
Learning unbiased features

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1 Introduction

A key element in transfer learning is representation learning; if representations can be developed that expose the relevant factors underlying the data, then new tasks and domains can be learned readily based on mappings of these salient factors. We propose that an important aim for these representations are to be *unbiased*. Different forms of representation learning can be derived from alternative definitions of unwanted bias, e.g., bias to particular tasks, domains, or irrelevant underlying data dimensions. One very useful approach to estimating the amount of bias in a representation comes from maximum mean discrepancy (MMD) [5], a measure of distance between probability distributions. We are not the first to suggest that MMD can be a useful criterion in developing representations that apply across multiple domains or tasks [1]. However, in this paper we describe a number of novel applications of this criterion that we have devised, all based on the idea of developing unbiased representations. These formulations include: a standard domain adaptation framework; a method of learning invariant representations; an approach based on noise-insensitive autoencoders; and a novel form of generative model. We suggest that these formulations are relevant for the transfer learning workshop for a few reasons: (a). they focus on deep learning; (b). the formulations include both supervised and unsupervised learning scenarios; and (c). they are well-suited to the scenario emphasized in the call-for-papers, where the learning task is not focused on the regime of limited training data but instead must manage large scale data, which may be limited in labels and quality.

2 Maximum Mean Discrepancy

Each of our approaches to learn unbiased features rely on a sample-based measure of the bias in the representation. A two sample test is a statistical test that tries to determine, given two datasets $\{X_n\} \sim P$ and $\{Y_m\} \sim Q$, whether the datasets have been generated from the same underlying distribution, i.e., if $P = Q$. Maximum mean discrepancy [5] is a useful distance measure between two distributions that can be used to perform two sample tests.

$$\begin{aligned} \text{MMD}(X, Y) &= \left\| \frac{1}{N} \sum_{n=1}^N \phi(X_n) - \frac{1}{M} \sum_{m=1}^M \phi(Y_m) \right\|^2 \\ &= \frac{1}{N^2} \sum_{n=1}^N \sum_{n'=1}^N \phi(X_n)^\top \phi(X_{n'}) + \frac{1}{M^2} \sum_{m=1}^M \sum_{m'=1}^M \phi(Y_m)^\top \phi(Y_{m'}) - \frac{2}{NM} \sum_{n=1}^N \sum_{m=1}^M \phi(X_n)^\top \phi(Y_m) \end{aligned} \quad (1)$$
$$(2)$$

Where $\phi(\cdot)$ is a feature expansion function. We can apply the kernel trick to each inner product in Equation (2) to use an implicit feature space. When the space defined by the kernel is a universal reproducing kernel Hilbert space then asymptotically MMD is 0 if and only if $P = Q$ [6].

	E→B	B→D	K→D	D→E	B→K	E→K
Linear SVM	71.0 ± 2.0	79.0 ± 1.9	73.6 ± 1.5	74.2 ± 1.4	75.9 ± 1.8	84.5 ± 1.0
RBF SVM	68.0 ± 1.9	79.1 ± 2.3	73.0 ± 1.6	76.3 ± 2.2	75.8 ± 2.1	82.0 ± 1.4
TCA	71.8 ± 1.4	76.9 ± 1.4	73.3 ± 2.4	75.9 ± 2.7	76.8 ± 2.1	80.2 ± 1.4
NN	70.0 ± 2.4	78.3 ± 1.6	72.7 ± 1.6	72.8 ± 2.4	74.1 ± 1.6	84.0 ± 1.5
NN MMD*	71.8 ± 2.1	77.4 ± 2.4	73.9 ± 2.4	78.4 ± 1.6	77.9 ± 1.6	84.7 ± 1.6
NN MMD	73.7 ± 2.0	79.2 ± 1.7	75.0 ± 1.0	79.1 ± 1.6	78.3 ± 1.4	85.2 ± 1.1

Table 1: Domain adaptation results for product review sentiment classification task. NN MMD*: neural net with MMD trained and tested on word count instead of TF-IDF features.

3 Applications

3.1 Domain Adaptation

In domain adaptation, we are given a set of labeled data from a source domain and a set of unlabeled data from a different target domain. The task is to learn a model that works well on the target domain.

In our framework, we want to learn unbiased features that are invariant to the nuances across different domains. The classifier trained on these features can then generalize well over all domains. We use deep neural networks as the classification model. MMD is used as a penalty on one hidden layer of the neural net to drive the distributions of features for the source and target domains to be close to each other. While the use of MMD is similar to that of [1], we use a neural network to learn both the features and classifier jointly. The distributed representation of a neural network is far more powerful than the linear transformation and clustering method proposed in [1].

