Conditional Variance Penalties and Domain Shift Robustness

Christina Heinze-Deml & Nicolai Meinshausen
Seminar for Statistics
ETH Zurich
Zurich, Switzerland
{heinzedeml,meinshausen}@stat.math.ethz.ch

Abstract

When training a deep neural network for supervised image classification, one can broadly distinguish between two types of latent features of images that will drive the classification. Following the notation of Gong et al. (2016), we can divide latent features into (i) ‘core’ or ‘conditionally invariant’ features $X_{\text{core}}$ whose distribution $X_{\text{core}} | Y$ conditional on the class $Y$, does not change substantially across domains and (ii) ‘style’ or ‘orthogonal’ features $X_{\text{style}}$ whose distribution $X_{\text{style}} | Y$ can change substantially across domains. These latter orthogonal features would generally include features such as position, rotation, image quality or brightness but also more complex ones like hair color or posture for images of persons. Guarding against future adversarial domain shifts implies that the influence of the second type of style features in the prediction has to be limited. In contrast to previous work, we assume that the domain itself is not observed and hence a latent variable. Therefore, we can not directly see the distributional change of features across different domains.

We do assume, however, that we can sometimes observe a typically discrete identifier or ID variable. We know in some applications, for example, that two images show the same person, and ID then refers to the identity of the person. In data augmentation, we generate several images from the same original image, and ID then refers to the relevant original image. The method requires only a small fraction of images to have an ID variable.

The causal framework of Gong et al. (2016) is adapted by adding the identifier ID variable to the model and making domain a latent variable. We group data samples if they share the same class and identifier $(Y, \text{ID}) = (y, id)$ and penalize the conditional variance of the prediction if we condition on $(Y, \text{ID})$. The regularization is equivalent to penalizing with an appropriate graph Laplacian. Using this grouping-by-ID approach is shown to protect against shifts in the distribution of the style variables for both regression and classification models. Specifically, the conditional variance penalty CoRE is shown to be equivalent to minimizing the risk under noise interventions in a regression setting and is shown to lead to adversarial risk consistency in a partially linear classification setting.

We show empirically that the CoRE penalty substantially improves performance in settings where domains changes occur in terms of image quality, brightness and color while we also look at more complex changes such as changes in movement and posture. The attractive feature is that the type of domain change on future data does not need to be known a priori.

Keywords: Domain shift; Dataset shift; Causal models; Distributional robustness; Anticausal prediction; Image classification
1. Introduction

Deep neural networks (DNNs) have achieved outstanding performance on prediction tasks like visual object and speech recognition (Krizhevsky et al., 2012; Szegedy et al., 2015; He et al., 2015). Issues can arise when the learned representations rely on dependencies that vanish in test distributions, see for example Quionero-Candela et al. (2009); Torralba and Efros (2011); Csurka (2017) and references therein. Such domain shifts can be caused by changing conditions such as color, background or location changes. Predictive performance is then likely to degrade. The “Russian tank legend” is an example where the training data was subject to sampling biases that were not replicated in the real world. Concretely, the story relates how a machine learning system was trained to distinguish between Russian and American tanks from photos. The accuracy was very high but only due to the fact that all images of Russian tanks were of bad quality while the photos of American tanks were not. The system learned to discriminate between images of different qualities but would have failed in practice (Emspak, 2016). For a directly equivalent example, see §7.2. Existing biases in datasets used for training machine learning algorithms tend to be replicated in the estimated models (Bolukbasi et al., 2016). For another example involving Google’s photo app, see Crawford (2016) and Emspak (2016). In §7 we show many examples where unwanted biases in the training data are picked up by the trained model. As any bias in the training data is in general used to discriminate between classes, these biases will persist in future classifications, raising also considerations of fairness and discrimination (Barocas and Selbst, 2016).

Addressing the issues outlined above, we propose Conditional variance Regularization (CoRe) to give differential weight to different latent features. Conceptually, we take a causal view of the data generating process and categorize the latent data generating factors into ‘conditionally invariant’ (core) and ‘orthogonal’ (style) features, as in (Gong et al., 2016). It is desirable that a classifier uses only the core features as they pertain to the target of interest in a stable and coherent fashion. Basing a prediction on the core features alone yields a stable predictive accuracy even if the style features are altered. CoRe yields an estimator which is approximately invariant under changes in the conditional distribution of the style features (conditional on the class labels). Consequently, it is robust with respect to adversarial domain shifts, arising through arbitrarily strong interventions on the style features. CoRe relies on the fact that for certain datasets we can observe ‘grouped observations’ in the sense that we observe the same object under different conditions. Rather than pooling over all examples, CoRe exploits knowledge about this grouping, i.e. that a number of instances relate to the same object. By penalizing between-object variation of the prediction less than variation of the prediction for the same object, we can steer the prediction to be based more on the latent core features and less on the latent style features.

The remainder of this manuscript is structured as follows: §2 starts with a few motivating examples, showing simple settings where the style features change in the test distribution such that standard empirical risk minimization approaches would fail. In §3 we review related work, introduce notation in §4 and in §5 we formally introduce conditional variance regularization CoRe. In §6 CoRe is shown to be equivalent to minimizing the risk under noise interventions in a regression setting and is shown to lead to adversarial risk consistency.

1. A different version of this story can be found in Yudkowsky (2008).
Figure 1: Three motivating examples: a linear example in (a) and (b), a nonlinear example in (c) and (d) and an example where the goal is to predict whether a person is wearing glasses in (e) and (f). The distributions are shifted in test data by style interventions where style in example (a/b) is the linear direction \((1, -0.75)\), the polar angle in example (c/d), and the image quality in example (e/f). In this latter example, a 5-layer CNN achieves 0% training error and 2% test error for images that are sampled from the same distribution as the training images (e), but a 65% error rate on images where the confounding between image quality and glasses is changed (f). See §7.2 for more details.

in a partially linear classification setting. In [7] we evaluate the performance of CoRe in a variety of experiments.

To summarize, our contributions are the following:

(i) **Causal framework.** We extend the causal framework of [Gong et al. 2016] to address situations where the domain variable itself is latent.

(ii) **Conditional variance penalties and distributional robustness.** We introduce conditional variance penalties, which are equivalent to a suitable graph Laplacian penalty. For classification, we show in Theorem 1 that we can achieve consistency under a risk definition that allows adversarial domain changes. For regression, we show in Theorem 2 that estimator achieves distributional robustness against intervention distributions where the noise variance of domain-specific noise is increased. A one-to-one correspondence between the penalty parameter and the set of distributions we are protected against is shown.

(iii) **Software.** We illustrate our ideas using synthetic and real-data experiments. A TensorFlow implementation of CoRe as well as code to reproduce some of the experimental results are available at [https://github.com/christinaheinze/core](https://github.com/christinaheinze/core).
2. Motivating examples

To motivate the methodology we propose, consider the examples shown in Figure 1. Example 1 shows a setting where a linear decision boundary is suitable. Panel [a] shows the training data where class 1 is associated with red points, dark blue points correspond to class 0. If we were asked to draw a decision boundary based on the training data, we would probably choose one that is approximately horizontal. The style feature here corresponds to a linear direction $(1, -0.75)^T$. Panel [b] shows the test set where the style feature is intervened upon for class 1 observations: class 1 is associated with orange squares, cyan squares correspond to class 0. Clearly, a horizontal decision boundary would have misclassified all test points of class 1.

Example 2 shows a setting where a nonlinear decision boundary is required. Here, the core feature corresponds to the distance from the origin while the style feature corresponds to the angle between the $x_1$-axis and the vector from the origin to $(x_1, x_2)$. Panel [c] shows the training data and panel [d] additionally shows the test data where the style—i.e. the distribution of the angle—is intervened upon. Clearly, a circular decision boundary yields optimal performance on both training and test set but is unlikely to be found by a standard classification algorithm when only using the training set for the estimation. We will return to these examples in §5.4.

Lastly, we mimic the Russian tank legend in the third example by manipulating the face images from the CelebA dataset (Liu et al., 2015): in the training set images of class “wearing glasses” are associated with a lower image quality than images of class “not wearing glasses”. Examples are shown in panel [e]. In the test set, this relation is reversed, i.e. images showing persons wearing glasses are of higher quality than images of persons without glasses, with examples in panel [f]. We will return to this example in §7.2 and show that training a convolutional neural network to distinguish between people wearing glasses or not works well on test data that are drawn from the same distribution (with error rates below 2%) but fails entirely on the shown test data, with error rates worse than 65%.

3. Related work

For general distributional robustness, the aim is to learn

$$\arg\min_\theta \sup_{F \in \mathcal{F}} E_F(\ell(Y, f_\theta(X)))$$

for a given set $\mathcal{F}$ of distributions, loss $\ell$, and prediction $f_\theta(x)$. The set $\mathcal{F}$ is the set of distributions on which one would like the estimator to achieve a guaranteed performance bound and the set is often taken to be of the form $\mathcal{F} = \mathcal{F}_\epsilon(P_0)$ with

$$\mathcal{F}_\epsilon(P_0) := \{\text{distributions } Q \text{ such that } D(Q, P_0) \leq \epsilon\},$$

with $\epsilon > 0$ a small constant and $D(Q, P_0)$ being, for example, a $\phi$-divergence (Namkoong and Duchi, 2017; Ben-Tal et al., 2013; Bagnell, 2005) or a Wasserstein-distance (Shafieezadeh-Abadeh et al., 2017; Sinha et al., 2017; Gao et al., 2017). The distribution $P_0$ can be the true (but generally unknown) population distribution $P$ from which the data were drawn or its empirical counterpart $P_n$. The distributionally robust targets (1) can often be expressed in penalized form; see Gao et al. (2017); Sinha et al. (2017); Xu et al. (2009).
In this work, we do not try to achieve robustness with respect to a set of distributions that are pre-defined by a Kullback-Leibler divergence or a Wasserstein metric as in (2). We try to achieve robustness against a set of distributions that are generated by interventions on latent style variables. As such the right distribution set \( F \) in (1) has to be learnt from data and we need a causal model to define the set of distributions we would like to protect ourselves against.

Similar to this work in terms of their goals are the work of Gong et al. (2016) and Domain-Adversarial Neural Networks (DANN) proposed in Ganin et al. (2016), an approach motivated by the work of Ben-David et al. (2007). The main idea of Ganin et al. (2016) is to learn a representation that contains no discriminative information about the origin of the input (source or target domain). This is achieved by an adversarial training procedure: the loss on domain classification is maximized while the loss of the target prediction task is minimized simultaneously. The data generating process assumed in Gong et al. (2016) is similar to our model, introduced in §4.2, where we detail the similarities and differences between the models (cf. Figure 2). Gong et al. (2016) identify the conditionally independent features by adjusting a transformation of the variables to minimize the squared MMD distance between distributions in different domains. The fundamental difference between these very promising methods and our approach is that we use a different data basis. The domain identifier is explicitly observable in Gong et al. (2016) and Ganin et al. (2016), while it is latent in our approach. In contrast, we exploit the presence of an identifier variable ID that relates to the identity of an object (for example identifying a person). In other words, we do not assume that we have data from different domains but just different realizations of the same object under different interventions.

