
Disentangling to Cluster: Gaussian Mixture Variational Ladder Auto-Encoders

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Abstract

In clustering we normally output one cluster variable for each datapoint. But it is not necessarily the case that there is only one way to partition a given dataset into cluster components. One could cluster by colour, or by object type, or some other aspect. These different attributes form a hierarchy, and we could wish to cluster in any of them. By disentangling the learnt latent representations of some dataset into different attributes we can then cluster in those latent spaces. We call this *disentangled clustering*. Extending Variational Ladder Autoencoders (Zhao et al., 2017), we propose a clustering algorithm, VLAC, that outperforms a Gaussian Mixture DGM in cluster accuracy over digit identity on the test set of SVHN. We also demonstrate learning clusters jointly over numerous layers of the hierarchy of latent variables for the data, and show component-wise generation from this hierarchical model.

1 Introduction

What do we mean when we talk of clustering a set of images? We have data $x \in \mathcal{D}$ available at train time. The model assigns some cluster variable $y \in 1, \dots, K$ to each datapoint x . We score our method using some existing ground-truth label information $t \in 1, \dots, T$ that was not available when we applied our clustering algorithm. Classically t would be one-hot label information for the training set.

But plausibly there are different ways to cluster the same set of images, so it is limiting to insist *a priori* that there is only one cluster variable y per datapoint and that the clustering algorithm must successfully match that y to t over some dataset. Consider clustering images of digits. While it might make sense to cluster them against the ground truth classes corresponding to what digit they represent, one could conceivably cluster based on other aspects: what colour is the digit? what colour is the background? what is the style of the typeface? And for objects more generally one could cluster a set of objects by colour, texture, object type, or some other attribute.

As we analyse more complex data, intuitively we can expect to find an increase in the number of different aspects on which one could plausibly cluster. To have one latent cluster variable capturing all the different aspects, the number of cluster components needed would be the product of the number of clusters for each aspect. For example for digits one might need one cluster component for each combination of digit identity and colour.

Because having such a large number of cluster components would be unwieldy and unparsimonious, we are interested in outputting a set of L cluster variables y_ℓ , one of which might correspond to a particular given ground truth label and others might capture other ways of clustering the data. This broadened conception of clustering, which we call *disentangled clustering*, requires us to learn sets of latent variables at different levels of the hierarchy of attributes so as to perform clustering over them.

So we wish for disentangled representations. Further we want these representations to be ordered in some way. The Variational Ladder Auto-Encoder (VLAE) [1] separates out subsets of latent variables of images via the degree of computation needed to map from each layer of latent variable to the image: ‘high level’ and ‘low level’ aspects of the image have their associated latent variables separated from each other by how expressive the mapping is between that latent variable and the data.

We augment VLAEs so they can perform clustering at each layer, by introducing mixture distributions for each subset of latent variables. We call this model *Variational Ladder Autoencoder for Clustering* or *VLAC*. We find that we can learn a clustering variable in the hierarchy that corresponds to the ground truth for SVHN [2], and that it is more amenable to clustering using our disentangled clustering variables than using a single entangled layer as in a GM-DGM.

Like some other deep generative models, we produce inference artifacts that can be applied after training to new data. This enable us to perform *test set clustering*, so here we might have a labelled test set that we evaluate our model on.

Related Work Our approach has some links to multi-view clustering [3, 4, 5, 6, 7, 8], where in analogy to multi-view learning one has a feature vector that is composed of distinct chunks of features each about some different aspect of that datapoint. These subsets of features can then be each be used to produce clustering assignments. Often the aim is to use these different sources of information to try to create the same clustering assignments [3, 4].

However, unlike multi-view clustering, in this work we do not have access to the already-chunked feature vector that divides up the different aspects one could cluster over – we are learning it. And further, in multi-view clustering the different views are used to bolster one overall clustering assignment for each datapoint. Here want to cluster distinctly in each learnt set of latent variables.