We tested the neural network with MMD penalty model on the Amazon product review sentiment classification dataset [2]. This dataset contains product reviews from 4 domains corresponding to 4 product categories (books, dvd, electronics, kitchen). Each review is labeled either positive or negative, and we preprocessed them as TF-IDF vectors. We tested a 2 hidden layer neural net model on the adaptation tasks between all pairs of source and target domains. For each task, a small portion of the the labeled source domain data is used as validation data for early stopping. Other hyper parameters are chosen to optimize the average target performance over 10 random splits of the data, in a setting similar to cross-validation. The best target accuracy with standard deviation for a few tasks are shown in Table 1. More results and experiment settings can be found in the appendix.

We compare our method with SVM models with no adaptation, neural net with the same architecture but no MMD penalty, and another popular domain adaptation baseline Transfer Component Analysis (TCA) [8]. The neural net model with MMD penalty dominates on most tasks. Even with the more basic word count features the “NN MMD” method still works better than most other baselines, demonstrating the ability of our model to learn features useful across domains.

3.2 Learning Invariant Features

In this application we use the proposed framework to learn features invariant to transformations on input data. More specifically, we want to learn features for human faces that are both good for identity recognition and invariant to different lighting conditions.

In the experiment we used the extended Yale B dataset, which contains faces of 38 people under various lighting conditions corresponding to light source from different directions. We created 5 groups of images, corresponding to light source in upper right, lower right, lower left, upper left and the front. Then for each group of images, we chose 1 image per person to form one domain for that lighting condition. In this way we had 5 domains with $5 \times 38 = 190$ images in total. All the other images (around 2000) are used for testing. The task is to recognize the identity of the person in image, i.e. a 38-way classification task. For this task, we did not use a validation set, but rather report the best result on test set to see where the limits of different models are. Note that the lighting conditions here can be modeled very well with a Lambertian model, however we did not use this strong model but rather choose to use a generic neural network to learn invariant features, so that the proposed method can be readily applied to other applications.

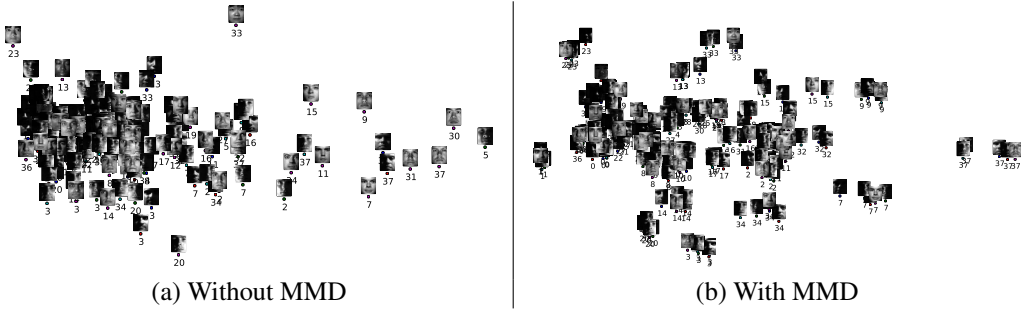


Figure 1: PCA projection of the representations of the second hidden layer for the training images. Each example is plotted with the person ID and the image. Zoom in to see the details.

The proposed model for this task is similar to the one used in the previous section, except that the MMD penalty is now applied to the distribution of hidden representations for 5 different domains rather than two. We used the following formulation which is a sum of MMD between each individual distribution and the average distribution across all domains

$$\text{MMD} = \sum_{s=1}^S \left\| \frac{1}{N_s} \sum_{i:d_i=s} \phi(h_i) - \frac{1}{N} \sum_n \phi(h_n) \right\|^2 \quad (3)$$

where s indexes domains, i indexes examples, $S = 5$ is the number of different domains, N_s is the number of examples from domain s , N is the total number of examples across all domains, d_i is the domain label for example i and h_i is the hidden representation computed from a neural network. We use a two hidden layer neural net with 256 and 128 ReLU units on each of them for this task. The MMD penalty with a Gaussian kernel is applied to the second hidden layer. Dropout [7] is used for all the methods compared here to regularize the network as overfitting is a big problem.

On this task, the baseline model trained without the MMD penalty achieves a test accuracy of 72% (100% training accuracy). Using the MMD penalty with Gaussian kernel, the best test accuracy improved significantly to around 82%. Using a linear kernel leads to a test accuracy to 78%.