Causal modeling has related aims to the setting of transfer learning and guarding against adversarial domain shifts. Specifically, causal models have the defining advantage that the predictions will be valid even under arbitrarily large interventions on all predictor variables (Haavelmo, 1944; Aldrich, 1989; Pearl, 2009; Schölkopf et al., 2012; Peters et al., 2016; Zhang et al., 2013; 2015; X. Yu, 2017; M. Rojas-Carulla, 2017; Magliacane et al., 2017). There are two difficulties in transferring these results to the setting of adversarial domain changes in image classification. The first hurdle is that the classification task is typically anti-causal since the image we use as a predictor is a descendant of the true class of the object we are interested in rather than the other way around. The second challenge is that we do not want to guard against arbitrary interventions on any or all variables but only would like to guard against a shift of the style features. It is hence not immediately obvious how standard causal inference can be used to guard against large domain shifts. Recently, various approaches have been proposed that leverage causal motivations for deep learning or use deep learning for causal inference. Chalupka et al. (2014) characterize learning the visual causes for a certain target behavior and thereby model perceiving systems. Various approaches focus on cause-effect inference where the goal is to find the causal relation between two random variables, \( X \) and \( Y \) (Lopez-Paz et al., 2017; Lopez-Paz and Oquab, 2017; Goudet et al., 2017). Lopez-Paz et al. (2017) propose the Neural Causation Coefficient (NCC) to estimate the probability of \( X \) causing \( Y \) and apply it to finding the causal relations

\[2. \text{ The distinction between 'conditionally independent' features and 'conditionally transferable' (which is the former modulo location and scale transformations) is for our purposes not relevant as we do not make a linearity assumption in general.} \]
between image features. Specifically, the NCC is used to distinguish between features of objects and features of the objects’ contexts. Lopez-Paz and Oquab (2017) note the similarity between structural equation modeling and CGANs (Mirza and Osindero 2014). One CGAN is fitted in the direction $X \rightarrow Y$ and another one is fitted for $Y \rightarrow X$. Based on a two-sample test statistic, the estimated causal direction is returned. Goudet et al. (2017) use generative neural networks for cause-effect inference, to identify $v$-structures and to orient the edges of a given graph skeleton. Bahadori et al. (2017) devise a regularizer that combines an $\ell_1$ penalty with weights corresponding to the estimated probability of the respective feature being causal for the target. The latter estimates are obtained by causality detection networks or scores such as estimated by the NCC. Besserve et al. (2017) draw connections between GANs and causal generative models, using a group theoretic framework. Kocaoglu et al. (2017) propose causal implicit generative models to sample from conditional as well as interventional distributions, using a conditional GAN architecture (CausalGAN). The generator structure needs to inherit its neural connections from the causal graph, i.e. the causal graph structure must be known. Louizos et al. (2017) propose the use of deep latent variable models and proxy variables to estimate individual treatment effects. Kilbertus et al. (2017) exploit causal reasoning to characterize fairness considerations in machine learning. Distinguishing between the protected attribute and its proxies, they derive causal non-discrimination criteria. The resulting algorithms avoiding proxy discrimination require classifiers to be constant as a function of the proxy variables in the causal graph, thereby bearing some structural similarity to our style features. Distinguishing between core and style features can be seen as some form of disentangling factors of variation. Estimating disentangled factors of variation has gathered a lot of interested in the context of generative modeling (Higgins et al., 2017; Chen et al., 2016; Bouchacourt et al., 2017). For example, Matsuo et al. (2017) propose a “Transform Invariant Autoencoder” where the goal is to reduce the dependence of the latent representation on a specified transform of the object in the original image. Specifically, Matsuo et al. (2017) predefine location as the style feature and the goal is to learn a latent representation that does not include $X^{\text{style}}$. Our approach is different as we do not predefine which features are considered style features. The style features in our approach could be location but also image quality, posture, brightness, background and contextual information or something entirely unknown. We try to learn a representation of style and core features from data by exploiting the grouping of training samples. Additionally, the approach in Matsuo et al. (2017) cannot effectively deal with a confounding situation where the distribution of the style features differs conditional on the class (this is a natural restriction for their work, however, as the class label is not even observed in the autoencoder setting). As in CoRE, Bouchacourt et al. (2017) exploit grouped observations. In a variational autoencoder framework, they aim to separate style and content—they assume that samples within a group share a common but unknown value for one of the factors of variation while the style can differ. Denton and Birodkar (2017) propose an autoencoder framework to disentangle style and content in videos using an adversarial loss term where the grouping structure induced by clip identity is exploited. Here we try to solve a classification task directly without estimating the latent factors explicitly as in a generative framework.
4. Setting

We first describe the general notation used before describing the causal graph that allows us to compare the setting of adversarial domain shifts to transfer learning, domain adaptation and adversarial examples.

4.1 Notation

Let $Y \in \mathcal{Y}$ be a target of interest. Typically $\mathcal{Y} = \mathbb{R}$ for regression or $\mathcal{Y} = \{1, \ldots, K\}$ in classification with $K$ classes. Let $X \in \mathbb{R}^p$ be a predictor, for example the $p$ pixels of an image. The prediction $\hat{y}$ for $y$, given $X = x$, is of the form $f_\theta(x)$ for a suitable function $f_\theta$ with parameters $\theta \in \mathbb{R}^d$, where the parameters $\theta$ correspond to the weights in a DNN. For regression, $f_\theta(x) \in \mathbb{R}$, whereas for classification $f_\theta(x)$ corresponds to the conditional probability distribution of $Y \in \{1, \ldots, K\}$. Let $\ell$ be a suitable loss that maps $y$ and $\hat{y} = f_\theta(x)$ to $\mathbb{R}^+$. A standard goal is to minimize the expected loss or risk

$$L(\theta) = E\left[\ell(Y, f_\theta(X))\right].$$

Let $(x_i, y_i)$ for $i = 1, \ldots, n$ be the samples that constitute the training data and $\hat{y}_i = f_\theta(x_i)$ the prediction for $y_i$. The standard approach is to simply pool over all available observations, ignoring any grouping information that might be available. The pooled estimator thus treats all examples identically by summing over the empirical loss as

$$\hat{\theta}_{pool} = \arg\min_\theta \frac{1}{n} \sum_{i=1}^n \left[ \ell(y_i, f_\theta(x_i)) \right] + \gamma \cdot \text{pen}(\theta),$$

where $\text{pen}(\theta)$ is a complexity penalty, for example a ridge term $\|\theta\|_2^2$ on the weights of a convolutional neural network. All examples that compare to the pooled estimator will include a ridge penalty as default. Different penalties can exploit underlying geometries, such as the Laplacian regularized least squares (Belkin et al., 2006). In fact, the proposed estimator will be of this form, exploiting grouping information in the data.

4.2 Causal graph

The full causal structural model for all variables is shown in the panel (b) of Figure 2. The domain variable $D$ is latent, in contrast to Gong et al. (2016) whose model is shown in panel (a) of Figure 2. We add the ID variable (identity of a person, for example), whose distribution can change conditional on $Y$. In Figure 2, $Y \rightarrow \text{ID}$ but in some settings it might be more plausible to consider $\text{ID} \rightarrow Y$. For our proposed method both options are possible. The ID variable is used to group observations. The variable is typically discrete and relates to the identity of the underlying object. The variable can be assumed to be latent in the setting of Gong et al. (2016).

The rest of the graph is in analogy to G̺ong et al. (2016). The prediction is anti-causal, that is the predictors $X$ that we use for $Y$ are non-ancestral to $Y$. In other words, the class label is causal for the image and not the other way around. The causal effect from the class label $Y$ on the image $X$ is mediated via two types of latent variables: the so-called core or ‘conditionally invariant’ features $X^{\text{core}}$ and the orthogonal or style features
Figure 2: Observed quantities are shown as shaded nodes; nodes of latent quantities are transparent. (a) Left: data generating process for the considered model as in Gong et al. (2016), where the effect of the domain on the orthogonal features $X_{\text{style}}$ is mediated via unobserved noise $\Delta$. The style interventions and all its descendants are shown as nodes with dashed borders to highlight variables that are affected by style interventions. Observed variables are shaded. Middle: our setting. The domain itself is unobserved but we can now observe the (typically discrete) ID variable we use for grouping. Right: the same model as in the middle if marginalizing out over the unobserved $X_{\text{core}}$.

$X_{\text{style}}$. The distinguishing factor between the two is that external interventions $\Delta$ are possible on the style features but not on the core features. If the interventions $\Delta$ have different distributions in different domains, then the distribution $P(X_{\text{core}}|Y)$ is constant across domains while $P(X_{\text{style}}|Y)$ can change across domains. The style features $X_{\text{style}}$ and $Y$ are confounded, in other words, by the latent domain $D$. In contrast, the core or ‘conditionally invariant’ features satisfy $X_{\text{core}} \perp \!\!\!\!\perp D|Y$. The style variable can include point of view, image quality, resolution, rotations, color changes, body posture, movement etc. and will in general be context-dependent. The style intervention variable $\Delta$ influences both the latent style $X_{\text{style}}$, and hence also the image $X$. In potential outcome notation, we let $X_{\text{style}}(\Delta = \delta)$ be the style under intervention $\Delta = \delta$ and $X(Y, \text{ID}, \Delta = \delta)$ the image for class $Y$, identity ID and style intervention $\Delta$. The latter is sometimes abbreviated as $X(\delta)$ for notational simplicity. Finally, $f_\theta(X(\Delta = \delta))$ is the prediction under the style intervention $\Delta = \delta$. For a formal justification of using a causal graph and potential outcome notation simultaneously see Richardson and Robins (2013).

To be specific, if not mentioned otherwise we will assume a causal graph as follows. For independent $\varepsilon_Y, \varepsilon_{\text{ID}}, \varepsilon_{\text{style}}$ in $\mathbb{R}, \mathbb{R}, \mathbb{R}^q$ respectively with positive density on their support.

---

3. The type of features we regard as style and which ones we regard as core features can conceivably change depending on the circumstances—for instance, is the color “gray” an integral part of the object “elephant” or can it be changed so that a colored elephant is still considered to be an elephant?
and continuously differentiable functions \( k_y, k_{id}, \) and \( k_{style}, k_{core}, k_x, \)

\[
Y \leftarrow k_y(D, \varepsilon_Y) \\
\text{identifier ID} \leftarrow k_{id}(Y, \varepsilon_{ID}) \\
core or conditionally invariant features \( X_{\text{core}} \leftarrow k_{core}(Y, \text{ID}) \)
\]

\[
\text{style or orthogonal features} \ X_{\text{style}} \leftarrow k_{style}(Y, \text{ID}, \varepsilon_{style}) + \Delta \\
\text{image} \ X \leftarrow k_x(X_{\text{core}}, X_{\text{style}}).
\]

Of these, \( Y, X \) and \( \text{ID} \) are observed whereas \( D, X_{\text{core}}, X_{\text{style}}, \Delta \) and the noise variables are latent. The model can be generalized by allowing further independent noise terms inside \( k_x \) and \( k_{core} \) but the model above is already fairly general and keeps notational simplicity more constrained than the fully general version.

4.3 Data

To summarize, we assume we have \( n \) samples \((x_i, y_i, \text{id}_i)\) for \( i = 1, \ldots, n \), where the observations \( \text{id}_i \) with \( i = 1, \ldots, n \) of variable \( \text{ID} \) can also contain unobserved values. Let \( m \leq n \) be the number of unique realizations of \((Y, \text{ID})\) and let \( S_1, \ldots, S_m \) be a partition of \( \{1, \ldots, n\} \) such that, for each \( j \in \{1, \ldots, m\} \), the realizations \((y_i, \text{id}_i)\) are identical for all \( i \in S_j \). The cardinality of \( S_j \) is denoted by \( n_j := |S_j| \geq 1 \). Then \( n = \sum_i n_i \) is again the total number of samples and \( c = n - m \), the total number of grouped observations. Typically \( n_i = 1 \) for most samples and occasionally \( n_i \geq 2 \) but one can also envisage scenarios with larger groups of the same identifier \((y, \text{id})\).

4.4 Domain adaptation, adversarial examples and adversarial domain shifts

In this work, we are interested in guarding against adversarial domain shifts. We use the causal graph to explain the related but not identical goals of domain adaptation, transfer learning and guarding against adversarial examples.

