DIVA: Domain Invariant Variational Autoencoders

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Abstract

We consider the problem of domain generalization, namely, how to learn representations given data from a set of domains that generalize to data from a previously unseen domain. We propose the Domain Invariant Variational Autoencoder (DIVA), a generative model that tackles this problem by learning three independent latent subspaces, one for the domain, one for the class, and one for any residual variations. We highlight that due to the generative nature of our model we can also incorporate unlabeled data from known or previously unseen domains. To the best of our knowledge this has not been done before in a domain generalization setting. This property is highly desirable in fields like medical imaging where labeled data is scarce. We experimentally evaluate our model on the rotated MNIST benchmark and a malaria cell images dataset where we show that (i) the learned subspaces are indeed complementary to each other, (ii) we improve upon recent works on this task and (iii) incorporating unlabelled data can boost the performance even further.

1 Introduction

Deep neural networks (DNNs) led to major breakthroughs in a variety of areas like computer vision and natural language processing. Despite their big success, recent research shows that DNNs learn the bias present in the training data. As a result they are not invariant to cues that are irrelevant to the actual task [2]. This leads to a dramatic performance decrease when tested on data from a different distribution with a different bias.

In domain generalization the goal is to learn representations from a set of similar distributions, here called domains, that can be transferred to a previously unseen domain during test time. A common motivating application, where domain generalization is crucial, is medical imaging [8][29]. For instance, in digital histopathology a typical task is the classification of benign and malignant tissue. However, the preparation of a histopathology image includes the staining and scanning of tissue which can greatly vary between hospitals. Moreover, a sample from a patient could be preserved in different conditions [7]. As a result, each patient data could be treated as a separate domain [21]. Another problem commonly encountered in medical imaging is class label scarcity. Annotating medical images is an extremely time consuming task that requires expert knowledge. However, obtaining domain labels is surprisingly cheap, since hospitals generally store information about the patient (e.g., age and sex) and the medical equipment (e.g., manufacturer and settings). Therefore, we are interested in extending the domain generalization framework to be able to deal with additional unlabeled data, as we hypothesize that it can improve performance.

In this paper, we propose to tackle domain generalization via a new deep generative model that we refer to as the Domain Invariant Variational Autoencoder (DIVA). We extend the variational autoencoder (VAE) framework [18][32] by introducing independent latent representations for a domain label, a class label and any residual variations in the input \( x \). Such partitioning of the latent space will encourage and guide the model to disentangle these sources of variation.

Preprint. Under review.
We are interested in learning representations that generalize from one domain to another. We follow the domain generalization definitions used in [29]. A domain is defined as a joint distribution \( p(d, x, y, z_d, z_x, z_y) = p_\theta(x | z_d, z_x, z_y) p_\theta(d | z_d) p(y | z_y) p(z_d) p(d) p(y) \). Right: Inference model. We propose to factorize the variational posterior as \( q_{\phi_d}(z_d | x) q_{\phi_x}(z_x | x) q_{\phi_y}(z_y | x) \). Dashed arrows represent the two auxiliary classifiers \( q_{\omega_d}(d | z_d) \) and \( q_{\omega_y}(y | z_y) \).

Finally, by virtue of having a generative model we can naturally handle the semi-supervised scenario, similarly to [19]. We evaluate our model on a version of the MNIST dataset where each domain corresponds to a specific rotation angle of the digits, as well as on a malaria cell images dataset where each domain corresponds to a different patient.

2 Towards domain generalization with generative models

We follow the domain generalization definitions used in [29]. A domain is defined as a joint distribution \( p(x, y) \) on \( X \times Y \), where \( X \) denotes an input space and \( Y \) an output space. Let \( \mathcal{D}_{X \times Y} \) be the set of all domains. The training set consists of samples \( S \) taken from \( N \) domains, \( S = \{ S^{(d)} \}_{d=1}^N \). The \( d \)th domain \( p^{(d)}(x, y) \) is represented by \( n_d \) samples, \( S^{(d)} = \{ (x_k^{(d)}, y_k^{(d)}) \}_{k=1}^{n_d} \). Here each of the \( N \) distributions \( p^{(d)}(x, y), \ldots, p^{(d)}(x, y), \ldots, p^{(d)}(x, y) \) are sampled from \( \mathcal{D}_{X \times Y} \). We further assume that \( p^{(d)}(x, y) \neq p^{(d)}(x, y) \), therefore, the samples in \( S \) are non-i.i.d. During test time we are presented with samples \( S^{(d)} \) from a previously unseen domain \( p^{(d)}(x, y) \).

We are interested in learning representations that generalize from \( p^{(d)}(x, y), \ldots, p^{(d)}(x, y) \) to this new domain. Training data are given as tuples \((d, x, y)\) in the case of supervised data or as \((d, x)\) in the case of unsupervised data.

2.1 DIVA: Domain Invariant VAE

Assuming a perfectly disentangled latent space [14], we hypothesize that there exists a latent subspace that is invariant to changes in \( d \), i.e., that is domain invariant. We propose a generative model with three independent sources of variation; \( z_d \), which is domain specific, \( z_y \), which is class specific and finally \( z_x \), which captures any residual variations left in \( x \). While \( z_x \) keeps an independent Gaussian prior \( p(z_x) \), \( z_d \) and \( z_y \) have conditional priors \( p_\theta_d(z_d | d) \), \( p_\theta_y(z_y | y) \) with learnable parameters \( \theta_d, \theta_y \).