We visualize the hidden representations for the training images learned with the Gaussian kernel MMD penalty in Figure 1. Note that examples for each person under very different lighting conditions are grouped together even though the MMD penalty only depends on lighting condition, and does not take into account identity.

3.3 Noise-Insensitive Autoencoders

Auto-encoders (AEs) are neural network models that have two basic components: an encoder, that maps data into a latent space, and a decoder, that maps the latent space back out into the original space. Auto-encoders are typically trained to minimize reconstruction loss from encoding and decoding. In many applications, reconstruction loss is merely a proxy and can lead to spurious representations. Researchers have spent a great deal of effort developing new regularization schemes to improve the learned representation [11, 12, 9]. Two such methods include denoising auto-encoders (DAEs) [12] and contractive auto-encoders (CAEs) [9]. With denoising auto-encoders, the data is perturbed with noise and the reconstruction loss is altered to measure how faithfully the original data can be recovered from the perturbed data. Contractive auto-encoders more explicitly penalize the latent representation so that it becomes invariant to infinitesimal perturbations in the original space. In the appendix, we show how the CAE penalty can be interpreted as a form of MMD penalty with a linear kernel.

We experiment with several single-layer auto-encoder variants, including an ordinary auto-encoder trained on reconstruction loss, a contractive auto-encoder, and a denoising auto-encoder. For comparison, we augment both the ordinary auto-encoder and denoising auto-encoder with the MMD penalty on their hidden layer, sampling a new set of perturbed hidden units with each weight update. We trained each model on 10,000 MNIST digits and tuned hyperparameters to minimize a denoising reconstruction loss on held-out data. Further details can be found in the appendix.

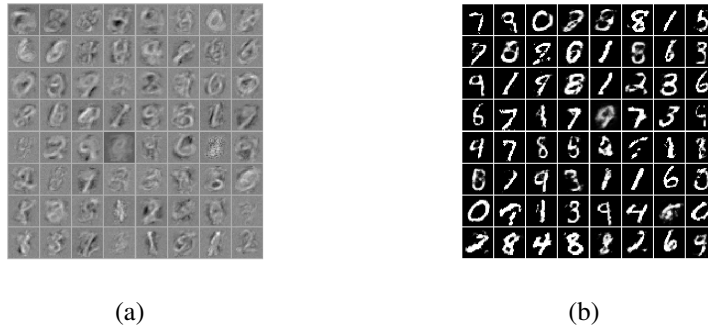


Figure 2: (a) visualization of some bottom layer weights; (b) independent samples from the model.

To measure the invariance to perturbation, we created a noisy copy of the test data and trained an SVM classifier on the latent representations to distinguish between clean and noisy data. A worse accuracy corresponds to a more unbiased latent representation. The MMD autoencoder outperformed the other approaches on this measure. Surprisingly, the denoising autoencoder performed the worst, demonstrating that denoising does not necessarily produce features that are invariant to noise. Also interesting is that a relatively low contraction penalty was chosen for the CAE, as higher penalties seemed to incur higher denoising reconstruction loss. This is likely due to the difference between the applied Bernoulli noise, and the infinitesimal noise assumed by the CAE. Plots of the filters can be found in the appendix.

Model	AE	DAE	CAE	MMD	MMD+DAE
SVM Accuracy	78.6	82.5	77.9	61.1	72.9

Table 2: SVM accuracy on distinguishing clean from noisy data. Lower accuracy means the learned features are more invariant to noise.

3.4 Learning Generative Deep Models

The last application we consider is to use the MMD criterion for learning generative models. Unlike previous sections where MMD is used to learn unbiased representations, in this application we use MMD to match the distribution of the generative model with the data distribution. The idea is MMD should be small on samples from a good generative model.

Here we train a generative deep model proposed in [4] on a subset of 1000 MNIST digits. The model contains a stochastic hidden layer h at the top with a fixed prior distribution $p(h)$, and a mapping f that deterministically maps h to x . The prior $p(h)$ and the mapping $f(x|h)$ together implicitly defines the distribution $p(x)$.

In [4] the authors proposed a minimax formulation to learn the mapping f , where one extra classifier looks at the data and the samples of the model and then try to do a good job of distinguishing them, and the parameters of f is updated to make this classifier do as bad as possible so that samples generated will be close to the data. As the formulation interleaves two optimization problems with opposite objectives, careful scheduling is required for the model to converge to a good point.