(i) **Domain adaptation and transfer learning.** Assume we have \( J \) different domains, each with a new distribution \( F_j \) for the joint distribution of \((Y, \Delta)\). The shift of \( F_j \) for different domains \( j = 1, \ldots, J \) causes a shift in both the distribution of \( X \) and in the conditional distribution \( Y | X \). If we consider domain adaptation and transfer learning together, the goal is generally to give the best possible prediction \( \hat{Y}_j(x) \) in each domain \( j = 1, \ldots, J \). In contrast, we do not aim to give the best possible prediction in each domain as we aim to infer a single prediction that should work as well as possible in a worst-case sense over a set of distributions generated by domain changes. Some predictive accuracy needs to be sacrificed compared to the best possible prediction in each domain.

(ii) **Standard adversarial examples.** The setting of adversarial examples in the sense of Szegedy et al. (2014) and Goodfellow et al. (2015) can also be described by the causal graph above by using \( X_{\text{style}}(\Delta) = \Delta \) and identifying \( X_{\text{style}} \) with pixel-by-pixel

4. Observations where the ID variable is unobserved are not grouped, that is each such observation is counted as a unique observation of \((Y, \text{ID})\).
additive effects. The magnitude of the intervention \(\Delta\) is then typically assumed to be within an \(\epsilon\)-ball in \(\ell_q\)-norm around the origin, with \(q = \infty\) or \(q = 2\) for example. If the input dimension is large, many imperceptible changes in the coordinates of \(X\) can cause a large change in the output, leading to a misclassification of the sample. The goal is to devise a classification in this graph that minimizes the adversarial loss

\[
E \left[ \max_{\Delta \in \mathbb{R}^\tau : \|\Delta\|_q \leq \epsilon} \ell \left( Y, f_\theta(X(\Delta)) \right) \right],
\]

where \(X(\Delta)\) is the image under the intervention \(\Delta\) and \(\hat{Y} = f_\theta(X(\Delta))\) is the estimated conditional distribution of \(Y\), given the image under the chosen interventions. See Sinha et al. (2017) for recent work on achieving robustness to a pre-defined class of distributions.

(iii) **Adversarial domain shifts.** Here we are interested in arbitrarily strong interventions \(\Delta \in \mathbb{R}^q\) on the style features \(X^{\text{style}}\), which are not known explicitly in general. Analogously to (5), the adversarial loss under arbitrarily large style interventions is

\[
L_{\text{adv}}(\theta) = E \left[ \max_{\Delta \in \mathbb{R}^q} \ell \left( Y, f_\theta(X(\Delta)) \right) \right].
\]

In contrast to (5) the interventions can be arbitrarily strong but we assume that the style features \(X^{\text{style}}\) can only change certain aspects of the image, while other aspects of the image (mediated by the core features) cannot be changed. In contrast to Ganin et al. (2016), we use the term “adversarial” to refer to adversarial interventions on the style features, while the notion of “adversarial” in domain adversarial neural networks describes the training procedure. Nevertheless, the motivation of Ganin et al. (2016) is equivalent to ours—that is, to protect against shifts in the distribution(s) of test data which we characterize by distinguishing between core and style features. We also look at random interventions \(\Delta\). Each distribution of the random interventions is inducing a distribution for \((X, Y)\). Let \(F\) be the set of all such induced distributions. We then try to minimize the worst-case across this distribution class, as in (1), with the difference to standard distributional robustness being that the set \(F\) takes a specific form induced by the causal graph.

The adversarial loss \(L_{\text{adv}}(\theta)\) of the pooled estimator (3) will in general be infinite; see §6.1 for a concrete example. Using panel (b) in Figure 2, one can show that the pooled estimator will work well in terms of the adversarial loss \(L_{\text{adv}}\) if both (i) \(Y \perp \perp X^{\text{core}}\) and (ii) \(Y \not\perp \perp X^{\text{style}}\). The first condition (i) implies that if the estimator learns to extract \(X^{\text{core}}\) from the image \(X\), there is no further information in \(X\) that explains \(Y\) and, therefore, the direction corresponding to \(X^{\text{style}}\) is not required for predicting \(Y\). The second condition (ii) prevents that the relations between \(Y\), \(X^{\text{core}}\), and \(X^{\text{style}}\) are deterministic and ensures that \(X^{\text{style}}\) cannot replace \(X^{\text{core}}\) in the first condition. From (i) and (ii), we see that the pooled estimator will work well in terms of the adversarial loss \(L_{\text{adv}}\) if (a) the edge from \(X^{\text{style}}\) to \(X\) is absent or if (b) both the edge from \(D\) to \(X^{\text{style}}\) and the edge from \(Y\) to \(X^{\text{style}}\) are absent (cf. Figure 2).
5. Conditional variance regularization

5.1 Invariant parameter space

In order to minimize the adversarial loss \( \ell \) we have to ensure \( f_\theta(x(\Delta)) \) is as constant as possible as a function of the style variable \( \Delta \) for all \( x \in \mathbb{R}^p \). Let \( I \) be the invariant parameter space

\[
I := \{ \theta : f_\theta(x(\Delta)) \text{ is constant as function of } \Delta \text{ for all } x \in \mathbb{R}^p \}.
\]

For all \( \theta \in I \), the adversarial loss \( \ell \) is identical to the loss under no interventions at all. More precisely, let \( X \) be a shorthand notation for \( X(\Delta = 0) \), the images in absence of external interventions:

\[
\text{if } \theta \in I, \text{ then } \mathbb{E}\left[ \max_{\Delta \in \mathbb{R}^q} \ell(Y,f_\theta(X(\Delta))) \right] = \mathbb{E}\left[ \ell(Y,f_\theta(X)) \right].
\]

The optimal predictor in the invariant space \( I \) is

\[
\theta^* = \arg\min_{\theta} \mathbb{E}\left[ \ell(Y,f_\theta(X)) \right] \text{ such that } \theta \in I.
\] (7)

If \( f_\theta \) is only a function of the core features \( X^{\text{core}} \), then \( \theta \in I \). The challenge is that the core features are not directly observable and we have to infer the invariant space \( I \) from data.

5.2 CoRe estimator

To get an approximation to the optimal invariant parameter vector (7), we use empirical risk minimization under an invariance constraint:

\[
\hat{\theta}^{\text{core}} = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \ell(y_i,f_\theta(x_i)) \text{ such that } \theta \in I_n,
\] (8)

where the first part is the empirical version of the expectation in (7). The unknown invariant parameter space \( I \) is approximated by an empirically invariant space \( I_n \). For all structural equation models of the form (4), the invariant space \( I \) is constrained by the space of models that have vanishing expected conditional variance in the sense that

\[
I \subseteq \{ \theta : C_\theta = 0 \}, \text{ where } C_\theta := \mathbb{E}(\text{Var}(f_\theta(X)|Y,ID))
\]

is the expected conditional variance of \( f_\theta(X) \), given \((Y,ID)\). As empirical approximation \( I_n = I_n(\tau) \) we use

\[
I_n(\tau) := \{ \theta : \hat{C}_\theta \leq \tau \}, \text{ where } \hat{C}_\theta := \hat{\mathbb{E}}(\text{Var}(f_\theta(X)|Y,ID))
\] (9)

is an estimate of the expected variance (details below). Setting \( \tau = 0 \) is equivalent to demanding that the conditional variance vanishes which implies that the estimated predictions for the class labels are identical across all images that share the same identifier \((y,\text{id})\) while slightly larger values of \( \tau \) allow for some small degree of variations. Under the right assumptions we get \( I_n(\tau) \to I \) for \( n \to \infty \) and \( \tau \to 0 \). We return to this question in \S 6.1.
One can equally use the Lagrangian form of the constrained optimization in (8), with a penalty parameter $\lambda$ instead of a constraint $\tau$, to get
\[
\hat{\theta}_{\text{core}} = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f_\theta(x_i)) + \lambda \cdot \hat{C}_\theta.
\] (10)

We will give an explicit interpretation of this conditional variance penalty $\lambda$ in §6.2. We can also add a standard ridge penalty in addition to the conditional variance penalty.

Before showing numerical examples, we first discuss the estimation of the expected conditional variance in §5.3 before returning to the simple examples of §2 in §5.4. Adversarial risk consistency in a classification setting for a partially linear version of (4) is shown in §6.1. Furthermore, we discuss the population limit of the penalized version in §6.2, where we show that the regularization parameter $\lambda \geq 0$ is proportional to the size of the future style interventions (or rather proportional to the magnitude of the noise on the style variables) that we want to guard against for future test data.

5.3 Estimating expected conditional variance as a graph Laplacian

Recall that $S_j \subseteq \{1, \ldots, n\}$ contains samples with identical realizations of $(Y, ID)$ for $j \in \{1, \ldots, m\}$. For each $j \in \{1, \ldots, m\}$, define the average across all $f_\theta(x_i), i \in S_j$ as $\mu_{\theta,j}$. As estimator of the conditional variance $\hat{C}_\theta$ we use
\[
\hat{C}_\theta := \frac{1}{m} \sum_{j=1}^{m} \frac{1}{|S_j|} \sum_{i \in S_j} (f_\theta(x_i) - \mu_{\theta,j})^2,
\]
where the right hand side can also be interpreted as the graph Laplacian (Belkin et al., 2006) of an appropriately weighted graph that fully connects all observations $i \in S_j$ for each $j \in \{1, \ldots, m\}$. If there are no groups of samples that share the same identifier $(y, id)$, the graph Laplacian is zero and we also define $\hat{C}_\theta$ to vanish in this case. The CoRE estimator is then identical to pooled estimation in this special case.

As an alternative to penalizing with the expected conditional variance of the predicted response, we can constrain $I$ by looking at the expected conditional variance of the loss
\[
I \subseteq \{\theta : C_\theta^\ell = 0\}, \quad \text{where} \quad C_\theta^\ell = E(\text{Var}(\ell(Y, f_\theta(X))|Y, ID))
\]
and get an empirical estimate as
\[
I_n^\ell(\tau) := \{\theta : \hat{C}_\theta^\ell \leq \tau\}, \quad \text{where} \quad \hat{C}_\theta^\ell = \hat{E}(\text{Var}(\ell(Y, f_\theta(X))|Y, ID)).
\] (11)

The penalty is then taking a similar form to Namkoong and Duchi (2017). A crucial difference of our approach is that we penalize with the expected conditional variance. That we take a conditional variance is here important as we try to achieve distributional robustness with respect to interventions on the style variables. Conditioning on ID allows to guard specifically against these interventions. An unconditional variance penalty, in contrast, can achieve robustness against a pre-defined class of distributions such as a ball of distributions defined in a Kullback-Leibler or Wasserstein metric; see for example Sinha et al. (2017) for an application in the context of adversarial examples. Some further discussion is in section §6.2. If not mentioned otherwise we use the conditional variance of the predictions as in (9) as a conditional variance penalty.
5.4 Classification example

We revisit the first and the second example from §2. Figure 3 shows the respective training and test sets with the estimated decision boundaries for different values of the penalty parameter $\lambda$. Additionally, grouped examples that share the same $(y, id)$ are visualized: two grouped observations are connected by a line or curve, respectively. In each example, there are eight such groups (only clearly visible in the nonlinear example). Panel (a) shows the linear decision boundaries for $\lambda = 0$, equivalent to the pooled estimator, and for CoRE with $\lambda = 10$. The pooled estimator misclassifies all test points of class 1 as can be seen in panel (b). In contrast, the decision boundary of the CoRE estimator aligns with the direction along which the grouped observations vary, classifying the test set with almost perfect accuracy. Panels (c) and (d) show the corresponding plots for the second example for penalty values $\lambda \in \{0, 0.05, 0.1, 1\}$. While all of them yield good performance on the training set, only a value of $\lambda = 1$, which is associated with a circular decision boundary, achieves almost perfect accuracy on the test set.