This will encourage information about the domain \( d \) and label \( y \) to be encoded into \( z_d \) and \( z_y \) respectively. Furthermore, as \( z_d \) and \( z_y \) are marginally independent by construction, we argue that the model will learn representations \( z_y \) that are invariant with respect to the domain \( d \). All three of these latent variables are then used by a single decoder \( p_\theta(x | z_d, z_x, z_y) \) for the reconstruction of \( x \).

Since we are interested in using neural networks for \( p_\theta(x | z_d, z_x, z_y) \), exact inference will be intractable. For this reason, we perform amortized variational inference with an inference network [18][32], i.e., we employ a VAE-type framework. We introduce three separate encoders \( q_{\phi_d}(z_d | x) \), \( q_{\phi_x}(z_x | x) \) and \( q_{\phi_y}(z_y | x) \) that serve as variational posteriors over these latent variables. Notice that we do not share their parameters as we empirically found that sharing parameters leads to a decreased generalization performance. For the prior and variational posterior distributions over the latent variables \( z_x, z_d, z_y \) we assume fully factorized Gaussians with parameters given as a function of their input. We coin the term Domain Invariant VAE (DIVA) for our overall model, which is depicted in Figure 1.
Given a specific dataset, all of the aforementioned parameters can be optimized by maximizing the following variational lower bound per input \(x\):

\[
L_x(d, x, y) = \mathbb{E}_{q_{\phi_d}(z_d|x)} q_{\phi_x}(z_x|x) q_{\phi_y}(z_y|x) \left[ \log p_{\theta}(x|z_d, z_x, z_y) \right] \\
- \beta KL (q_{\phi_d}(z_d|x)||p_{\theta_d}(z_d|d)) - \beta KL (q_{\phi_x}(z_x|x)||p(z_x)) \\
- \beta KL (q_{\phi_y}(z_y|x)||p_{\theta_y}(z_y|y)).
\] (1)

Notice that we have introduced a weighting term, \(\beta\). This is motivated by the \(\beta\)-VAE [13] and serves as a constraint that controls the capacity of the latent spaces of DIVA. Larger values of \(\beta\) limit the capacity of each \(z\) and in the ideal case each dimension of \(z\) captures one of the conditionally independent factors in \(x\). The \(\beta\)-VAE framework offers a trade-off between the information preservation, i.e., how well one can reconstruct \(x\) from the \(z\)’s, and the capacity, i.e., how well the \(z\)’s compress information about \(x\).

To further encourage separation of \(z_d\) and \(z_y\) into domain and class specific information respectively, we add two auxiliary objectives. During training \(z_d\) is used to predict the domain \(d\) and \(z_y\) is used to predict the class \(y\) for a given input \(x\):

\[
\mathcal{F}_{\text{DIVA}}(d, x, y) := L_x(d, x, y) + \alpha_d \mathbb{E}_{q_{\phi_d}(z_d|x)} \left[ \log q_{\omega_d}(d|z_d) \right] + \alpha_y \mathbb{E}_{q_{\phi_y}(z_y|x)} \left[ \log q_{\omega_y}(y|z_y) \right],
\] (2)

where \(\alpha_d, \alpha_y\) are weighting terms for each of these auxiliary objectives. Since our main goal is a domain invariant classifier, during inference we only use the encoder \(q_{\phi_d}(z_d|x)\) and the auxiliary classifier \(q_{\omega_y}(y|z_y)\). For the prediction of the class \(y\) for a new input \(x\) we use the mean of \(z_y\).

[24] and [8] claim that learning a disentangled representation, i.e., \(q_{\phi}(z) = \prod_{i} q_{\phi_i}(z_i)\), in an unsupervised fashion is impossible for arbitrary generative models. Inductive biases, e.g., some form of supervision or constraints on the latent space, are necessary to find a specific set of solutions that matches the true generative model. Consequently, DIVA is using domain labels \(d\) and class labels \(y\) in addition to input data \(x\) during training. Furthermore, we enforce the factorization of the marginal distribution of \(z\) in the following form: \(q_{\phi}(z) = q_{\phi_d}(z_d)q_{\phi_x}(z_x)q_{\phi_y}(z_y)\), which prevents the impossibility described in [24]. We argue that the strong inductive biases in DIVA make it possible to learn disentangled representations that match the ground truth factors of interest, namely, the domain factors \(z_d\) and class factors \(z_y\).

### 2.2 Semi-supervised DIVA

In [19] an extension to the VAE framework was introduced that allows to use labeled as well as unlabeled data during training. While [19] introduced a two step procedure, [25] presented a way of optimizing the decoder of the VAE and the auxiliary classifier jointly. We use the latter approach to learn from supervised data \(\{(d_n, x_n, y_n)\}\) as well as from unsupervised data \(\{(d_m, x_m)\}\). Analogically to [25], we use \(q_{\omega_y}(y|z_y)\) to impute \(y\):

\[
L_u(d, x) = \mathbb{E}_{q_{\phi_d}(z_d|x)} q_{\phi_x}(z_x|x) q_{\phi_y}(z_y|x) \left[ \log p_{\theta}(x|z_d, z_x, z_y) \right] \\
- \beta KL (q_{\phi_d}(z_d|x)||p_{\theta_d}(z_d|d)) - \beta KL (q_{\phi_x}(z_x|x)||p(z_x)) \\
+ \mathbb{E}_{q_{\phi_y}(z_y|x)} \left[ \log p_{\theta_y}(y) \right] - \log q_{\omega_y}(y|z_y),
\] (3)

