 shows the (negative) LM as a function of the training set size at $\beta=1$. Once again, we observe two qualitatively different forms of behavior. In the CD splits, 3-layer networks almost uniformly outperform 1-layer networks. In the case of CV splits, there is a cross-over. The 1-layer model performs better for smaller (sparser) datasets, but is overtaken by the 3-layer model for larger (denser) datasets.

Figure 10 shows $RD$ curves for 1-layer and 3-layer architectures, evaluated on test sets of CV and CD splits with different $N_{\text{train}}$. We observe changes in both the position and the shape of the $RD$ curves as we decrease $N_{\text{train}}$. In the case of CV splits, reducing the number of training data hurts generalization (shifts the $RD$ curve to the top) for both 1-layer and 3-layer architectures, whereas in CD splits the effect of $N_{\text{train}}$ is much less pronounced. This is consistent with the interpretation that reducing $N_{\text{train}}$ in CV splits increases difficulty of the generalization problem, whereas the difficulty in CD splits stays similar.

We similarly observe that both $N_{\text{train}}$ and network depth influence the shape of the $RD$ curves. From previous experiments we know overfitting becomes more pronounced as we reduce $N_{\text{train}}$ in the CV splits. Indeed, for the 1-layer architecture, the $RD$ curve transforms from a well-known Pareto-optimal curve, to a U-shaped curve as we reduce $N_{\text{train}}$. If we interpret $D$ as a measure of empirical risk, and $R$ as a measure of complexity, then these U-shaped curves are consistent with a classic bias-variance trade-off.

This trend does not hold for 3-layer architectures; whereas for large $N_{\text{train}}$ we observe qualitatively similar results across both splits and architectures, there is no clearly defined U-shaped curve that appears for smaller $N_{\text{train}}$ values. However, we do observe a slight “bump” in some of these curves (see Figures A13 and A14). For example, the $N_{\text{train}}=16k$ curve dips and briefly increases near $\beta = 1$, but then decreases once more for smaller $\beta$ values. While we emphasize that these results are far from conclusive, this could in fact be evidence of a double-U-shaped risk curve as observed by Belkin et al. (2019). This would signify that
the 3-layer model resides in a “modern interpolation” regime for $\beta < 1$ (see Figures A13 and A14).

5 Conclusion

This empirical study, in which we trained over 3000 VAE instances, evaluates to what extent VAEs are able to generalize to novel examples in domains with a large combinatorial space of feature values. One of the main questions in this context is whether increasing model capacity generally aids generalization, or whether VAEs can also be susceptible to overfitting. Our results demonstrate that the answer to this question is not clear cut; increasing model capacity can either improve or deteriorate generalization, depending on the degree of KL regularization and the difficulty of the generalization task.

The key factor that determines the difficulty of a generalization problem is the relationship between the amount of training data and the dimensionality of the data distribution. When we have a sufficiently large amount of data, the training set will contain close analogs to most test examples. In this regime, interpolation between memorized examples will yield good generalization performance. However, in many practical problems of interest, the data will be characterized by a large number of generative factors, which give rise to a combinatorial explosion of possible feature combinations. In this regime, generalization fundamentally requires reasoning about examples that correspond to unseen combinations of features, for which there are no close analogs in the training data.

To probe these two regimes, we provide a Tetrominoes dataset, in which the train/test splits are designed to control both the amount of training data and the density of the data in feature space. Our results show that when the generalization problem is easy, increasing model capacity improves generalization. However, both the choice of evaluation metric and the degree of KL regularization become more decisive as the generalization problem gets more difficult. When we consider a standard VAE objective ($\beta = 1$) and measure generalization performance in terms of the log-marginal likelihood, 1-layer networks outperform 3-layer networks. We see that 3-layer networks can memorize training...
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Figure 9: Training set size versus negative test LM (at \(\beta=1\)), for CD and CV splits with 1-layer and 3-layer models (lower is better).

data, which adversely affects performance when the generalization task is difficult.

On the other hand, when we characterize the generalization performance in terms of RD curves, the story is more nuanced: When we decrease the KL regularization coefficient \(\beta\), 2-layer and 3-layer networks outperform 1-layer networks in terms of distortion (i.e. the reconstruction loss) and the evidence lower bound.