6. Adversarial risk consistency and distributional robustness

We show two properties of the CoRE estimator. First, adversarial risk consistency is shown for logistic models. Second, we show that the population CoRE estimator protects optimally against an increase in the variance of the noise in the style variable in a regression setting.

6.1 Adversarial risk consistency for classification and logistic loss

We analyze the adversarial loss, defined in Eq. (6), for the pooled and the CoRE estimator in a one-layer network for binary classification (logistic regression). The proof is given in §A.
Assume the structural equation for the image $X \in \mathbb{R}^p$ is linear in the style features $X^{\text{style}} \in \mathbb{R}^q$ (with generally $p \gg q$) and we use logistic regression to predict the class label $Y \in \{-1, 1\}$. Let the interventions $\Delta \in \mathbb{R}^q$ act additively on the style features $X^{\text{style}}$ (this is only for notational convenience) and let the style features $X^{\text{style}}$ act in a linear way on the image $X$ via a matrix $W \in \mathbb{R}^{p \times q}$ (this is an important assumption without which results are more involved). The core or ‘conditionally invariant’ features are $X^{\text{core}} \in \mathbb{R}^r$, where in general $r \leq p$ but this is not important for the following. For independent $\varepsilon_Y, \varepsilon_{\text{ID}}, \varepsilon_{\text{style}}, \varepsilon_X$ in $\mathbb{R}, \mathbb{R}, \mathbb{R}^q, \mathbb{R}^p$ respectively with positive density on their support and continuously differentiable functions $k_y, k_{\text{id}}, k_{\text{style}}, k_{\text{core}}, k_x$.

\[
\begin{align*}
\text{class } Y & \leftarrow k_y(D, \varepsilon_Y) \\
\text{identifier ID} & \leftarrow k_{\text{id}}(Y, \varepsilon_{\text{ID}}) \\
\text{core or conditionally invariant features } X^{\text{core}} & \leftarrow k_{\text{core}}(Y, \varepsilon_{\text{ID}}) \\
\text{style or orthogonal features } X^{\text{style}} & \leftarrow k_{\text{style}}(Y, \varepsilon_{\text{ID}}) + \Delta \\
\text{image } X & \leftarrow k_x(X^{\text{core}}, \varepsilon_X) + WX^{\text{style}}. 
\end{align*}
\]

Of these, $Y$, $X$, and ID are observed whereas $D$, $X^{\text{core}}$, $X^{\text{style}}$, $\Delta$ and the noise variables are latent. The distribution of $\Delta$ can depend on the unobserved domain.

We assume a logistic regression as a prediction of $Y$ from the image data $X$:

\[
f_\theta(x) := \frac{\exp(x^t \theta)}{1 + \exp(x^t \theta)}.
\]

Given training data with $n$ samples, we estimate $\theta$ with $\hat{\theta}$ and use here a logistic loss $\ell_\theta(y_i, x_i) = \log(1 + \exp(-y_i(x_i^t \theta)))$ for training and testing. We want to compare the following losses on test data

\[
L(\theta) = E\left[\ell(Y, f_\theta(X))\right] \\
L_{\text{adv}}(\theta) = E\left[\max_{\Delta \in \mathbb{R}^q} \ell(Y, f_\theta(X(\Delta)))\right],
\]

where the $X$ in the first loss is a shorthand notation for $X(\Delta = 0)$, that is the images in absence of interventions on the style variables. The first loss is thus a standard logistic loss in absence of adversarial interventions. The second loss is the loss under adversarial style or domain interventions as we allow arbitrarily large interventions on $X^{\text{style}}$ here. The corresponding benchmarks are

\[
L^* = \min_\theta L(\theta), \quad \text{and} \quad L^*_{\text{adv}} = \min_\theta L_{\text{adv}}(\theta).
\]

The formulation of Theorem 1 relies on the following assumptions.

**Assumption 1** We require the following conditions:

(A1) Assume $\Delta$ is sampled from a distribution for training data in $\mathbb{R}^q$ with positive density (with respect to the Lebesgue measure) in an $\epsilon$-ball in $\ell_2$-norm around the origin for some $\epsilon > 0$. 

14
(A2) Assume the matrix \( W \) has full rank \( q \).

(A3) For a fixed number \( n \) of samples, the samples of \((Y, ID, X)\) are drawn iid from a distribution such that the number \( m \leq n \) of unique realizations of \((Y, ID)\) is smaller than \( n - q \) with probability \( p_n \) and \( p_n \to 1 \) for \( n \to \infty \).

The last assumption guarantees that the number \( c = n - m \) of grouped examples is at least as large as the dimension of the style variables. If we have too few or no grouped examples (small \( c \)), we cannot estimate the conditional variance accurately. Under these assumptions we can prove adversarial risk consistency.

**Theorem 1 (Adversarial risk consistency)** Under model (12) and Assumption 1, with probability 1 with respect to the training data, the pooled estimator (3) has infinite adversarial loss

\[
L_{adv}(\hat{\theta}_{pool}) = \infty.
\]

The CoRe estimator (8) with \( \tau = 0 \) in (9) is adversarial loss consistent, in the sense that for \( n \to \infty \),

\[
L_{adv}(\hat{\theta}_{core}) \to_p L^*_{adv}.
\]

A proof is given in §A. The respective ridge penalties in both estimators (3) and (10) are assumed to be vanishing for the proof, but the proof can easily be generalized to include ridge penalties that vanish sufficiently fast for large sample sizes. The Lagrangian regularizer \( \lambda \) is assumed to be infinite for the CoRe estimator. Again, this could be generalized to finite values if the adversarial interventions \( \Delta \) are constrained to be in a region with finite \( \ell_2 \)-norm. An equivalent result can be derived for misclassification loss instead of logistic loss, where the adversarial misclassification error of the pooled estimator is then 1 while the adversarial misclassification error of the CoRe estimator will converge to the optimal adversarial value.

6.2 Population limit: optimal robustness against increases of the style-noise variance

We look at a partially linear version of the causal graph and least squares loss as a special case, using the marginalized version of the causal graph as in panel (c) of Figure 2. Let \( Y \in \mathbb{R} \) be a continuous target variable, \( ID \in \mathbb{Z} \) an integer-valued identity variable, and \( X^{style} \in \mathbb{R}^r \) the style or orthogonal features and the observed vector \( X \in \mathbb{R}^p \). Let \( \epsilon_Y, \epsilon_ID, \epsilon_{style} \) be independent mean-zero random vectors in \( \mathbb{R}, \mathbb{R}, \mathbb{R}^r \) respectively with positive density on their respective support, variance \( \sigma_Y^2 \) for \( \epsilon_Y \) and non-singular covariance \( \Sigma_{style} \) for \( \epsilon_{style} \).

We look at the population limit of the CoRe estimator in its penalized form (10)

\[
\theta_{core}(\lambda) = \arg\min_{\theta \in \mathbb{R}^p} E[\ell(Y, b^T X)] + \lambda \cdot C_\theta,
\]

where again \( C_\theta := E(\text{Var}(f_\theta(X)|Y, ID)) \) is the expected conditional variance and \( \ell(y, z) = (y - z)^2 \). We analyze the case where interventions \( \Delta \) are random and follow the same distribution as the noise \( \epsilon_{style} \), just with a different scaling that can depend on the domain.

---

5. We can also add an independent noise term \( \epsilon_X \) for \( X \) but choose to omit it here to retain notational simplicity.
Specifically, as a special case of the marginalized version of the causal graph in panel (c) of Figure 2, consider a partially linear version of (4) with a constant marginal distribution of $Y$ in all domains

$$
Y \leftarrow \varepsilon_Y \in \mathbb{R} \\
\text{ID} \leftarrow k_{id}(Y, \varepsilon_{ID}) \\
X_{\text{style}} \leftarrow k_{style}(Y, \text{ID}) + \varepsilon_{\text{style}} + \kappa \cdot \varepsilon'_{\text{style}} \\
X \leftarrow k_{x}(Y, \text{ID}) + B X_{\text{style}}
$$

(14)

for suitable functions $k_{id} : \mathbb{R} \times \mathbb{R} \mapsto \mathbb{Z}$, $k_{style} : \mathbb{R} \times \mathbb{Z} \mapsto \mathbb{R}^r$, $k_{x} : \mathbb{R} \times \mathbb{Z} \times \mathbb{R}^p \mapsto \mathbb{R}^p$ and matrix $B \in \mathbb{R}^{p \times r}$. As mentioned above, the interventions $\Delta$ are modeled as random interventions $\kappa \varepsilon'_{\text{style}}$, where $\varepsilon'_{\text{style}}$ has the same distribution as $\varepsilon_{\text{style}}$ but the two random variables are independent. The scaling $\kappa \geq 1$ is variable. In a standard setting, we might have $\kappa = 0$ for training data but we suppose that $\kappa$ can increase in the future. In a new domain, for example, it might be larger. We would like to have a prediction of $Y$ that works well even if the scaling $\kappa$ of the ‘style noise’ increases substantially. Let $E_\kappa$ denote the expectation under model (14) with parameter $\kappa \in \mathbb{R}^\mathbb{+}$.

**Theorem 2 (Distributional robustness)** Under model (14), the population CORE estimator (13) is optimal against the class of distributions generated by varying the style noise level $\kappa$ in $[0, \sqrt{\lambda}]$,

$$
\theta_{\text{core}}(\lambda) = \arg\min_b \sup_{\kappa \leq \sqrt{\lambda}} E_\kappa(\ell(Y, b^T X)).
$$

A proof is given in [13].

The CORE estimator hence optimizes the worst case among all noise scalings of the style variable. The value of the penalty $\lambda$ determines the level up to which we are protected when the noise variance increases. More precisely, a penalty $\lambda = \kappa^2$ is mimicking an increase in the variance of the noise in the style variable and allows using the current training data (with $\kappa = 0$) to optimize the loss under arbitrarily large values of the additional style variance $\kappa^2$. In this sense, there is a clear interpretation of the penalty factor $\lambda$ in the CORE estimator (10). Choosing $\lambda = 0$ means that we expect the variance of the style variable to remain unchanged, whereas using a strong penalty $\lambda \to \infty$ assumes that the variance of the style variable will grow very large in the future and the performance of the estimator will then not be affected even under arbitrarily strong interventions on the style variable.

A similar result is shown in Rothenhäusler et al. (2018) who propose “anchor regression”. Anchor regression penalizes the ordinary least squares objective with a quantity that relies on so-called “anchors” $A$ which are exogeneous variables. This quantity corresponds to the change in loss under shift interventions of a given strength. Anchor regression is shown to yield optimal predictive performance under such interventions. While the theoretical results have a similar form as the estimator is shown to be distributionally robust, they do not follow as corollaries from each other. Both CORE and anchor regression rely on the presence of “auxiliary variables” — in CORE, we exploit the grouping information given by ID while anchor regression relies on the exogeneous anchor variable $A$. However, ID and $A$ play almost orthogonal roles. In anchor regression, the aim is to achieve predictive...
stability if the variance term explained by $A$ is varying. In CoRE, the aim is to retain the variance term explained by ID as we expect the variance under a constant ID = id to grow in the future. The interventions considered in anchor regression are shift interventions and it protects against specific distributional shifts up to a given strength. In Theorem 2 we consider noise interventions on the latent style variable.