Various deep learning clustering algorithms have been proposed for clustering, including: Gaussian Mixture DGMs [9, 10, 11], GM-VAE [12], VaDE [13], IMSAT [14], DEC [15] and the current state-of-the-art ACOL-GAR [16].

Many recent papers on learning disentangled representations are based around rewarding statistical independence between latent variables. Examples of this include Factor VAE [17], β -TCVAE [18] and HFVAE [19]. These approaches do not learn hierarchies of disentangled factors, having only one stochastic layer, but are orthogonal to the method of disentangling by computation given by VLAEs.

2 VLAC: Clustering with Gaussian Mixture Variational Ladder Autoencoders

VLAEs To gain a more expressive model over a vanilla VAE that has a single set of latent variables z [20, 21], it is natural to consider having a hierarchy of latent variables $z \rightarrow \mathbf{z} = \{z_\ell\}$ for $\ell \in 1, \dots, L$ each with dimensionality d_ℓ^z . The simplest VAE with a hierarchy of conditional stochastic variables in the generative model is the Deep Latent Gaussian Model [21]. Here we have a Markov chain in the generative model: $p_\theta(x, \mathbf{z}) = p_\theta(x|z_1) \prod_{\ell=1}^{L-1} [p_\theta(z_\ell|z_{\ell+1})]p(z_L)$ Performing inference in this model is challenging. The latent variables further from the data can fail to learn anything informative [22, 23]: in the worst case a single-layer VAE can train in isolation within this hierarchical model: each $p_\theta(z_\ell|z_{\ell+1})$ distribution can become a fixed distribution not depending on z_{i+1} such that each KL divergence present in the objective between corresponding z_ℓ layers is driven to a local minima. [23] gives a proof of this separation for the case where the model is perfectly trained ($\text{KL}(q_\phi(z, x) || p_\theta(x, z)) = 0$).

The Variational Ladder Autoencoder (VLAE) [23] avoid this collapse in hierarchical VAEs. Here we have a ‘flat hierarchy’ in \mathbf{z} . Instead of having the set of z_ℓ variables conditioned on each other, the prior for $\mathbf{z} = \{z_\ell\}$ is a set of independent standard Gaussians: $p(\mathbf{z}) = \prod_{\ell=1}^L \mathcal{N}(z_\ell|0, \mathcal{I})$, $|z_\ell| = d_\ell^z$. and inside the conditional distribution $p_\theta(x|\mathbf{z})$ there is a ladder [24, 25, 22] over z_ℓ variables. This separates out aspects of the data by the degree of computation needed to map between their latent representation and x . Thus $p_\theta(x|\mathbf{z})$ is defined implicitly by:

$$\tilde{z}_L = f_L^\theta(z_L) \tag{1}$$

$$\tilde{z}_\ell = f_\ell^\theta(z_\ell, \tilde{z}_{\ell+1}) \tag{2}$$

$$x \sim p(x|f_0^\theta(\tilde{z}_1)) \tag{3}$$

for $\ell \in 1, \dots, L - 1$. The posterior follows a similar structure, but in reverse:

$$h_\ell = g_\ell^\phi(h_{\ell-1}) \quad (4)$$

$$z_\ell \sim \mathcal{N}(z_\ell | \mu_\ell^\phi(h_\ell), \sigma_\ell^\phi(h_\ell)) \quad (5)$$

for $\ell \in 1, \dots, L$ and where $h_0 = x$.