where we use Monte Carlo sampling with the reparametrization trick [13] for the continuous latents \(z_d, z_x, z_y\) and explicitly marginalize over the discrete variable \(y\). The final objective combines the supervised and unsupervised variational lower bound as well as the two auxiliary objectives. By assuming \(N\) labeled and \(M\) unlabeled data tuples we arrive at the following objective

\[
\mathcal{F}_{\text{SS-DIVA}} = \sum_{n=1}^{N} \mathcal{F}_{\text{DIVA}}(x_n, y_n, d_n) + \sum_{m=1}^{M} L_u(x_m, d_m) + \alpha_d \mathbb{E}_{q_{\phi_d}(z_d|x_m)} \left[ \log q_{\omega_d}(d_m|z_d) \right].
\] (4)

### 3 Related Work

The majority of proposed deep learning methods for domain generalization fall into one of two categories: 1) Learning a single domain invariant representation, e.g., using adversarial methods
While DIVA falls under this category there is a key difference: we do not explicitly regularize $z_y$ using $d$. Instead we learn complementary representations $z_d$, $z_x$ and $z_y$ utilizing a generative architecture. 2) Ensembling models, each trained on an individual domain from the training set [9, 27]. The size of models in this category scales linearly with the amount of training domains. This leads to slow inference if the number of training domains is large. However, the size of DIVA is independent of the number of training domains. In addition, during inference time we only use the mean of the encoder $q_{\phi_y}(z_y|x)$ and the auxiliary classifier $q_{\phi_z}(y|z_y)$.

An area that is closely related to domain generalization is that of the statistical parity in fairness. The goal of fair classification is to learn a meaningful representation that at the same time cannot be used to associate a data sample to a certain group [19]. The major difference to domain generalization is the intention behind that goal, e.g., to protect groups of individuals vs. being robust to variations in the input. Consequently, DIVA is closely related to the fair VAE [25]. In contrast to the fair VAE, which is using a hierarchical latent space, DIVA is using a partitioned latent space.

In the last two years we have seen a steady increase of methods using latent subspaces in generative models. [30] as well as [1] show that a partitioned latent space in combination with a few labeled examples leads to better disentangled representations. [15] show that such an approach leads to models that are more robust to out-of-distribution inputs. Furthermore, they show that such an approach can be used in combination with invertible networks [16]. In addition, [1] show the compatibility of the approach with flow based models [31]. Last, [2] propose a multi-level approach, where one latent space is used for individual samples and another one is shared among samples from the same group.

4 Experiments

We evaluate the performance of DIVA on two datasets: rotated MNIST [11] and malaria cell images [30]. In both cases we first investigate if DIVA is able to successfully learn disentangled representations. Furthermore, we compare DIVA to other methods in a supervised and semi-supervised setting. While for the rotated MNIST dataset DIVA's graphical model is matching the ground truth generative model, the malaria cell images dataset poses a more challenging and realistic scenario, where the ground truth generative model is unknown.

4.1 Rotated MNIST

The construction of the rotated MNIST dataset follows [11]. We sample 100 images from each of the 10 classes from the original MNIST training dataset. This set of images is denoted $M_{0^\circ}$. To create five additional domains the images in $M_{0^\circ}$ are rotated by 15, 30, 45, 60 and 75 degrees. In order to evaluate their domain generalization abilities, models are trained on five domains and tested on the remaining 6th domain, e.g., train on $M_{0^\circ}$, $M_{15^\circ}$, $M_{30^\circ}$, $M_{45^\circ}$ and $M_{60^\circ}$, test on $M_{75^\circ}$. The evaluation metric is the classification accuracy on the test domain. All experiments are repeated 10 times. Detailed information about hyperparameters, architecture and training schedule can be found in the Appendix.

4.1.1 Qualitative disentanglement

First of all, we visualize the three latent spaces $z_d$, $z_x$ and $z_y$, to see if DIVA is able to successfully disentangle them. In addition, we want to see if DIVA utilizes $z_x$ in a meaningful way, since it is not directly connected to any downstream task. For the following visualizations we restrict the size of each latent space $z_d$, $z_x$ and $z_y$ to 2 dimensions. Therefore, we can plot the latent supspaces directly without applying dimensionality reduction, see Figure 2. Here, we trained DIVA on 5000 images from five domains: $M_{0^\circ}$, $M_{15^\circ}$, $M_{30^\circ}$, $M_{45^\circ}$ and $M_{60^\circ}$.