While Theorem 2 was derived for regression under squared error loss, a similar result can be obtained for classification under (truncated) squared error loss. The (truncated) quadratic loss $\ell(Y, f_\theta(X)) = (Y - f_\theta(X))^2$ is classification-calibrated [Bartlett et al., 2003] and the truncation is even unnecessary in our case. For example, if $Y \in \{0, 1\}$, let $f_\theta(x) \in [0, 1]$ be the predicted probability of $Y = 1$, given $X = x$. Taking a first-order Taylor approximation of $f_\theta$ one can derive an analogous result to Theorem 2 where the approximation error of the Taylor expansion hinges on the magnitude of the future interventions and hence on the penalty level of the CoRE estimator. For loss functions other than truncated squared error loss one could make a similar argument but one would have to use the conditional variance of the loss as a penalty as in (11). This approach would then be similar to Namkoong and Duchi (2017), with the important difference that we work with conditional variances instead of unconditional variances. Conditioning on the ID variable is crucial in our context as we do not want to protect against general shifts in distribution but specifically against shifts in the distribution of the style variable. Conditioning on ID allows us to distinguish between the conditional variance caused by the unknown style variable (which we assume will change in the future) and the conditional variance caused by the randomness of ID (which we expect to stay constant in the future). Exploring the possibility of using the conditional variance of the loss instead of the prediction for general loss functions would be interesting follow-up work.

7. Experiments

We perform an array of different experiments, showing the applicability and advantage of the conditional variance penalty for two broad settings:

1. Settings where we do not know what the style variables correspond to but still want to protect against a change in their distribution in the future. In the examples we show cases where the style variable ranges from brightness (§7.7), image quality (§7.2), movement (§7.3) and fashion (§7.4), which are all not known explicitly to the method. We also include genuinely unknown style variables in §7.1 (in the sense that they are unknown not only to the methods but also to us as we did not explicitly create the style interventions).

2. Settings where we do know what type of style interventions we would like to protect against. This is usually dealt with by data augmentation (adding images which are, say, rotated or shifted compared to the training data if we want to protect against rotations or translations in the test data (Schölkopf et al., 1996)). The conditional variance penalty is here exploiting that some augmented samples were generated from the same original sample and we use as ID variable the index of the original image. We show that this approach generalizes better than simply pooling the augmented
Figure 4: Eyeglass detection for CelebA dataset. The goal is to predict whether a person wears glasses or not. Random samples from training and test data are shown. Groups of observations in the training data that have common \((Y, ID)\) correspond to pictures of the same person with either glasses on or off. These are labelled by red boxes in the training data and the conditional variance penalty is calculated across these groups of pictures.

Details of the network architectures can be found in Appendix \( \S \) C. All reported error rates are averaged over five runs of the respective method. A TensorFlow (Abadi et al., 2015) implementation of CoRe can be found at https://github.com/christinaheinze/core.

7.1 Eyeglasses detection with small sample size

We use a subsample of the CelebA dataset (Liu et al., 2015), without editing the images. We try to classify images according to whether the person in the image is wearing glasses or not. For construction of the ID variable we exploit the fact that several photos of the same person are available and set ID to be the identifier of the person in the dataset. Figure 4 shows examples from both the training and the test data set. The conditional variance is estimated across groups of observations that share a common \((Y, ID)\), which here corresponds to pictures of the same person, where all pictures show the person either with glasses (if \(Y = 1\)) or all pictures show the person without glasses (\(Y = 0\)).

The standard approach would be to pool all examples. The only additional information we exploit is that some observations can be grouped. We include \(m = 10\) identities in the training set, resulting in a total sample size \(n = 321\) as there are approximately 30 images of each person. If using a 5-layer convolutional neural network (details can be found in Table C.1) and pooling all data with a standard ridge penalty, the test error on unseen images is 24.76%. Using ImageNet pre-trained features from Inception V3 does not yield lower error rates. Exploiting the group structure with the CoRe penalty (in addition to a
Training data ($n = 20000$):  Test set 1 ($n = 5344$):  Test set 2 ($n = 5344$):

5-layer CNN training error: 0%  5-layer CNN test error: 2%  5-layer CNN test error: 65%
with add. CoRe penalty: 10%  with add. CoRe penalty: 13%  with add. CoRe penalty: 29%

Figure 5: Eyeglass detection for CelebA dataset with image quality interventions (which are unknown to any procedure used). The JPEG compression level is lowered for $Y = 1$ (glasses) samples on training data and test set 1 and lowered for $Y = 0$ (no glasses) samples for test set 2. To the human eye, these interventions are barely visible but the CNN that uses pooled data without CoRe penalty has exploited the correlation between image quality and outcome $Y$ to achieve a (arguably spurious) low test error of 2% on test set 1. However, if the correlation between image quality and $Y$ breaks down, as in test set 2, the CNN that uses pooled data without a CoRe penalty has a 65% misclassification rate. The training data on the left show paired observations in two red boxes: these observations share the same label $Y$ and show the same person ID. They are used to compute the conditional variance penalty for the CoRe estimator that does not suffer from the same degradation in performance for test set 2.

ridge penalty) reduces the test error to 16.89%. Results are not very sensitive to the specific choice of the penalty, as discussed further in D.6.

The surprising aspect here is that both training and test data are drawn from the same distribution so we would not expect a distributional shift. The distributional shift in this example is caused by statistical fluctuations alone (by chance the background of eyeglass wearers might, for example, be darker in the training sample than test samples, the eyeglass wearers might be more outdoors, might be more women than men etc.). The following examples are more concerned with biases that will persist even if the number of training and test samples is very large. A second difference to the subsequent examples is the grouping structure—in this example, we consider only a few identities, namely $m = 10$, with a relatively large number of associated observations ($n_i \approx 30$ for all $i$). In the following examples, $m$ is much larger while $n_i$ is typically smaller than five.

### 7.2 Eyeglasses detection with known and unknown image quality intervention

We revisit the third example from §2. We again use the CelebA dataset and consider the problem of classifying whether the person in the image is wearing eyeglasses. In contrast to §7.1 we modify the images in the following way: in the training set and in test set 1,
we sample the image quality\[i^\ast\] for all samples \{i : y_i = 1\} (all samples that show glasses) from a Gaussian distribution with mean \(\mu = 30\) and standard deviation \(\sigma = 10\). Samples with \(y_i = 0\) (no glasses) are unmodified. In other words, if the image shows a person wearing glasses, the image quality tends to be lower. In test set 2, the quality is reduced in the same way for \(y_i = 0\) samples (no glasses), while images with \(y_i = 1\) are not changed. Figure 5 shows examples from the training set and test sets 1 and 2. This setting mimics the confounding that occurred in the Russian tank legend (cf. §1). For the CoRE penalty, we calculate the conditional variance across images that share the same ID if \(Y = 1\), that is across images that show the same person wearing glasses on all images. Observations with \(Y = 0\) (not wearing glasses) are not grouped. Two examples are shown in the red box of Figure 5. Here, we have \(c = 5000\) grouped observations among a total sample size of \(n = 20000\).

Figure 6 shows misclassification rates for CoRE and the pooled estimator on test sets 1 and 2. The pooled estimator (only penalized with an \(\ell_2\) penalty) achieves low error rates of 2\% on test set 1, but suffers from a 65\% misclassification error on test set 2, as now the relation between \(Y\) and the implicit \(X^{style}\) variable (image quality) has been flipped. The CoRE estimator has a larger error of 13\% on test set 1 as image quality as a feature is penalized by CoRE implicitly and the signal is less strong if image quality has been removed as a dimension. However, in test set 2 the performance of the CoRE estimator is 28\% and improves substantially on the 65\% error of the pooled estimator. The reason is again the same: the CoRE penalty ensures that image quality is not used as a feature to the same extent as for the pooled estimator. This increases the test error slightly if the samples are generated from the same distribution as training data (as here for test set 1) but substantially improves the test error if the distribution of image quality, conditional on the class label, is changed on test data (as here for test set 2).

**Eyeglasses detection with known image quality intervention** To compare to the above results, we repeat the experiment by changing the grouped observations as follows. Above, we grouped images that had the same person ID when \(Y = 1\). We refer to this scheme of grouping observations with the same \((Y,ID)\) as ‘Grouping setting 2’. Here, we use an explicit augmentation scheme and augment \(c = 5000\) images with \(Y = 1\) in the following way: each image is paired with a copy of itself and the image quality is adjusted as described above. In other words, the only difference between the two images is that image quality differs slightly, depending on the value that was drawn from the Gaussian distribution with mean \(\mu = 30\) and standard deviation \(\sigma = 10\), determining the strength of the image quality intervention. Both the original and the copy get the same value of identifier variable ID. We call this grouping scheme ‘Grouping setting 1’. Compare the left panels of Figures 5 and 6 for examples.

While we used explicit changes in image quality in both above and here, we referred to grouping setting 2 as ‘unknown image quality interventions’ as the training sample as in the left panel of Figure 5 does not immediately reveal that image quality is the important style variable. In contrast, the augmented data samples (grouping setting 1) we use here differ only in their image quality for a constant \((Y,ID)\).

---

6. We use ImageMagick (https://www.imagemagick.org) to change the quality of the compression through 
convert -quality q_{ij} input.jpg output.jpg where \(q_{ij} \sim N(30, 100)\).
Training data (n = 20000):  Test set 1 (n = 5344):  Test set 2 (n = 5344):

5-layer CNN training error: 0%  5-layer CNN test error: 2%  5-layer CNN test error: 65%
with added CoRe penalty: 3%  with added CoRe penalty: 7%  with add. CoRe penalty: 13%

Figure 6: Eyeglass detection for CelebA dataset with image quality interventions. The only difference to Figure 5 is in the training data where the paired images now use the same underlying image in two different JPEG compressions. The compression level is drawn from the same distribution. The CoRe penalty performs better than for the experiment in Figure 5 since we could explicitly control that only $X^{\text{style}} \equiv \text{image quality}$ varies between grouped examples. On the other hand, the performance of the pooled estimator is not changed in a noticeable way if we add augmented images as the (spurious) correlation between image quality and outcome $Y$ still persists in the presence of the extra augmented images. Thus, the pooled estimator continues to be susceptible to image quality interventions.

Figure 6 shows examples and results. The pooled estimator performs more or less identical to the previous dataset. The explicit augmentation did not help as the association between image quality and whether eyeglasses are worn is not changed in the pooled data after including the augmented data samples. The misclassification error of the CoRe estimator is substantially better than the error rate of the pooled estimator. The error rate on test set 2 of 13% is also improving on the rate of 28% of the CoRe estimator in grouping setting 2. We see that using grouping setting 1 works best since we could explicitly control that only $X^{\text{style}} \equiv \text{image quality}$ varies between grouped examples. In grouping setting 2, different images of the same person can vary in many factors, making it more challenging to isolate image quality as the factor to be invariant against.

7.3 Stickmen image-based age classification with unknown movement interventions

In this example we consider synthetically generated stickmen images; see Figure 7 for some examples. The target of interest is $Y \in \{\text{adult, child}\}$. The core feature $X^{\text{core}}$ is here the height of each person. The class $Y$ is causal for height and height cannot be easily intervened on or change in different domains. Height is thus a robust predictor for differentiating between children and adults. As style feature we have here the movement of a person (distribution of angles between body, arms and legs). For the training data we created a dependence between age and the style feature ‘movement’, which can be thought to arise through a hidden common cause $D$, namely the place of observation. The data generating
Training data \((n = 20000)\):  
Test set 1 \((n = 20000)\):  
Test set 2 \((n = 20000)\):

5-layer CNN training error: 4%  
5-layer CNN test error: 3%  
5-layer CNN test error: 41%  
with added CoRe penalty: 4%  
with added CoRe penalty: 4%  
with added CoRe penalty: 9%

Figure 7: Classification into \{adult, child\} based on stickmen images, where children tend to be smaller and adults taller. In training and test set 1 data, children tend to have stronger movement whereas adults tend to stand still. In test set 2 data, adults show stronger movement. The two red boxes in the panel with the training data show two out of the \(c = 50\) pairs of examples over which the conditional variance is calculated. The CoRe penalty leads to a network that generalizes better for test set 2 data, where the spurious correlation between age and movement is reversed, if compared to the training data.