We propose to directly minimize the MMD between the data and the model samples. Given a fixed sample of h , we can backpropagate through the MMD penalty and the whole network, to drive the model samples to be close to the data. This method utilizes a single consistent objective and completely avoids the minimax problem. Details of our architecture and training can be found in the appendix.

Figure 2 visualizes some bottom layer weights of the network and a set of samples generated from the model. We can see that with this method the model learns some meaningful features and is able to generate realistic samples.

References

- [1] Mahsa Baktashmotlagh, Mehrtash T Harandi, Brian C Lovell, and Mathieu Salzmann. Unsupervised domain adaptation by domain invariant projection. In *IEEE International Conference on Computer Vision (ICCV)*, pages 769–776, 2013.
- [2] John Blitzer, Mark Dredze, and Fernando Pereira. Biographies, bollywood, boom-boxes and blenders: Domain adaptation for sentiment classification. In *ACL*, volume 7, pages 440–447, 2007.
- [3] John Duchi, Elad Hazan, and Yoram Singer. Adaptive subgradient methods for online learning and stochastic optimization. *The Journal of Machine Learning Research*, 12:2121–2159, 2011.
- [4] Ian J Goodfellow, Jean Pouget-Abadie, Mehdi Mirza, Bing Xu, David Warde-Farley, Sherjil Ozair, Aaron Courville, and Yoshua Bengio. Generative adversarial networks. In *Advances in Neural Information Processing Systems (NIPS)*, 2014.
- [5] Arthur Gretton, Karsten M Borgwardt, Malte Rasch, Bernhard Schölkopf, and Alex J Smola. A kernel method for the two-sample-problem. In *Advances in Neural Information Processing Systems (NIPS)*, 2006.
- [6] Arthur Gretton, Karsten M Borgwardt, Malte J Rasch, Bernhard Schölkopf, and Alexander Smola. A kernel two-sample test. *The Journal of Machine Learning Research*, 13(1):723–773, 2012.
- [7] Geoffrey E. Hinton, Nitish Srivastava, Alex Krizhevsky, Ilya Sutskever, and Ruslan Salakhutdinov. Improving neural networks by preventing co-adaptation of feature detectors. *arXiv preprint arXiv:1207.0580*, 2012.
- [8] Sinno Jialin Pan, Ivor W Tsang, James T Kwok, and Qiang Yang. Domain adaptation via transfer component analysis. *IEEE Transactions on Neural Networks*, 22(2):199–210, 2011.
- [9] Salah Rifai, Pascal Vincent, Xavier Muller, Xavier Glorot, and Yoshua Bengio. Contractive autoencoders: Explicit invariance during feature extraction. In *International Conference on Machine Learning (ICML)*, 2011.
- [10] Oren Rippel, Michael A. Gelbart, and Ryan P. Adams. Learning ordered representations with nested dropout. In *International Conference on Machine Learning (ICML)*, 2014.
- [11] Kevin Swersky, Marc’Aurelio Ranzato, David Buchman, Benjamin M. Marlin, and Nando de Freitas. On autoencoders and score matching for energy based models. In *International Conference on Machine Learning (ICML)*, 2011.
- [12] Pascal Vincent, Hugo Larochelle, Isabelle Lajoie, Yoshua Bengio, and Pierre-Antoine Manzagol. Stacked denoising autoencoders: Learning useful representations in a deep network with a local denoising criterion. *The Journal of Machine Learning Research*, 11:3371–3408, 2010.