From these initial qualitative results we conclude that DIVA is disentangling the information contained in $x$ as intended, as $z_d$ is only containing information about $d$ and $z_y$ only information about $y$. In the case of the rotated MNIST dataset $z_x$ captures any residual variation that is not explained by the domain $d$ or the class $y$. In addition, we are able to generate conditional reconstructions with DIVA. The results along with more details can be found in the Appendix.
Figure 2: 2D embeddings of all three latent subspaces. In the top row embeddings are colored according to their domain, in the bottom row they are colored according to their class. First column: $z_d$ encoded by $q_{\phi_d}(z_d|x)$. The top plot shows five distinct clusters, where each cluster corresponds to a single domain. In the bottom plot no clustering is visible. Second column: $z_x$ encoded by $q_{\phi_x}(z_x|x)$. We observe a correlation between the rotation angle of each MNIST digit and $z_x[0]$ in the top plot. Upon visual inspection of the original inputs $x$, we find a correlation between the line thickness digit and $z_x[0]$ as well as a correlation between the digit width and $z_x[1]$ in the bottom plot. As a result, we observe a clustering of embeddings with class ‘1’ at the lower left part of the plot. Third column: $z_y$ encoded by $q_{\phi_y}(z_y|x)$. In the top plot no clustering is visible. The bottom plot shows ten distinct clusters, where each cluster corresponds to a class.

Table 1: Comparison with other state-of-the-art domain generalization methods. Methods in the first half of the table (until the vertical line) use only labeled data. The second half of the table shows results of DIV A when trained semi-supervised (+ X times the amount of unlabeled data). We report the average and standard error of the classification accuracy.

| Test $|\mathcal{M}_d|^\circ$ | DA | LG | HEX | ADV | DIV A | DIV A(+1) | DIV A(+3) | DIV A(+5) | DIV A(+9) |
|------|------|-----|-----|-----|------|---------|----------|----------|----------|----------|
| $M_{0^\circ}$ | 86.7 | 89.7 | 90.1 | 89.9 | **93.5 ± 0.3** | 93.8 ± 0.4 | 93.9 ± 0.5 | 93.2 ± 0.5 | 93.0 ± 0.4 |
| $M_{15^\circ}$ | 98.0 | 97.8 | 98.9 | 98.6 | **99.3 ± 0.1** | 99.4 ± 0.1 | 99.5 ± 0.1 | 99.5 ± 0.1 | 99.6 ± 0.1 |
| $M_{30^\circ}$ | 97.8 | 98.0 | 98.9 | 98.8 | **99.1 ± 0.1** | 99.3 ± 0.1 | 99.3 ± 0.1 | 99.3 ± 0.1 | 99.3 ± 0.1 |
| $M_{45^\circ}$ | 97.4 | 97.1 | 98.8 | 98.7 | **99.2 ± 0.1** | 99.0 ± 0.2 | 99.2 ± 0.1 | 99.3 ± 0.1 | 99.3 ± 0.1 |
| $M_{60^\circ}$ | 96.9 | 96.6 | 98.3 | 98.6 | **99.3 ± 0.1** | 99.4 ± 0.1 | 99.4 ± 0.1 | 99.4 ± 0.1 | 99.2 ± 0.2 |
| $M_{75^\circ}$ | 89.1 | 92.1 | 90.0 | 90.4 | **93.0 ± 0.4** | 93.8 ± 0.4 | 93.8 ± 0.2 | 93.5 ± 0.4 | 93.2 ± 0.3 |
| **Avg** | **94.3** | **95.3** | **95.8** | **95.2** | **97.2 ± 1.3** | **97.5 ± 1.1** | **97.5 ± 1.2** | **97.4 ± 1.3** | **97.3 ± 1.3** |

4.1.2 Comparison to other methods

We compare DIV A against the well known domain adversarial neural networks (DA) [10] as well as three recently proposed methods: LG [35], HEX [37] and ADV [37].

For the first half of Table 1 (until the vertical line) we only use labeled data. The first column indicates the rotation angle of the test domain. We report test accuracy on $y$ for all methods. For DIV A we report the mean and standard error for 10 repetitions. DIV A achieves the highest accuracy across all test domains and the highest average test accuracy among all proposed methods.

The second half of Table 1 showcases the ability of DIV A to use unlabeled data. For this experiment we add: The same amount (+1) of unlabeled data as well as three (+3), five (+5) and nine (+9) times
the amount of unlabeled data to our training set. We first add the unlabeled data to $\mathcal{M}_0^\circ$ and create the data for the other domains as described in Section 4.1. In Table 1 we can clearly see a performance increase when unlabeled data is added to the training set. The effect seems to become smaller when the amount of unlabeled data is much larger than the amount of labeled data as seen in the last two columns of Table 1.

### 4.1.3 Additional unlabeled domains

In Section 4.1.2 we show that the performance of DIV A increases when it is presented with additional unlabeled data for each domain. As a result each training domain consists of labeled and unlabeled examples. In this section we investigate a more challenging scenario: We add an additional domain to our training set that consists of only unlabeled examples. Coming back to our introductory example of medical imaging, here we would add unlabeled data from a new patient or new hospital to the training set. In contrast to the experiment in Section 4.1.2 where we would add unlabeled data from each known patient or hospital to the training set.