The process is illustrated in Figure D.6. For instance, the images of children might mostly show children playing while the images of adults typically show them in more “static” postures. The left panel of Figure 7 shows examples from the training set where large movements are associated with children and small movements are associated with adults. Test set 1 follows the same distribution, as shown in the middle panel. A standard CNN will exploit this relationship between movement and the label \(Y\) of interest, whereas this is discouraged by the conditional variance penalty of CoRe. The latter is pairing images of the same person in slightly different movements as shown by the red boxes in the leftmost panel of Figure 7. If the learned model exploits this dependence between movement and age for predicting \(Y\), it will fail when presented images of, say, dancing adults. The right panel of Figure 7 shows such examples (test set 2). The standard CNN suffers in this case from a 41% misclassification rate, as opposed to the 3% on test set 1 data. For as few as \(c = 50\) paired observations, the network with an added CoRe penalty, in contrast, achieves also 4% on test set 1 data and succeeds in achieving an 9% performance on test set 2, whereas the pooled estimator fails on this dataset with a test error of 41%.

These results suggest that the learned representation of the pooled estimator uses movement as a predictor for age while CoRe does not use this feature due to the conditional variance regularization. Importantly, including more grouped examples would not improve the performance of the pooled estimator as these would be subject to the same bias and hence also predominantly have examples of heavily moving children and “static” adults (also see Figure D.7 which shows results for \(c \in \{20, 500, 2000\}\)).

7.4 Gender classification with unknown confounding

We work again with the CelebA dataset. This time we consider the problem of classifying whether the person in the image is male or female. We create a confounding on training and test set 1 by including mostly images of men wearing glasses and women not wearing
Training data \((n = 17000)\): Test data I \((n = 4224)\): Test data II \((n = 1120)\):

| Model            | Error Rate | Model            | Error Rate | Model            | Error Rate |
|------------------|------------|------------------|------------|------------------|------------|
| 5-layer CNN      | 0%         | 5-layer CNN      | 3%         | 5-layer CNN      | 44%        |
| with added CoRe penalty: 9% | with added CoRe penalty: 8% | with add. CoRe penalty: 26% |
| Inception v3     | 2%         | Inception v3     | 2%         | Inception v3     | 42%        |
| with added CoRe penalty: 9% | with added CoRe penalty: 8% | with add. CoRe penalty: 23% |

Figure 8: Classification for \(Y \in \{\text{woman, man}\}\). There is an unknown confounding here as men are very likely to wear glasses in training and test set 1 data, while it is women that are likely to wear glasses in test set 2. Estimators that pool all observations are making use of this confounding and hence fail for test set 2. The conditional variance penalty for the CoRe estimator is computed over groups of images of the same person (and consequently same class label), such as the images in the red box on the left. Here, \(c = 500\).

glasses. In test set 2 the association between gender and glasses is flipped: women always wear glasses while men never wear glasses. Examples from the training and test sets 1 and 2 are shown in Figure 8.

To compute the conditional variance penalty, we use again images of the same person. The ID variable is, in other words, the identity of the person and gender \(Y\) is constant across all examples that have a constant ID. Conditioning on \((Y, ID)\) is hence identical to conditioning on ID alone. Another difference to the other experiments is that we consider a binary style feature here.

For this example, we computed the relevant results both with a 5-layer CNN if trained end-to-end as well as for using Inception V3 pre-trained features and retraining the last softmax layer. Interestingly, the results do not change much and both models lead to misclassification error rates above 40% for test set 2 data and \(c = 500\) paired examples. Adding the CoRe penalty has the desired effect in both models, as the performance is much more stable across all data sets. Additional results for different sample sizes and different numbers of paired examples can be found in Appendix §D.2.

7.5 MNIST: more sample efficient data augmentation

The goal of using CoRe in this example is to make data augmentation more efficient in terms of the required samples. In data augmentation, one creates additional samples by modifying the original inputs, e.g. by rotating, translating, or flipping the images (Schölkopf et al. [1996]). In other words, additional samples are generated by interventions on style features. Using this augmented data set for training results in invariance of the estimator with
Training data ($n = 10200$):

- 3-layer CNN training error: 0%
  - with added CoRE penalty: 1%

Test set ($n = 10000$):

- 3-layer CNN test error: 22%
  - with added CoRE penalty: 10%

Figure 9: Data augmentation for MNIST images. The left shows training data with a few rotated images. Evaluating on only rotated images from the test set, a standard network achieves only 22% accuracy. We can add the CoRE penalty by computing the conditional variance over images that were generated from the same original image. The test error is then lowered to 10% on the test data of rotated images.

respect to the transformations (style features) of interest. For CoRE we can use the grouping information that the original and the augmented samples belong to the same object. This enforces the invariance with respect to the style features more strongly compared to normal data augmentation which just pools all samples. We assess this for the style feature ‘rotation’ on MNIST [LeCun et al., 1998] and only include $c = 200$ augmented training examples for $m = 10000$ original samples, resulting in a total sample size of $n = 10200$. The degree of the rotations is sampled uniformly at random from $[35, 70]$. Figure 9 shows examples from the training set. By using CoRE the average test error on rotated examples is reduced from 22% to 10%. Very few augmented sample are thus sufficient to lead to stronger rotational invariance. The standard approach of creating augmented data and pooling all images requires, in contrast, many more samples to achieve the same effect. Additional results for $m \in \{1000, 10000\}$ and $c$ ranging from 100 to 5000 can be found in Figure D.5 in Appendix §D.3.

7.6 Elmer the Elephant

In this example, we want to assess whether invariance with respect to the style feature ‘color’ can be achieved. In the children’s book ‘Elmer the elephant’ one instance of a colored elephant suffices to recognize it as being an elephant, making the color ‘gray’ no longer an integral part of the object ‘elephant’. Motivated by this process of concept formation, we would like to assess whether CoRE can exclude ‘color’ from its learned representation by penalizing conditional variance appropriately.

We work with the ‘Animals with attributes 2’ (AwA2) dataset [Xian et al., 2017] and consider classifying images of horses and elephants. We include additional examples by

7. [https://en.wikipedia.org/wiki/Elmer_the_Patchwork_Elephant](https://en.wikipedia.org/wiki/Elmer_the_Patchwork_Elephant)
Training data \((n = 1850)\): \hspace{1em} Test data I \((n = 414)\): \hspace{1em} Test data II \((n = 414)\):

5-layer CNN training error: 0% \hspace{1em} 5-layer CNN test error: 24% \hspace{1em} 5-layer CNN test error: 52%
with added CoRe penalty: 0% \hspace{1em} with add. CoRe penalty: 30% \hspace{1em} with add. CoRe penalty: 30%

Figure 10: Elmer-the-Elephant dataset. The left panel shows training data with a few additional grayscale elephants. The pooled estimator learns that color is predictive for the animal class and achieves test error of 24% on test set 1 where this association is still true but suffers a misclassification error of 53% on test set 2 where this association breaks down. By adding the CoRe penalty, the test error is consistently around 30%, irrespective of the color distribution of horses and elephants.

adding grayscale images for \(c = 250\) images of elephants. These additional examples do not distinguish themselves strongly from the original training data as the elephant images are already close to grayscale images. The total training sample size is 1850.

Figure 10 shows examples and misclassification rates from the training set and test sets for CoRe and the pooled estimator on different test sets. Examples from these and more test sets can be found in Figure D.10. Test set 1 contains original, colored images only. In test set 2 images of horses are in grayscale and the colorspace of elephant images is modified, effectively changing the color gray to red-brown. We observe that the pooled estimator does not perform well on test set 2 as its learned representation seems to exploit the fact that ‘gray’ is predictive for ‘elephant’ in the training set. This association is no longer valid for test set 2. In contrast, the predictive performance of CoRe is hardly affected by the changing color distributions. More details can be found in Appendix §D.6.

It is noteworthy that a colored elephant can be recognized as an elephant by adding a few examples of a grayscale elephant to the very lightly colored pictures of natural elephants. If we just pool over these examples, there is still a strong bias that elephants are gray. The CoRe estimator, in contrast, demands invariance of the prediction for instances of the same elephant and we can learn color invariance with a few added grayscale images.

7.7 Eyeglasses detection: unknown brightness intervention

As in §7.2 we work with the CelebA dataset and try to classify whether the person in the image is wearing eyeglasses. Here we analyze a confounded setting that could arise as follows. Say the hidden common cause \(D\) of \(Y\) and \(X^{\text{style}}\) is a binary variable and indicates whether the image was taken outdoors or indoors. If it was taken outdoors, then the person tends to wear (sun-)glasses more often and the image tends to be brighter. If the image was taken indoors, then the person tends not to wear (sun-)glasses and the image tends to be darker. In other words, the style variable \(X^{\text{style}}\) is here equivalent to brightness and
Training data ($n = 20000$):  Test set 1 ($n = 5344$):  Test set 2 ($n = 5344$):

5-layer CNN training error: 0%  5-layer CNN test error: 4%  5-layer CNN test error: 37%
with added CoRe penalty: 6%  with added CoRe penalty: 6%  with add. CoRe penalty: 25%

Figure 11: Eyeglass detection for CelebA dataset with brightness interventions (which are unknown to any procedure used). On training data and test set 1 data, images where people wear glasses tend to be brighter whereas on test set 2 images where people do not wear glasses tend to be brighter.

Figure 11 shows examples from the training set and test sets. As previously, we compute the conditional variance over images of the same person, sharing the same class label (and the CoRe estimator is hence not using the knowledge that brightness is important). Two alternatives for constructing grouped observations in this setting are discussed in §D.1. We use $c = 2000$ and $n = 20000$. For the brightness intervention, we sample the value for the magnitude of the brightness increase resp. decrease from an exponential distribution with mean $\beta = 20$. In the training set and test set 1, we sample the brightness value as $b_{i,j} = [100 + y_i e_{i,j}]$ where $e_{i,j} \sim \text{Exp}(\beta^{-1})$ and $y_i \in \{-1, 1\}$, where $y_i = 1$ indicates presence of glasses and $y_i = -1$ indicates absence. For test set 2, we use instead $b_{i,j} = [100 - y_i e_{i,j}]$, so that the relation between brightness and glasses is flipped.

Figure 11 shows misclassification rates for CoRe and the pooled estimator on different test sets. Examples from all test sets can be found in Figure D.2. First, we notice that the pooled estimator performs better than CoRe on test set 1. This can be explained by the fact that it can exploit the predictive information contained in the brightness of an image while CoRe is restricted not to do so. Second, we observe that the pooled estimator does not perform well on test set 2 as its learned representation seems to use the image’s brightness as a predictor for the response which fails when the brightness distribution in the test set differs significantly from the training set. In contrast, the predictive performance of CoRe is hardly affected by the changing brightness distributions. Results for $\beta \in \{5, 10, 20\}$ and $c \in \{200, 5000\}$ can be found in Figure D.3 in Appendix §D.1.

8. Specifically, we use ImageMagick (https://www.imagemagick.org) and modify the brightness of each image by applying the command `convert -modulate b_{i,j},100,100 input.jpg output.jpg` to the image.
8. Conclusion

Distinguishing the latent features in an image into core and style features, we have proposed conditional variance regularization (CoRE) to achieve robustness with respect to arbitrarily large interventions on the style or conditionally invariant features. The main idea of the CoRE estimator is to exploit the fact that we often have instances of the same object in the training data. By demanding invariance of the classifier amongst a group of instances that relate to the same object, we can achieve invariance of the classification performance with respect to adversarial interventions on style features such as image quality, fashion type, color, or body posture. The training also works despite sampling biases in the data.

There are two main applications areas:

1. If the style features are known explicitly, we can achieve the same classification performance as standard data augmentation approaches with substantially fewer augmented samples, as shown for example in §7.5. Additionally, the augmented images do not need to be balanced carefully for the CoRE estimator, as shown for example in §7.6 where adding grayscale images to a set of grayish elephants leads to invariance to color with the CoRE approach while a pooled estimator is still using color to predict the animal class with the same dataset.