	D→B	E→B	K→B	B→D	E→D	K→D
Linear SVM	78.3 ± 1.4	71.0 ± 2.0	72.9 ± 2.4	79.0 ± 1.9	72.5 ± 2.9	73.6 ± 1.5
RBF SVM	77.7 ± 1.2	68.0 ± 1.9	73.2 ± 2.4	79.1 ± 2.3	70.7 ± 1.8	73.0 ± 1.6
TCA	77.5 ± 1.3	71.8 ± 1.4	68.8 ± 2.4	76.9 ± 1.4	72.5 ± 1.9	73.3 ± 2.4
NN	76.6 ± 1.8	70.0 ± 2.4	72.8 ± 1.5	78.3 ± 1.6	71.7 ± 2.7	72.7 ± 1.6
NN MMD*	76.5 ± 2.5	71.8 ± 2.1	72.8 ± 2.4	77.4 ± 2.4	74.3 ± 1.7	73.9 ± 2.4
NN MMD	78.5 ± 1.5	73.7 ± 2.0	75.7 ± 2.3	79.2 ± 1.7	75.3 ± 2.1	75.0 ± 1.0
	B→E	D→E	K→E	B→K	D→K	E→K
Linear SVM	72.4 ± 3.0	74.2 ± 1.4	82.7 ± 1.3	75.9 ± 1.8	77.0 ± 1.8	84.5 ± 1.0
RBF SVM	72.8 ± 2.5	76.3 ± 2.2	82.5 ± 1.4	75.8 ± 2.1	76.0 ± 2.2	82.0 ± 1.4
TCA	72.1 ± 2.6	75.9 ± 2.7	79.8 ± 1.4	76.8 ± 2.1	76.4 ± 1.7	80.2 ± 1.4
NN	70.1 ± 3.1	72.8 ± 2.4	82.3 ± 1.0	74.1 ± 1.6	75.8 ± 1.8	84.0 ± 1.5
NN MMD*	75.6 ± 2.9	78.4 ± 1.6	83.0 ± 1.2	77.9 ± 1.6	78.0 ± 1.9	84.7 ± 1.6
NN MMD	76.8 ± 2.0	79.1 ± 1.6	83.9 ± 1.0	78.3 ± 1.4	78.6 ± 2.6	85.2 ± 1.1

Table 3: Domain adaptation results for product review sentiment classification task. NN MMD*: neural net with MMD trained and tested on word count instead of TF-IDF features.

4 Appendix

4.1 More Details of the Domain Adaptation Experiments

The dataset contains 2000 product reviews in each of the 4 domains. Each product review is represented as a bag of words and bigrams. We preprocessed the data and ignored all words and bigrams occurring less than 50 times across the whole dataset. Then computed the new word-count vectors and TF-IDF vectors for each product review and use these vectors as input representations of the data.

To make the experiment results robust to sampling noise, we generated 10 random splits of the dataset, where each domain is split into 1500 examples for training, 100 for validation and 400 for testing. For each domain adaptation task from one source domain to a target domain, the training data in the source domain is used as labeled source domain data, and the training data without labels in the target domain is used as unlabeled target domain data. The validation data in the source domain is used for early stopping in neural network training, and the prediction accuracy on the test data from target domain is used as the evaluation metric. For each of the methods we considered in the experiments, hyper parameters are tuned to optimize the average target domain prediction accuracy across all 10 random splits, and the best average accuracy is reported, which is a setting similar to cross-validation for domain adaptation tasks.

We used a fully connected neural network with two hidden layers, 128 hidden units on the first layer and 64 hidden units on the second. All hidden units are rectified linear units (ReLU). The MMD penalty is applied on the second hidden layer. We used Gaussian kernels for MMD. The final objective is composed of a classification objective on the source domain and a MMD penalty for the source and target domains. The model is trained using stochastic gradient descent, where the initial learning rate is fixed and gradually adapted according to AdaGrad [3]. The hyperparameters of the model include the scale parameter in Gaussian kernel and the weight for the MMD penalty. The learning rate, momentum, weight-decay and dropout rate for neural network training are fixed for all the experiments.

For TCA baseline, we tried both linear kernels and Gaussian RBF kernels, and found that linear kernels actually works better, so the reported results are all from linear kernel TCA models. The projection matrix after kernel transformation projects the examples down to 64 dimensions (same as the 2nd hidden layer of the neural net above). Then a Gaussian kernel RBF SVM is trained on the mean-std normalized projected features (we’ve tried linear SVMs as well but found RBF SVMs work better). We found the normalization step to be critical to the performance of TCA as the scale of the features can differ by a few orders of magnitudes.

Full results on all source-target pairs are shown in Table 3. NN MMD with word count features are shown as “NN MMD*”. Overall all methods gets a significant boost from using TF-IDF features. But NN MMD method is able to learn useful features for domain adaptation even with word count features, and performs better than the baselines on most tasks.