In the following, we are looking at two different experimental setups, in both cases $\mathcal{M}_{75^\circ}$ is the test domain: For the first experiment we choose the domains $\mathcal{M}_0^\circ$, $\mathcal{M}_{15^\circ}$, $\mathcal{M}_{45^\circ}$ and $\mathcal{M}_{60^\circ}$ to be part of the labeled training set. In addition, unlabeled data from $\mathcal{M}_{30^\circ}$ is used. In Table 2 we can see that even in the case where the additional domain is dissimilar to the test domain DIV A is able to slightly improve. For the second experiment we choose the domains $\mathcal{M}_0^\circ$, $\mathcal{M}_{15^\circ}$, $\mathcal{M}_{30^\circ}$ and $\mathcal{M}_{45^\circ}$ to be part of the labeled training set. In addition, unlabeled data from $\mathcal{M}_{60^\circ}$ is used. When comparing the results in Table 2 to the results in Table 1 we notice a drop in accuracy of about 20% for DIV A trained with only labeled data. However, when trained with unlabeled data from $\mathcal{M}_{60^\circ}$ we see an improvement of about 7%. The comparison shows that DIV A can successfully learn from samples of a domain without any labels.

| Unsupervised domain | DIVA supervised | DIVA semi-supervised |
|---------------------|-----------------|----------------------|
| $\mathcal{M}_{30^\circ}$ | 93.1 ± 0.5 | 93.3 ± 0.4 |
| $\mathcal{M}_{60^\circ}$ | 73.8 ± 0.8 | 80.6 ± 1.1 |

### 4.2 Malaria Cell Images

The majority of medical imaging datasets consist of images from a multitude of patients. In a domain generalization setting each patient is viewed as an individual domain. While we focus on patients as domains in this paper, this type of reasoning can be extended to, e.g., hospitals as domains. We, among others [30, 21], argue that machine learning algorithms trained with medical imaging datasets should be evaluated on a subset of hold-out patients. This presents a more realistic scenario since the algorithm is tested on images from a previously unseen domain. In the following, we use a malaria cell images dataset [30] as an example of a dataset consisting of samples from multiple patients. The images in this dataset were collected and photographed at Chittagong Medical College Hospital, Bangladesh. It consists of 27558 single red blood cell images taken from 150 infected and 50 healthy patients. The images were manually annotated by a human expert. To facilitate the counting of parasitized and uninfected cells, the cells were stained using Giemsa stain which turns the parasites inside the cell pink. In addition, the staining process leads to a variety of colors of the cell itself. While the color of the cell is relatively constant for a single patient, it can vary greatly between patients, see Figure 3. This variability in appearance of the cells can be easily ignored by a human observer, however, machine learning models can fail to generalize across patients. In our experiments we will use the patient ID as the domain label $d$. We argue that for this specific dataset the patient ID is a good proxy of appearance variability. In addition, there is no extra cost for obtaining the patient ID for each cell.

Subsequently, we use a subset of the malaria cell images dataset that consists of the 10 patients with the highest amount of cells. The amount of cells per patient varies between 400 and 700 and there are 5922 cell images in total. The choice of this subset is motivated by the similar amount of cells as well as the similar marginal label distributions per patient. The latter being a necessary condition
for successful domain generalization [39]. Furthermore we rescale all images to $64 \times 64$ pixels. We apply no further data augmentation.

### 4.2.1 Qualitative disentanglement

We investigate the three latent subspaces $z_d$, $z_x$ and $z_y$ to see if DIVA is able to successfully disentangle them. In addition, we want to see if DIVA utilizes $z_x$ in a meaningful way, since it is not directly connected to any downstream task. Figure 3 shows the reconstructions of $x$ using all three latent subspaces as well as reconstructions of $x$ using only a single latent subspace at a time. First, we find that DIVA is able to reconstruct the original cell images using all three subspaces (Figure 3, first row). Second, we find that the three latent subspaces are indeed disentangled: $z_d$ is containing the color of the cell (Figure 3, second row), $z_x$ the shape of the cell (Figure 3, third row) and $z_y$ the location of the parasite (Figure 3, fourth row). The holes in the reconstructions using only $z_x$ indicate that there is no probability mass in $z_d$ and $z_y$ at 0, similar to Figure 2. From the reconstructions in Figure 3 we conclude that DIVA is able to learn disentangled representations that match the ground truth factors of interest, here, the appearance of the cell and the presence of the parasite.

$$
\begin{align*}
x & \sim p_{\theta}(z_d, z_x, z_y) \\
x & \sim p_{\theta}(z_d, 0, 0) \\
x & \sim p_{\theta}(0, z_x, 0) \\
x & \sim p_{\theta}(0, 0, z_y)
\end{align*}
$$

Figure 3: Reconstructions of $x$ using all three latent subspaces as well as reconstructions of $x$ using only a single latent subspace at a time.

### 4.2.2 Supervised case

To further evaluate domain generalization abilities, models are trained on nine domains (patient IDs) and tested on the remaining 10th domain. The evaluation metrics are the classification accuracy, F1 score and ROC AUC on the hold out test domain. All experiments are repeated five times. We chose the baseline architecture to consist of eight ResNet blocks [12] followed by two linear layers. Furthermore, we compare to a domain adversarial neural network (DA) with the same architecture as the baseline, where the additional domain classifier consists of two linear layers. In case of DIVA, $q_{\phi_y}(z_y|x)$, $q_{\phi_y}(z_x|x)$ and $q_{\phi_y}(z_d|x)$ are parameterized by eight ResNet blocks followed by a single linear layer. Furthermore, the auxiliary classifiers $q_{\omega_d}(d|z_d)$ and $q_{\omega_y}(y|z_y)$ consist of a single linear layer each. During inference all three models have the same architecture. Detailed information about hyperparameters, architecture and training schedule can be found in the Appendix.