2. Perhaps more interesting are settings in which it is unknown what the style features are, with examples in §7.1, §7.2, §7.3, §7.4, and §7.7. CoRE regularization forces predictions to be based on features that do not vary strongly between instances of the same object. We could show in the examples and in Theorems 1 and 2 that this regularization achieves distributional robustness with respect to changes in the distribution of the (unknown) style variables.

An interesting line of work would be to use larger models such as Inception or large ResNet architectures (Szegedy et al., 2015; He et al., 2016). These models have been trained to be invariant to an array of explicitly defined style features. In §7.4 we include results which show that using Inception V3 features does not guard against interventions on more implicit style features. We would thus like to assess what benefits CoRE can bring for training Inception-style models end-to-end, both in terms of sample efficiency and in terms of generalization performance. While we showed some examples where the necessary grouping information is available, an interesting possible future direction would be to use video data since objects display temporal constancy and the temporal information can hence be used for grouping and conditional variance regularization.
Acknowledgments

We thank Brian McWilliams, Jonas Peters, and Martin Arjovsky for helpful comments and discussions and CSCS for provision of computational resources. A preliminary version of this work was presented at the NIPS 2017 Interpretable ML Symposium and we thank participants of the symposium for very helpful discussions.

References

M. Abadi, A. Agarwal, P. Barham, E. Brevdo, Z. Chen, C. Citro, G. S. Corrado, A. Davis, J. Dean, M. Devin, S. Ghemawat, I. Goodfellow, A. Harp, G. Irving, M. Isard, Y. Jia, R. Jozefowicz, L. Kaiser, M. Kudlur, J. Levenberg, D. Mané, R. Monga, S. Moore, D. Murray, C. Olah, M. Schuster, J. Shlens, B. Steiner, I. Sutskever, K. Talwar, P. Tucker, V. Vanhoucke, V. Vasudevan, F. Viégas, O. Vinyals, P. Warden, M. Wattenberg, M. Wicke, Y. Yu, and X. Zheng. TensorFlow: Large-scale machine learning on heterogeneous systems, 2015. URL https://www.tensorflow.org/. Software available from tensorflow.org.

J. Aldrich. Autonomy. Oxford Economic Papers, 41:15–34, 1989.

J. Bagnell. Robust supervised learning. In Proceedings of the national conference on artificial intelligence, volume 20, page 714. Menlo Park, CA; Cambridge, MA; London; AAAI Press; MIT Press; 1999, 2005.

M. T. Bahadori, K. Chalupka, E. Choi, R. Chen, W. F. Stewart, and J. Sun. Causal regularization. ArXiv e-prints, 2017. URL http://arxiv.org/abs/1702.02604.

S. Barocas and A. D. Selbst. Big Data’s Disparate Impact. 104 California Law Review 671, 2016.

P.L. Bartlett, M.I. Jordan, and J.D. McAuliffe. Convexity, classification, and risk bounds. Technical report, Department of Statistics, U.C. Berkeley, 2003.

M. Belkin, P. Niyogi, and V. Sindhwani. Manifold regularization: A geometric framework for learning from labeled and unlabeled examples. Journal of machine learning research, 7(Nov):2399–2434, 2006.

S. Ben-David, J. Blitzer, K. Crammer, and F. Pereira. Analysis of representations for domain adaptation. In Advances in Neural Information Processing Systems 19. 2007.

A. Ben-Tal, D. Den Hertog, A. De Waegenaere, B. Melenberg, and G. Rennen. Robust solutions of optimization problems affected by uncertain probabilities. Management Science, 59(2):341–357, 2013.

M. Besserve, N. Shajarisales, B. Schölkopf, and D. Janzing. Group invariance principles for causal generative models. ArXiv e-prints, 2017. URL http://arxiv.org/abs/1705.02212.
T. Bolukbasi, K.-W. Chang, J. Y. Zou, V. Saligrama, and A. T. Kalai. Man is to computer programmer as woman is to homemaker? debiasing word embeddings. In Advances in Neural Information Processing Systems 29. 2016.

D. Bouchacourt, R. Tomioka, and S. Nowozin. Multi-level variational autoencoder: Learning disentangled representations from grouped observations. ArXiv e-prints, 2017. URL http://arxiv.org/abs/1705.08841.

K. Chalupka, P. Perona, and F. Eberhardt. Visual Causal Feature Learning. Uncertainty in Artificial Intelligence, 2014.

X. Chen, Y. Duan, R. Houthooft, J. Schulman, I. Sutskever, and P. Abbeel. InfoGAN: Interpretable Representation Learning by Information Maximizing Generative Adversarial Nets. In Advances in Neural Information Processing Systems 29. 2016.

K. Crawford. Artificial intelligence’s white guy problem. The New York Times, June 25 2016, 2016. URL https://www.nytimes.com/2016/06/26/opinion/sunday/artificial-intelligences-white-guy-problem.html.

G. Csurka. A comprehensive survey on domain adaptation for visual applications. In Domain Adaptation in Computer Vision Applications., pages 1–35. 2017.

E. L. Denton and V. Birodkar. Unsupervised learning of disentangled representations from video. In Advances in Neural Information Processing Systems 30. 2017.

J. Emspak. How a machine learns prejudice. Scientific American, December 29 2016, 2016. URL https://www.scientificamerican.com/article/how-a-machine-learns-prejudice/.

Y. Ganin, E. Ustinova, H. Ajakan, P. Germain, H. Larochelle, F. Laviolette, M. Marchand, and V. Lempitsky. Domain-adversarial training of neural networks. Journal of Machine Learning Research, 17(1), 2016.

R. Gao, X. Chen, and A. Kleywegt. Wasserstein distributional robustness and regularization in statistical learning. arXiv preprint arXiv:1712.06050, 2017.

M. Gong, K. Zhang, T. Liu, D. Tao, C. Glymour, and B. Schölkopf. Domain adaptation with conditional transferable components. In International Conference on Machine Learning, 2016.

I. Goodfellow, J. Shlens, and C. Szegedy. Explaining and harnessing adversarial examples. In International Conference on Learning Representations, 2015.

O. Goudet, D. Kalainathan, P. Caillou, D. Lopez-Paz, I. Guyon, M. Sebag, A. Tritas, and P. Tubaro. Learning Functional Causal Models with Generative Neural Networks. ArXiv e-prints, 2017. URL https://arxiv.org/abs/1709.05321.

T. Haavelmo. The probability approach in econometrics. Econometrica, 12:S1–S115 (supplement), 1944.
K. He, X. Zhang, S. Ren, and J. Sun. Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification. *ICCV*, 2015.

K. He, X. Zhang, S. Ren, and J. Sun. Deep residual learning for image recognition. *CVPR*, 2016.

I. Higgins, L. Matthey, A. Pal, C. Burges, X. Glorot, M. Botvinick, S. Mohamed, and A. Lerchner. beta-VAE: Learning Basic Visual Concepts with a Constrained Variational Framework. *International Conference on Learning Representations*, 2017.

N. Kilbertus, M. Rojas-Carulla, G. Parascandolo, M. Hardt, D. Janzing, and B. Schölkopf. Avoiding discrimination through causal reasoning. *Advances in Neural Information Processing Systems*, 2017.

D. P. Kingma and J. Ba. Adam: A method for stochastic optimization. *ICLR*, 2015.

M. Kocaoglu, C. Snyder, A. G. Dimakis, and S. Vishwanath. CausalGAN: Learning Causal Implicit Generative Models with Adversarial Training. *ArXiv e-prints*, 2017. URL https://arxiv.org/abs/1709.02023.

A. Krizhevsky, I. Sutskever, and G. E Hinton. Imagenet classification with deep convolutional neural networks. In *Advances in Neural Information Processing Systems 25*, 2012.

Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner. Gradient-based learning applied to document recognition. *Proceedings of the IEEE*, 1998.

Z. Liu, P. Luo, X. Wang, and X. Tang. Deep learning face attributes in the wild. In *Proceedings of International Conference on Computer Vision (ICCV)*, 2015.

D. Lopez-Paz and M. Oquab. Revisiting Classifier Two-Sample Tests. *International Conference on Learning Representations (ICLR)*, 2017.

D. Lopez-Paz, R. Nishihara, S. Chintala, B. Schölkopf, and L. Bottou. Discovering causal signals in images. In *The IEEE Conference on Computer Vision and Pattern Recognition (CVPR 2017)*, 2017.

C. Louizos, U. Shalit, J. M. Mooij, D. Sontag, R. Zemel, and M. Welling. Causal effect inference with deep latent-variable models. *Advances in Neural Information Processing Systems*, 2017.

R. Turner J. Peters M. Rojas-Carulla, B. Schölkopf. Causal transfer in machine learning. *ArXiv e-prints*, 2017. URL https://arxiv.org/abs/1507.05333

S. Magliacane, T. van Ommen, T. Claassen, S. Bongers, P. Versteeg, and J. M. Mooij. Causal transfer learning. *ArXiv e-prints*, 2017. URL https://arxiv.org/abs/1707.06422.

T. Matsuo, H. Fukuhara, and N. Shimada. Transform invariant auto-encoder. *ArXiv e-prints*, 2017. URL http://arxiv.org/abs/1709.03754.
M. Mirza and S. Osindero. Conditional Generative Adversarial Nets. ArXiv e-prints, 2014. URL https://arxiv.org/abs/1411.1784.

H. Namkoong and J.C. Duchi. Variance-based regularization with convex objectives. In Advances in Neural Information Processing Systems, pages 2975–2984, 2017.

J. Pearl. Causality: Models, Reasoning, and Inference. Cambridge University Press, New York, USA, 2nd edition, 2009.

J. Peters, P. Bühlmann, and N. Meinshausen. Causal inference using invariant prediction: identification and confidence intervals. Journal of the Royal Statistical Society, Series B (with discussion), to appear, 2016.

J. Quionero-Candela, M. Sugiyama, A. Schwaighofer, and N. D. Lawrence. Dataset Shift in Machine Learning. The MIT Press, 2009.

T. Richardson and J. M. Robins. Single world intervention graphs (SWIGs): A unification of the counterfactual and graphical approaches to causality. Center for the Statistics and the Social Sciences, University of Washington Series. Working Paper 128, 30 April 2013, 2013.

D. Rothenhäusler, P. Bühlmann, N. Meinshausen, and J. Peters. Anchor regression: heterogeneous data meets causality. arXiv preprint arXiv:1801.06229, 2018.

B. Schölkopf, D. Janzing, J. Peters, E. Sgouritsa, K. Zhang, and J. Mooij. On causal and anticausal learning. In Proceedings of the 29th International Conference on Machine Learning (ICML), pages 1255–1262, 2012.

B. Schölkopf, C. Burges, and V. Vapnik. Incorporating invariances in support vector learning machines. pages 47–52. Springer, 1996.

S. Shafieezadeh-Abadeh, D. Kuhn, and P. Esfahani. Regularization via mass transportation. arXiv preprint arXiv:1710.10016, 2017.

A. Sinha, H. Namkoong, and J. Duchi. Certifiable distributional robustness with principled adversarial training. arXiv preprint arXiv:1710.10571, 2017.

C. Szegedy, W. Zaremba, I. Sutskever, J. Bruna, D. Erhan, I. Goodfellow, and R. Fergus. Intriguing properties of neural networks. In International Conference on Learning Representations, 2014.

C. Szegedy, W. Liu, Y. Jia, P. Sermanet, S. Reed, D. Anguelov, D. Erhan, V. Vanhoucke, and A. Rabinovich. Going deeper with convolutions. In Computer Vision and Pattern Recognition (CVPR), 2015.