VLAC: Variational Ladder Autoencoder for Clustering To enable us to cluster, we alter the generative model above so we have a mixture distribution in z_ℓ : $p_\theta(x, \mathbf{z}) \rightarrow p_\theta(x, \mathbf{z}, \mathbf{y}) = p(x|\mathbf{z}) \prod_{\ell=1}^L p_\theta(z_\ell|y_\ell)p(y_\ell)$. $p(z_\ell|y_\ell) = \mathcal{N}(z_\ell|\mu_{y_\ell}, \sigma_{y_\ell})$ and $p(y_\ell) = \text{Cat}(1/K_\ell)$. Where $\mathbf{K} = \{K_\ell\}$ is the vector of the dimensionalities of our discrete variables $\{y_\ell\}$. Our variational posterior is now $q_\phi(\mathbf{z}, \mathbf{y}|x)$. We choose to factorise this as $q_\phi(\mathbf{z}|\mathbf{y}, x)q_\phi(\mathbf{y}|x)$. Each of these is a product over our L layers. $q_\phi(\mathbf{y}|x) = \prod_{\ell=1}^L q_\phi(y_\ell|x)$, $q_\phi(y_\ell|x) = \text{Cat}(\pi_\ell^\phi(x))$. $q_\phi(\mathbf{z}|\mathbf{y}, x) = \prod_{\ell=1}^L q_\phi(z_\ell|x, \{y_i\}_{i \leq \ell})$, and so the new counterparts to Eqs (4-5) are:

$$h_1 = g_1^\phi(x) \quad (6)$$

$$h_\ell = g_\ell^\phi(h_{\ell-1}, y_{\ell-1}) \text{ for } \ell > 1 \quad (7)$$

$$z_\ell \sim \mathcal{N}(z_\ell | \mu_\ell^\phi(h_\ell, y_\ell), \sigma_\ell^\phi(h_\ell, y_\ell)) \quad (8)$$

See Figure 1 for a graphical representation of this model for $L = 2$. After training the $q_\phi(y_\ell|x)$ networks are inference artifacts that can be applied to new datapoints.

Thus the ELBO for our model is:

$$\mathcal{L}(x) = \mathbb{E}_{\mathbf{z} \sim q} \log p_\theta(x|\mathbf{z}) - \sum_{\ell=1}^L \mathbb{E}_{\mathbf{y} \sim q} \text{KL}(q_\phi(z_\ell|x, \{y_i\}_{i \leq \ell}) || p(z_\ell|y_\ell)) - \sum_{\ell=1}^L \text{KL}(q_\phi(y_\ell|x) || p(y_\ell)) \quad (9)$$

If all $K_\ell = 1$ then VLAC reduces to a VLAE. It is not necessary to have $K_\ell > 1$ for all layers in VLAC.

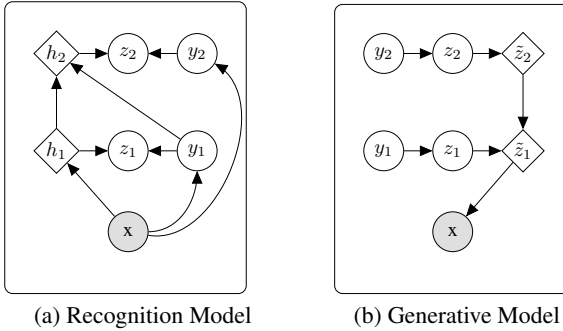


Figure 1: VLAC with $L = 2$

Evaluation Metrics Following [13, 26, 16] we use unsupervised cluster accuracy (ACC), also known as cluster purity, to evaluate our models:

$$\text{ACC} = \max_{P \in \mathcal{P}} \frac{\sum_{i=1}^{|\mathcal{D}|} \mathbb{I}[t_i = P y_i]}{|\mathcal{D}|} \quad (10)$$

where P is a $T \times K$ rectangular permutation matrix that attributes each y to a ground truth class t .

3 Experiments

We trained our model with $L = 4$ and convolutional g and deconvolutional f networks. For full implementation details, see the code at¹. We use the Gumbel-Softmax Trick/CONCRETE sampling [27, 28] to stochastically estimate the expectations over the discrete variables, rather than exactly marginalise them out. This avoids us having to calculate numerous forward passes through the model.

We apply our model to SVHN [2], as it gives variations in style of one type of object while also having distinct ground-truth class structure (here t indexes digit identity) that we can benchmark against.

When running our implementation of a VLAE over SVHN we observed that the 3rd layer was associated most clearly with variation in digit identity. In our experiments we ran VLAC with $\mathbf{K}^{\text{1layer}} = [1, 1, 50, 1]$ and $\mathbf{K}^{\text{2layer}} = [1, 5, 50, 1]$. We evaluate the cluster accuracy in y_3 against t , over the test set.