In Figure 4 we find that the results are not equally distributed across all test domains. For the baseline method the difference in accuracy between the best performing domain and the worst performing domain is about 10%. This example shows how a non-domain invariant model fails when the test domain considerably deviates from the training domains. Upon visual inspection of domain ‘0’ we find that cells from this patient show a unique dark pink stain that is different from all other domains. In this particular case DIVA’s performance improves significantly across all three metrics. We believe that the improvement of DIVA as well as of DA stems from the increased invariance with respect to the visual appearance of the cells. Last, DIVA is able to improve on average across all three metrics when compared to the baseline and DA, although the improvements are within the standard error, see Appendix for more details.

### 4.2.3 Semi-supervised case

As described in Section 4.1.3 we are interested in learning from domains with no class labels, since such an approach can drastically lower the amount of labeled data needed to learn a domain invariant representation, i.e., a model that generalizes well across patients. For the semi-supervised experiments
we randomly select one, two, three, four and five domains from the nine training domains. The samples from the selected domains are subsequently treated as unlabeled. Samples from supervised domains are presented as \((d, x, y)\) whereas samples from unsupervised domains are presented as \((d, x)\). Note that in the case of five unsupervised domains more than 50% of the training dataset is unlabeled. In all five experiments we choose the test domain to be domain ‘1’, since all three methods show very similar results on this domain across all three metrics in a supervised setting, see Figure 4. All experiments are repeated five times. Each time another subset of domains is selected, which results in the large standard errors seen in Figure 5. The architecture and hyperparameters for all models are the same as for the experiments in Section 4.2.2. In Figure 5, we see a steady decline in performance of the baseline model across all three metrics. However, we find that DIVA and DA benefit from jointly learning from labeled and unlabeled data. As a result DIVA and DA show better performance especially for experiment with three, four and five unsupervised domains compared to the baseline model. Furthermore, we argue that the improvement of DIVA over DA arises from the way the additional unlabeled data is utilized. In case of DA the unlabeled data \((d, x)\) is only used to train the domain classifier and the feature extractor in an adversarial manner. In Section 2.2, we show that due to DIVA’s generative nature \(q_{\phi_{z}}(z_{y}|x), p_{\theta_{y}}(z_{y}|y)\) can be updated using \(q_{\omega_{z}}(y|z_{y})\) to marginalize over \(y\) for an unlabeled sample \(x\). In addition, the unlabeled data \((d, x)\) is used to update \(q_{\phi_{z}}(z_{d}|x), p_{\theta_{d}}(z_{d}|d), q_{\omega_{z}}(d|z_{d}), q_{\phi_{z}}(z_{x}|x)\) and \(p_{\theta}(x|z_{d}, z_{x}, z_{y})\) in the same way as in the supervised case.

5 Conclusion

We have proposed DIVA as a generative model with three latent subspaces. We evaluated DIVA on rotated MNIST and a malaria cell images dataset. In both cases DIVA is able to learn disentangled representations that match the ground truth factors of interest, represented by the class \(y\) and the domain \(d\). By learning representations \(z_{y}\) that are invariant with respect to the domain \(d\), DIVA is able to improve upon other methods on both datasets. Furthermore, we show that we can boost DIVA’s performance by incorporating unlabeled samples, even from entirely new domains for which no labeled examples are available. This property is highly desirable in fields like medical imaging where the labeling process is very time consuming and costly.
Acknowledgments

The authors thank Patrick Forré, Rianne van den Berg, Marco Federici, Daniel Worrall and Bas Veeling for helpful discussions and comments.

Maximilian Ilse was funded by the Nederlandse Organisatie voor Wetenschappelijk Onderzoek (Grant DLMedIa: Deep Learning for Medical Image Analysis).

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Appendix

5.1 Rotated MNIST

5.1.1 Training procedure

All DIV A models are trained for 500 epochs. The training is terminated if the training loss for $y$ has not improved for 100 epochs. As proposed in [5], we linearly increase $\beta$ from 0.0 to 1.0 during the first 100 epochs of training. We set $\alpha_d = 2000$. As seen in [26], we adjust $\alpha_y$ according to the ratio of labeled (N) and unlabeled data (M),

$$\alpha_y = \gamma \frac{M + N}{N},$$  \hspace{1cm} (5)

where we set $\gamma = 3500$. Last, $z_d$, $z_x$ and $z_y$ each have 64 latent dimensions. All hyperparameters were determined by training DIV A on $M_{15^\circ}, M_{30^\circ}, M_{45^\circ}$ and testing on $M_{60^\circ}$. We searched over the following parameters: $\alpha_d$, $\alpha_d = \{1500, 2000, 2500, 3000, 3500, 4000\}$; $z_d = z_x = z_y = \{16, 32, 64\}$; $\beta_{max} = \{1, 5, 10\}$.

All models were trained using ADAM [17] (with default settings), a pixel-wise cross entropy loss and a batch size of 100.

5.1.2 Architecture

To enable a fair experiment, the encoder $q_{\phi_y}(z_y|x)$ and auxiliary classifier $q_{\omega_y}(y|z_y)$ form a DNN with the same number of layers and weights as described in [37].