Our experiments confirm the intuition that the density in latent space is a key determinant of the difficult of a generalization task. Decreasing the amount of training data whilst keeping the volume in feature space constant leads to a deterioration in generalization performance. However if we decrease the amount of training data whilst keeping the density in feature space constant, the effect on generalization performance is minor. Moreover, we observe qualitative changes in the shape of RD curves. For 1-layer architectures, there exists a minimum that is consistent with a classic bias-variance trade-off. For 3-layer networks, we do observe a small violation of monotonicity that could be consistent with the transition to a “modern interpolation” regime that has been observed in certain classes of highly overparameterized models. This suggests that immediate next steps in this line of work might be to ascertain to what extent similar properties hold for more complex models such as VAEs with autoregressive decoders, as well as for non-simulated datasets where the intrinsic dimensionality of the data is high.

Acknowledgements

We would like to thank reviewers of a previous version of this manuscript for their detailed comments, as well as Sarthak Jain and Heiko Zimmermann for helpful discussions. This project was supported by the Intel Corporation, the DARPA LwLL program, NIH grant R01CA199673 from NCI, and startup funds from Northeastern University.

Figure 10: RD curves evaluated on the test set for different splits as a function of layer depth. White stars indicate the RD value for a standard VAE (\(\beta=1\)).

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Table A1: List of Figures and their short descriptions presented in Appendix.

| Figure | Description |
|--------|-------------|
| A1     | Analysis of $\ell_2$ distance between training and test examples |
| A2     | Samples from test set and their nearest neighbours in training set |
| A3     | The deviation in pixel space caused by each feature in Tetrominoes |
| A4     | Analysis of $\ell_2$ distance caused by each feature in Tetrominoes |
| A5     | Visualization of latent space in mini-MNIST |
| A6     | Comparing the BCE loss for the 9-removal experiment |
| A7     | Reconstructions and weighted averages $\mu$ for MNIST |
| A8     | Reconstructions and nearest neighbours in training set for Tetrominoes datasets |
| A9     | Additional violin plots for analyzing the reconstructions |
| A10    | Heatmaps of LM |
| A11    | Heatmaps of $R$ and $D$ |
| A12    | $RD$-curves shown in alternative view |
| A13    | $RD$-curves shown for both training and test set |
| A14    | $RD$-curves shown for different $N_{train}$ |

A Implementation Details

All experiments were ran on NVIDIA 1080Ti and K80 GPUS, using Pytorch 1.1.0 and ProbTorch commit f9f5c9. Most models are trained with 32-bit precision. A few models (deep $\beta$-VAEs with $\beta < 0.1$) that didn’t train were retrained using 64-bit precision.

B Tetrominoes dataset

Table A2: Names, and training and test set sizes of datasets used in the paper.

| Dataset | Training | Test  |
|---------|----------|-------|
| CV      |          |       |
| 8k/157k | 8193     | 155647|
| 16k/147k| 16384    | 147456|
| 25k/139k| 24577    | 139263|
| 33k/131k| 32768    | 131072|
| 41k/123k| 40960    | 122880|
| 49k/115k| 49153    | 114687|
| 57k/106k| 57344    | 106496|
| Default | 81920    | 81920 |

CD     |          |       |
| 8k/8k  | 8159     | 8275  |
| 16k/16k| 16405    | 16286 |
| 25k/25k| 24642    | 24592 |

Checkerboard | 82021 | 81819 |

In this section, we take a closer look at the “difficulty” of generalization problem in the Tetrominoes dataset.
One can argue that generalization “difficulty” in any dataset is essentially linked to the closeness of training and test set in pixel space. This of-course depends not only on the nature of the dataset, but on size of both training and test sets. Moreover, we need to define the notion of closeness between training and test set in advance. One approach to quantify this concept is the following: for every example in the test, what is the distance to the closest example in training set for a given distance metric? Based on this, we define the difficulty of a generalization problem as:

\[ \text{Difficulty}(\hat{p}_{\text{train}}(x), \hat{p}_{\text{test}}(x), d(\cdot, \cdot)) = \mathbb{E}_{x \sim \hat{p}_{\text{train}}(x), x' \sim \hat{p}_{\text{test}}(x)}[d(x, x')] \] (5)

In Figure A1 we show the normalized $\ell_2$ histograms of test examples to their nearest neighbour in training set for different amount of training data. In Figure A2 we show test samples and their nearest $\ell_2$ neighbour in training set for different splits.
Figure A2: Test samples with minimum (left), median (middle), and maximum (right) $\ell_2$ norm between their nearest neighbour in training set. In each column, the test sample is displayed on the left, and the nearest neighbour is displayed on the right.
B.1 Which features are cause the most different in pixel space?