4.2 Relationship Between Contractive Auto-Encoders and MMD

It is straightforward to show that the contractive auto-encoder can be written as an MMD penalty with a linear kernel. First take e_i to be an elementary vector with a 1 at index i and 0 everywhere else. We will take a Taylor expansion of a hidden unit $h_j(x)$ around e_i [10]:

$$h_j(x + \epsilon e_i) \approx h_j(x) + \epsilon e_i^\top \nabla h_j(x) + o(\epsilon^2), \quad (4)$$

$$\frac{h_j(x + \epsilon e_i) - h_j(x)}{\epsilon} \approx e_i^\top \nabla h_j(x), \quad (5)$$

$$h_j(x + \epsilon e_i) - h_j(x) \approx \epsilon \frac{\partial h_j(x)}{\partial x_i}. \quad (6)$$

Squaring both sides and summing over each hidden dimension and data dimension recovers the contractive auto-encoder penalty.

$$\sum_j \sum_i (h_j(x + \epsilon e_i) - h_j(x))^2 \approx \epsilon^2 \sum_j \sum_i \left(\frac{\partial h_j(x)}{\partial x_i} \right)^2. \quad (7)$$

The left hand side can be rewritten as an MMD penalty $\|h(x) - \tilde{h}(x)\|^2$, where $\tilde{h}(x) = [h_1(x + \epsilon e_1), h_2(x + \epsilon e_1), \dots, h_K(x + \epsilon e_D)]$, assuming K hidden units and D data dimensions. Since there is no feature expansion, this is equivalent to using a linear kernel.

4.3 Auto-Encoder Training Details

We use a stochastic variant of the contraction penalty, where we sample $\tilde{h}(x)$ from a noise distribution. As in [12], we use Bernoulli noise where each data dimension is zeroed out with probability p , which is tuned along with the other hyperparameters. We use MMD with a Gaussian kernel $K(h(x), \tilde{h}(x)) = \exp(-\frac{1}{\sigma^2} \|h(x) - \tilde{h}(x)\|^2)$. The networks each have one layer of 100 sigmoidal hidden units and are trained using stochastic gradient descent with momentum.

4.4 Auto-Encoder Weight Filters

Figure 3 shows the weight filters, the weights from the each hidden unit to the data visualized as images. The MMD filters tend to be cleaner and more localized than the other variants.

4.5 Training Details for the Generative Experiments

We learn a generative deep model with 32 stochastic hidden units with independent uniform prior distributions in $[-1, 1]$, the deterministic mapping is implemented by a feedforward network with two ReLU layers with 64 and 128 units each, and then a final sigmoid layer of 784 units (MNIST images are of size $28 \times 28 = 784$). We use a Gaussian kernel for the MMD. For training, a set of new samples h is generated from $p(h)$ after every 200 updates to f .

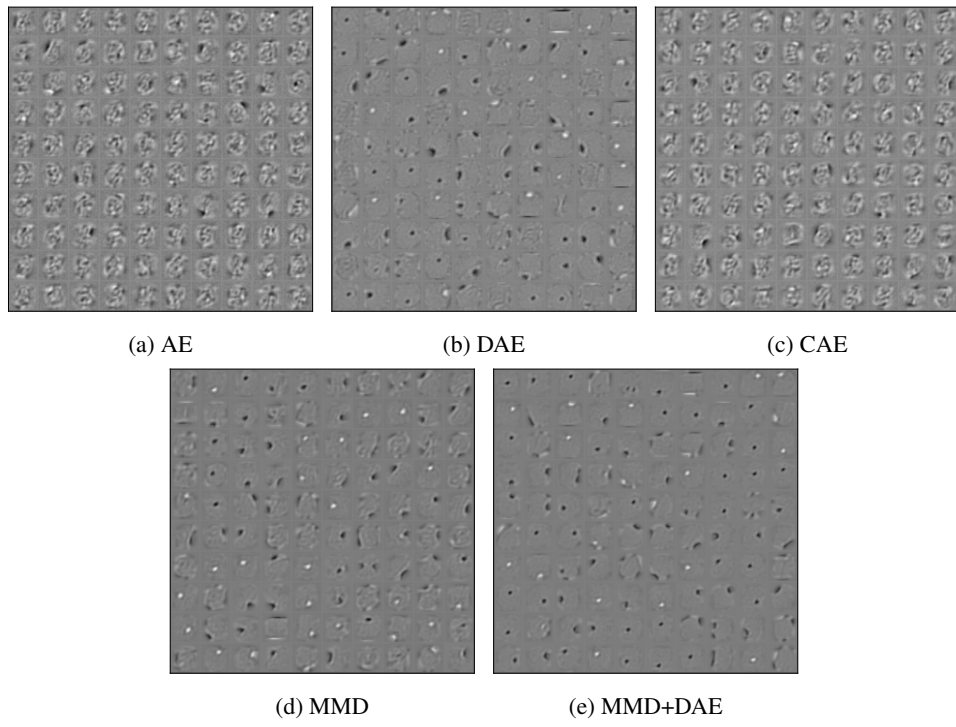


Figure 3: Visualization of the weight matrices for each variety of auto-encoder.