Table 3: Architecture for $p_{\theta}(x|z_d, z_x, z_y)$. The parameter for Linear is output features. The parameters for ConvTranspose2d are output channels and kernel size. The parameter for Upsample is the upsampling factor. The parameters for Conv2d are output channels and kernel size.

| block | details |
|-------|---------|
| 1     | Linear(1024), BatchNorm1d, ReLU |
| 2     | Upsample(2) |
| 3     | ConvTranspose2d(128, 5), BatchNorm2d, ReLU |
| 4     | Upsample(2) |
| 5     | ConvTranspose2d(256, 5), BatchNorm2d, ReLU |
| 6     | Conv2d(256, 1) |

Table 4: Architecture for $p_{\theta_d}(z_d|d)$ and $p_{\theta_y}(z_y|y)$. Each network has two heads one for the mean and one for the scale. The parameter for Linear is output features.

| block | details |
|-------|---------|
| 1     | Linear(64), BatchNorm1d, ReLU |
| 2.1   | Linear(64) |
| 2.2   | Linear(64), Softplus |

Table 5: Architecture for $q_{\phi_d}(z_d|x)$, $q_{\phi_x}(z_x|x)$ and $q_{\phi_y}(z_y|x)$. Each network has two heads one for the mean one and for the scale. The parameters for Conv2d are output channels and kernel size. The parameters for MaxPool2d are kernel size and stride. The parameter for Linear is output features.

| block | details |
|-------|---------|
| 1     | Conv2d(32, 5), BatchNorm2d, ReLU |
| 2     | MaxPool2d(2, 2) |
| 3     | Conv2d(64, 5), BatchNorm2d, ReLU |
| 4     | MaxPool2d(2, 2) |
| 5.1   | Linear(64) |
| 5.2   | Linear(64), Softplus |
Table 6: Architecture for $q_{ω_d}(d|z_d)$ and $q_{ω_y}(y|z_y)$. The parameter for Linear is output features.

| block | details |
|-------|---------|
| 1     | ReLU, Linear(5 for $q_{ω_d}(d|z_d)$)/10 for $q_{ω_y}(y|z_y)$), Softmax |

5.1.3 Conditional generation

Yet another way to gain insight into the disentanglement abilities of DIVA is conditional generation. We first train DIVA with $β = 10$ using $M_0°$, $M_{15°}$, $M_{30°}$, $M_{45°}$ and $M_{60°}$ as training domains. After training we perform two experiments. In the first one we are fixing the class and varying the domain. In the second experiment we are fixing the domain and varying the class.

Change of class The first row of Figure 6 (left) shows the input images $x$ for DIVA. First, we generate embeddings $z_d$, $z_x$ and $z_y$ for each $x$ using $q_{φ_d}(z_d|x)$, $q_{φ_x}(z_x|x)$ and $q_{φ_y}(z_y|x)$. Second, we replace $z_y$ with a sample $z'_y$ from the conditional prior $p_{θ_y}(z_y|y)$. Last, we generate new images from $z_d$, $z_x$ and $z'_y$ using the trained encoder $p_{θ}(x|z_d, z_x, z_y)$. In Figure 6 (left) rows 2 to 11 correspond to the classes ’0’ to ’9’. We observe that the rotation angle (encoded in $z_d$) and the line thickness (encoded in $z_x$) are well preserved, while the class of the image is changing as intended.

![Image of reconstructions](image)

Figure 6: Reconstructions. Left: First row is input, row 2 to 11 correspond to labels ’0’ to ’9’. Right: First row is input, row 2 to 6 correspond to domains 0, 15, 30, 45, 60.

Change of domain We repeat the experiment from above but this time we keep $z_x$ and $z_y$ fixed while changing the domain. After generating embeddings $z_d$, $z_x$ and $z_y$ for each $x$ in the first row of Figure 6 (right), we replace $z_d$ with a sample $z'_d$ from the conditional prior $p_{θ_d}(z_d|d)$. Finally, we generate new images from $z'_d$, $z_x$ and $z_y$ using the trained encoder $p_{θ}(x|z_d, z_x, z_y)$. In Figure 6 (right) rows 2 to 6 correspond to the domains $M_0°$ to $M_{60°}$. Again, DIVA shows the desired behaviour: While the rotation angle is changing the class and style of the original image is maintained.

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5.1.4 Qualitative Disentanglement: Test domain

In this section, we visualize the $z_d$ and $z_y$ for data points $x$ from the test domain $M_{75^s}$ for the model trained in Section 4.1.1. Figure 8 shows 1000 embeddings $z_y$ encoded by $q_{\phi_y}(z_y|x)$. Figure 7 shows 1000 embeddings $z_d$ encoded by $q_{\phi_d}(z_d|x)$.

Figure 7: 1000 two-dimensional embeddings $z_d$ encoded by $q_{\phi_d}(z_d|x)$ for $x$ from the test domain $M_{75^s}$. The color of each point indicates the associated class.

Figure 8: 1000 two-dimensional embeddings $z_y$ encoded by $q_{\phi_y}(z_y|x)$ for $x$ from the test domain $M_{75^s}$. The color of each point indicates the associated class.
5.2 Malaria cell images

5.2.1 Supervised experiments

Average results for all three metrics can be found in Table 7.