One crucial factor in the difficulty of generalization in a dataset is the change caused in image space that is caused by moving in feature space. Not only this property can be different for different features, but it may also depend on the location in features space that change is happening (see Figure A3). In order to have a better understating of which features are more difficult to generalize to, we performed the following experiments. For all 163,840 tetromino images, we changed a single feature by a single unit. Figure A3 shows the $\ell_2$ distance between the corresponding images.

![Figure A3: Effect of each feature individual feature in pixel space. (Top) Original image. (Middle) A single feature in the original image modified by one unit. (Bottom) $\ell_2$ distance between images in the top and middle.](image)

Figure A3: Effect of each feature individual feature in pixel space. (Top) Original image. (Middle) A single feature in the original image modified by one unit. (Bottom) $\ell_2$ distance between images in the top and middle.

![Figure A4: Histograms of $\ell_2$ distance between each tetromino image and the same tetromino modified in a single feature by 1 unit. We can observe that size causes the least difference in pixel space. x and y-positions seem to be the second and third most influential factors. Angle causes the most difference in pixel space.](image)

Figure A4: Histograms of $\ell_2$ distance between each tetromino image and the same tetromino modified in a single feature by 1 unit. We can observe that size causes the least difference in pixel space. x and y-positions seem to be the second and third most influential factors. Angle causes the most difference in pixel space.
C Additional Experimental Results

C.1 Mini-MNIST

Figure A5: Data memorization in a VAE with latent dimension trained on 100 MNIST examples. (left) Inference marginal $q_\phi(z) = \frac{1}{N} \sum_n q_\phi(z \mid x_n)$. (right) Partitioning of the latent space. To close approximation, the decoder reconstructs a memorized nearest neighbor from the training data (for approximately 96% of the shown region, the largest weight is $w_{\text{max}} > 0.99$).

C.2 Binary Cross Entropy

Figure A6: Distribution of binary cross entropy loss between input image $x$ and the decoder output $\hat{x}$, vs the loss between weighted average image $\mu$ and $\hat{x}$; calculated over test set consisting of images of 9s. The reconstructions are closer to the input than the weighted average for the shallow VAE (most of the mass of blue distribution lies below the line). On the other hand, the reconstructions are closer closer to the weighted average than the input for the deep VAE (most of the mass of green distribution lies above the line).
C.3 Test examples, nearest neighbours, and reconstructions

Figure A7: Decoder outputs and weighted average images for VAEs with different architectures.

Figure A8: Distributions of distance between test data and output of the decoder ($\|\hat{x} - x\|$) and distance between test data and output of the infinite capacity decoder ($\|\hat{x} - \mu\|$, $\mu$ from Equation (3)), partitioned according distance to nearest training sample ($\|x - x_{\text{tr}}\|$) into 4 bins of equal sizes. Values in x-axis are the limits of the bins.
Figure A9: Reconstruction of test samples from all datasets for shallow and deep VAEs. Rows show examples with increasing reconstruction loss, randomly selected from the 10th (top), 40th to 60th (middle), and 90th (bottom) percentiles.
C.4 Log Marginal Likelihoods

Figure A10: Log Marginal likelihood for Training and Test sets for different values of $\beta$. 
C.5 RD Analysis

Figure A11: RD values on evaluated on the test set for different values of $\beta$. 

\begin{figure}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|c|c|c|c|c|c|c|}
\hline
# Layers & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 \\
\hline
64.9 & 64.8 & 65.0 & 65.1 & 65.9 & 67.0 & 67.9 & 69.1 & 69.9 & 76.2 & 82.2 & 95.3 \\
57.2 & 57.3 & 57.5 & 58.0 & 59.2 & 60.5 & 61.9 & 63.5 & 63.9 & 69.6 & 75.8 & 97.0 \\
56.5 & 56.4 & 56.5 & 57.6 & 60.3 & 61.3 & 61.6 & 63.4 & 62.6 & 71.8 & 78.1 & 93.9 \\
\hline
\end{tabular}
\end{figure}
Figure A12: The same RD curves observed in Figure 7 shown with two alternative views. The first view compares the effect of network capacity for datasets with different levels of difficulty (Top). The second view is the effect of making the generalization problem more difficult in models with different capacity (bottom).
Figure A13: RD curves on train and test set with the Default, CV, and Checkerboard splits in models with 1, 2, and 3 layers.
Figure A14: Estimated $RD$ curves for different number of training data for when the volume is kept constant and reduce to keep the density the same. The uppermost panel is ($N_{\text{train}} = 8k$) and the lowest is for ($N_{\text{train}} = 57k$)