¹To be made available publicly on github if accepted.

Table 1: Test set cluster accuracy on SVHN for our approach and baselines.

Model	Accuracy
VLAC with $\mathbf{K}^{1\text{layer}}$	0.637 ± 0.042
VLAC with $\mathbf{K}^{2\text{layer}}$	0.648 ± 0.027
Equivalent GM-DGM with $ K = 50$	0.570 ± 0.032
IMSAT [14]	0.573 ± 0.040
DEC [29]	0.560 ± 0.016
ACOL-GAR [16]	0.768 ± 0.013

In addition to published baseline results, we also compared against a single- z -layer Gaussian mixture DGM [9, 10] with an encoder-decoder structure matching that of the sub-networks needed for the 3rd layer of VLAC with $K_3 = 50$.

Further we also perform class-conditional generation from the layers with $K_\ell > 1$, sampling from the appropriate cluster in $p(z_\ell|y_\ell)$.

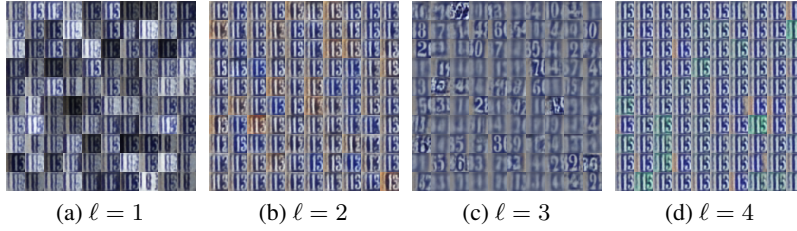


Figure 2: Manipulations of the latent representation of a datapoint in each layer of VLAC $\mathbf{K}^{2\text{layer}}$. For each layer sample from the prior for that layer while keeping all other layers fixed.

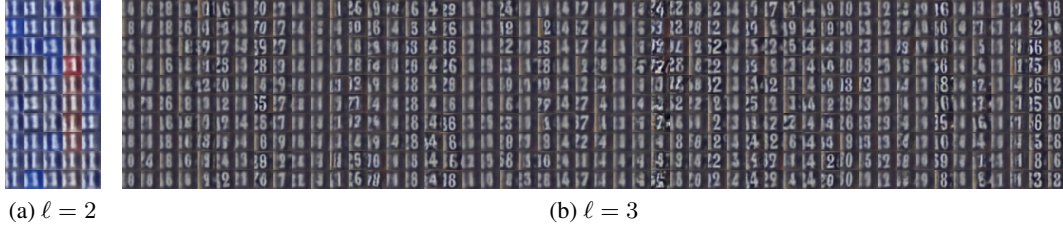


Figure 3: Sampling in the mixture layers of VLAC with $\mathbf{K}^{2\text{layer}}$, sampling from the prior by cluster component for one layer and keeping all other layers fixed with one sample from their priors. One column per cluster component

4 Discussion

Our model does not achieve state of the art clustering for SVHN. However, we can see that from the $\mathbf{K}^{1\text{layer}}$ results that clustering inside a ladder of stochastic variables is better than an equivalent GM-DGM baseline. And as VLAC with $\mathbf{K}^{2\text{layer}}$ gets better test set accuracy than VLAC with $\mathbf{K}^{1\text{layer}}$, we see that having a hierarchy of clusters increases performance further still.

From Figures 2-3 we can see that our model does separate out class information, first that class variation is mostly associated with one layer (as in a vanilla VLA) and then different ground truth classes correspond to cluster components within that layer. Figure 3a shows that the model has also discovered clusters describing the colour temperature of the image. Overall we are pleased to have demonstrated the benefits of clustering in disentangled spaces, and hope that this inspires more research both into how to cluster datasets over different aspects of the data and how disentangling can be used to improve performance of various classical machine learning tasks when working with image datasets.

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