Table 7: Results of the supervised experiments. We report the average and standard error for all three metrics.

| Metric     | Baseline | DA    | DIV A |
|------------|----------|-------|-------|
| Accuracy   | 93.7 ± 1.0 | 94.2 ± 0.8 | 94.5 ± 0.7 |
| F1 Score   | 96.4 ± 0.6 | 96.7 ± 0.5 | 96.9 ± 0.4 |
| ROC AUC    | 96.8 ± 0.9 | 96.8 ± 0.7 | 96.9 ± 0.9 |

5.2.2 Training procedure: DIV A

All DIV A models are trained for 500 epochs. The training is terminated if the validation accuracy for $y$ has not improved for 100 epochs. As proposed in [5], we linearly increase $\beta$ from 0.0 to 1.0 during the first 100 epochs of training. We set $\alpha_d = \alpha_y = 50000$. Last, $z_d$, $z_x$ and $z_y$ each have 64 latent dimensions. We searched over the following parameters: $\alpha_d$, $\alpha_d = \{12500, 25000, 50000, 75000\}$; $z_d = z_x = z_y = \{32, 64\}$; $\beta_{\text{max}} = \{1, 5, 10\}$. All hyperparameters were determined using a validation set that consists of 20% of the training set. All models were trained using ADAM [17] (with default settings), a mixture of discretized logistics [34] loss and a batch size of 100.

5.2.3 Training procedure: Baseline and DA

In case of the supervised experiments in Section 4.2.2 all models are trained for 500 epochs. The training is terminated if the validation accuracy for $y$ has not improved for 100 epochs. In case of the semi-supervised experiments in Section 2.2 the amount of epochs is adjusted to match the number of parameter updates of DIV A. For DA we follow the same training procedure as described in [10]. In the supervised case, first, a labeled batch randomly sampled from the training distributions is used to update the class classifier, domain classifier and the feature extractor in an adversarial fashion. Second, a second batch randomly sampled from the training distributions is used to update only the domain classifier and the feature extractor in an adversarial fashion. In the semi-supervised case samples from the unsupervised domains form the second batch together with samples from the supervised domains. We use the same domain adaptation parameter $\lambda$ schedule as described in [10]. Determined by hyperparameter search we find that DA performs better when $\lambda \cdot \epsilon$ is used. Here, $\epsilon = 0.001$. We searched over the following values of $\epsilon = \{0.1, 0.05, 0.01, 0.005, 0.001, 0.0005, 0.0001\}$.

5.2.4 Architecture

In the following we will describe the architecture of DIV A in detail. Note that the architecture for the baseline model is the same as $q_{\phi_y}(z_y|x)$ (we only use the mean of $z_y$) followed by $q_{\omega_y}(y|z_y)$ where $z_y$ has 1024 dimensions. DA is using $q_{\phi_y}(z_y|x)$ without the linear layer as a feature extractor. The class classifier and the domain classifier consist of two linear layers. The feature extractor for all models consist of 8 ResNet blocks [12]. During training weight norm [33] is used for all convolutional layers.
Table 8: Architecture for $p_\theta(x|z_d, z_x, z_y)$. The parameter for Linear is output features. The parameters for ResidualConvTranspose2d are output channels and kernel size. The parameters for Conv2d are output channels and kernel size.

| block | details |
|-------|---------|
| 1     | Linear(1024), LeakyReLU |
| 2     | ResidualConvTranspose2d(64, 3), LeakyReLU |
| 3     | ResidualConvTranspose2d(64, 3), LeakyReLU |
| 4     | ResidualConvTranspose2d(64, 3), LeakyReLU |
| 5     | ResidualConvTranspose2d(128, 3), LeakyReLU |
| 6     | ResidualConvTranspose2d(128, 3), LeakyReLU |
| 7     | ResidualConvTranspose2d(128, 3), LeakyReLU |
| 8     | ResidualConvTranspose2d(128, 3), LeakyReLU |
| 9     | ResidualConvTranspose2d(128, 3), LeakyReLU |
| 10    | Conv2d(100, 3) |
| 11    | Conv2d(100, 1) |

Table 9: Architecture for $p_{\phi_d}(z_d|d)$ and $p_{\phi_y}(z_y|y)$. Each network has two heads one for the mean and one for the scale. The parameter for Linear is output features.

| block | details |
|-------|---------|
| 1     | Linear(64), LeakyReLU |
| 2.1   | Linear(64) |
| 2.2   | Linear(64), Softplus |

Table 10: Architecture for $q_{\phi_d}(z_d|x)$, $q_{\phi_z}(z_x|x)$ and $q_{\phi_y}(z_y|x)$. Each network has two heads one for the mean one and for the scale. The parameters for Conv2d are output channels and kernel size. The parameters for ResidualConvTranspose2d are output channels and kernel size. The parameter for Linear is output features.

| block | details |
|-------|---------|
| 1     | Conv2d(32, 3), LeakyReLU |
| 2     | ResidualConvTranspose2d(32, 32), LeakyReLU |
| 3     | ResidualConvTranspose2d(32, 32), LeakyReLU |
| 4     | ResidualConvTranspose2d(64, 3), LeakyReLU |
| 5     | ResidualConvTranspose2d(64, 3), LeakyReLU |
| 6     | ResidualConvTranspose2d(64, 3), LeakyReLU |
| 7     | ResidualConvTranspose2d(64, 3), LeakyReLU |
| 8     | ResidualConvTranspose2d(64, 3), LeakyReLU |
| 9.1   | Linear(64) |
| 9.2   | Linear(64), Softplus |

Table 11: Architecture for $q_{\omega_d}(d|z_d)$ and $q_{\omega_y}(y|z_y)$. The parameter for Linear is output features.

| block | details |
|-------|---------|
| 1     | LeakyReLU, Linear(9 for $q_{\omega_d}(d|z_d)/2$ for $q_{\omega_y}(y|z_y)$), Softmax |