A. Torralba and A. A. Efros. Unbiased look at dataset bias. In Computer Vision and Pattern Recognition (CVPR), 2011.

M. Gong K. Zhang D. Tao X. Yu, T. Liu. Transfer learning with label noise. ArXiv e-prints, 2017. URL https://arxiv.org/abs/1707.09724.
Y. Xian, C. H. Lampert, B. Schiele, and Z. Akata. Zero-shot learning - A comprehensive evaluation of the good, the bad and the ugly. ArXiv e-prints, 2017. URL http://arxiv.org/abs/1707.00600.

H. Xu, C. Caramanis, and S. Mannor. Robust regression and lasso. In Advances in Neural Information Processing Systems, pages 1801–1808, 2009.

E. Yudkowsky. Artificial intelligence as a positive and negative factor in global risk. Global catastrophic risks, 1, 2008.

K. Zhang, B. Schölkopf, K. Muandet, and Z. Wang. Domain adaptation under target and conditional shift. In International Conference on Machine Learning, 2013.

K. Zhang, M. Gong, and B. Schölkopf. Multi-source domain adaptation: A causal view. In Proceedings of the Twenty-Ninth AAAI Conference on Artificial Intelligence, 2015.
APPENDIX

Appendix A. Proof of Theorem [1]

First part. To show the first part, namely that with probability 1,

\[ L_{adv}(\hat{\theta}_{pool}) = \infty, \]

we need to show that \( W^t\hat{\theta}_{pool} \neq 0 \) with probability 1. The reason this is sufficient is as follows: if \( W^t\theta \neq 0 \), then \( L_{adv}(\theta) = \infty \) as we can then find a \( v \in \mathbb{R}^q \) such that \( \gamma := \theta^tWv \neq 0 \). Setting \( \Delta_k = \kappa v \) for \( \kappa \in \mathbb{R} \), we get \( x(\Delta_k)^t\theta = x(\Delta = 0)^t\theta + \kappa \gamma \). Hence \( \log(1 + \exp(-y \cdot x(\Delta_k)^t\theta)) \rightarrow \infty \) for either \( \kappa \rightarrow \infty \) or \( \kappa \rightarrow -\infty \).

To show that \( W^t\hat{\theta}_{pool} \neq 0 \) with probability 1, let \( \hat{\theta}^* \) be the oracle estimator that is constrained to be orthogonal to the column space of \( W \):

\[ \hat{\theta}^* = \arg\min_{\theta : W^t\theta = 0} L_n(\theta) \quad \text{with} \quad L_n(\theta) := \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f_\theta(x_i(\Delta_i))). \quad (15) \]

We show \( W^t\hat{\theta}_{pool} \neq 0 \) by contradiction. Assume hence that \( W^t\hat{\theta}_{pool} = 0 \). If this is indeed the case, then the constraint \( W^t\theta = 0 \) in (15) becomes non-active and we have \( \hat{\theta}_{pool} = \hat{\theta}^* \). This would imply that taking the directional derivative of the training loss with respect to any \( \delta \in \mathbb{R}^p \) in the column space of \( W \) should vanish at the solution \( \hat{\theta}^* \). In other words, define the gradient as \( g(\theta) = \nabla_\theta L_n(\theta) \in \mathbb{R}^p \). The implication is then that for all \( \delta \) in the column-space of \( W \),

\[ \delta^t g(\hat{\theta}^*) = 0 \quad (16) \]

and we will show the latter condition is violated.

As we work with the logistic loss and \( \mathcal{Y} \in \{-1, 1\} \), the loss is given by \( \ell(y_i, f_\theta(x_i(\Delta_i))) = \log(1 + \exp(-y_i x_i(\Delta_i)^t\theta)) \). Define \( r_i(\theta) := y_i/(1 + \exp(y_i x_i(\Delta_i)^t\theta)) \). For all \( i = 1, \ldots, n \) we have \( r_i \neq 0 \). Then

\[ g(\hat{\theta}^*) = \frac{1}{n} \sum_{i=1}^{n} r_i(\hat{\theta}^*) x_i(\Delta_i). \quad (17) \]

Let \( x_i(0) \) for \( i = 1, \ldots, n \) be training data in absence of any interventions, that is under \( \Delta_i = 0 \). We call these data in the following the (counterfactual) intervention-free training data. Since the interventions only have an effect on the column space of \( W \) in \( X \), the oracle estimator \( \hat{\theta}^* \) is identical under the true training data and the intervention-free training data \( x(0) \). By assumption, \( x_i - x_i(0) = W\Delta_i \) and [17] can hence also be written as

\[ \delta^t g(\hat{\theta}^*) = \frac{1}{n} \sum_{i=1}^{n} r_i(\hat{\theta}^*) x_i(0)^t\delta + \frac{1}{n} \sum_{i=1}^{n} r_i(\hat{\theta}^*) \Delta_i^t W^t\delta. \quad (18) \]

Since \( \delta \) is in the column-space of \( W \), there exists \( u \in \mathbb{R}^q \) such that \( \delta = Wu \) and we can write [18] as

\[ \delta^t g(\hat{\theta}^*) = \frac{1}{n} \sum_{i=1}^{n} r_i(\hat{\theta}^*) x_i(0)^tWu + \frac{1}{n} \sum_{i=1}^{n} r_i(\hat{\theta}^*) \Delta_i^t W^tWu. \quad (19) \]
From (A2) we have that the eigenvalues of $W^tW$ are all positive. Also $r_i(\hat{\theta}^\ast)$ is not a function of the interventions $\Delta$, since, as above, the estimator $\hat{\theta}^\ast$ is identical whether trained on the original data $x_i$ or on the intervention-free data $x_i(0)$. If we condition on everything except for the random interventions by conditioning on $(x_i(0), y_i)$ for $i = 1, \ldots, n$, then the rhs of (19) can be written as

$$a^t u + B^t u,$$

where $a \in \mathbb{R}^q$ is fixed (again conditional on the intervention-free training data) and $B = \frac{1}{n} \sum_{i=1}^n r_i(\hat{\theta}^\ast)\Delta_i W^t W \in \mathbb{R}^q$ is a random vector and $B \neq -a \in \mathbb{R}^q$ with probability 1 as the interventions $\Delta_i$ are, by (A1), drawn from a continuous distribution. Hence the left hand side of (19) has a continuous distribution for any $\delta$ in the column-space of $W$, and the left hand side of (19) is not identically 0 with probability 1 for any given $\delta$ in the column-space of $W$. This shows that the implication (16) is incorrect with probability 1 and hence completes the proof of the first part by contradiction.

**Second part.** For the second part, we first show that with probability at least $p_n$, as defined in (A3), $\hat{\theta}^\ast = \hat{\theta}^\ast$ with $\hat{\theta}^\ast$ defined as in (15). Note that the invariant space for this model is the linear subspace $I = \{\theta : W^t \theta = 0\}$ and by their respective definitions,

$$\hat{\theta}^\ast = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^n \ell(y_i, f_\theta(x_i)) \text{ such that } \theta \in I,$$

$$\hat{\theta}^\ast = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^n \ell(y_i, f_\theta(x_i)) \text{ such that } \theta \in I_n.$$

Since we use $I_n = I_n(\tau)$ with $\tau = 0$,

$$I_n = \{\theta : \hat{\theta}(\text{Var}(f_\theta(X)|Y,\text{ID})) = 0\}.$$  

This implies that for $\theta \in I_n$ it holds that $f_\theta(x_i) = f_\theta(x_i')$ if $i, i' \in S_j$ for some $j \in \{1, \ldots, m\}$ (recall that $(y_i, \text{id}_i) = (y_i', \text{id}_i')$ if $i, i' \in S_j$ as the subsets $S_j$, $j = 1, \ldots, m$, collect all observations that have a unique realization of $(Y, \text{ID})$). Since $f_\theta(x) = f_\theta(x')$ implies $(x - x')^t \theta = 0$, it follows that $(x_i - x_i')^t \theta = 0$ if $i, i' \in S_j$ for some $j \in \{1, \ldots, m\}$ and hence

$$I_n \subseteq \{\theta : (x_i - x_i')^t \theta = 0 \text{ if } i, i' \in S_j \text{ for some } j \in \{1, \ldots, m\}\}.$$

Since $X^\text{style}$ has a linear influence on $X$ in (12), $x_i - x_i' = W(\Delta_i - \Delta_i')$ if $i, i'$ are in the same group $S_j$ of observations for some $j \in \{1, \ldots, m\}$. Note that the number of grouped examples $n - m$ is equal to or exceeds the rank $q$ of $W$ with probability $p_n$, using (A3), and $p_n \to 1$ for $n \to \infty$. By (A2), it follows then with probability at least $p_n$ that $I_n \subseteq \{\theta : W^t \theta = 0\} = I$. As, by definition, $I \subseteq I_n$ is always true, we have with probability $p_n$ that $I = I_n$. Hence, with probability $p_n$ (and $p_n \to 1$ for $n \to \infty$), $\hat{\theta}^\ast = \theta^\ast$. It thus remains to be shown that

$$L_{\text{adv}}(\hat{\theta}^\ast) \to_p L_{\text{adv}}^\ast. \quad (20)$$

Since $\hat{\theta}^\ast$ is in $I$, we have $\ell(y, x(\Delta)) = \ell(y, x(0))$, where $x(0)$ are the previously discussed intervention-free data. Hence

$$\hat{\theta}^\ast = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^n \ell(y_i, f_\theta(x_i(0))) \text{ such that } \theta \in I,$$

$$34$$
that is the estimator is unchanged if we use the data without interventions \((\Delta_i = 0)\) as training data. Define the population-optimal vector as

\[
\theta^* = \arg\min_{\theta} E\left[ \max_{\Delta} \ell(Y, f_\theta(X(\Delta))) \right] \text{ such that } \theta \in I,
\]

which can for the same reason be written as

\[
\theta^* = \arg\min_{\theta} E\left[ \ell(Y, f_\theta(X(\Delta = 0))) \right] \text{ such that } \theta \in I.
\]  

Hence (21) and (22) can be written as

\[
\hat{\theta}^* = \arg\min_{\theta, \theta \in I} L_n^{(0)}(\theta) \text{ where } L_n^{(0)}(\theta) := \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f_\theta(x_i(0))) \\
\theta^* = \arg\min_{\theta, \theta \in I} L^{(0)}(\theta) \text{ where } L^{(0)}(\theta) := E[\ell(Y, f_\theta(X(\Delta = 0)))].
\]

Comparing (21) and (22), by uniform convergence of \(L_n^{(0)}\) to the population loss \(L^{(0)}\), we have \(L^{(0)}(\hat{\theta}^*) \to_p L^{(0)}(\theta^*)\). By definition of \(I\) and \(\theta^*\), we have \(L^{*}_{adv} = L_{adv}(\theta^*) = L^{(0)}(\theta^*)\). As \(\hat{\theta}^*\) is in \(I\), we also have \(L_{adv}(\hat{\theta}^*) = L^{(0)}(\hat{\theta}^*)\). Since, from above, \(L^{(0)}(\hat{\theta}^*) \to_p L^{(0)}(\theta^*)\), this also implies \(L_{adv}(\hat{\theta}^*) \to_p L_{adv}(\theta^*) = L^{*}_{adv}\). Using the previously established result that \(\hat{\theta}^{core} = \hat{\theta}^*\) with probability at least \(p_n\) and \(p_n \to 1\) for \(n \to \infty\), this completes the proof.

**Appendix B. Proof of Theorem 2**

Let \(\hat{Y} = \theta^t X\) be the prediction under parameter vector \(\theta\). Let \(E_\kappa\) be again the expectation with respect to random \((Y, X)\) under model (14),

\[
\begin{align*}
Y &\leftarrow \varepsilon_Y \in \mathbb{R} \\
ID &\leftarrow k_{id}(Y, \varepsilon_{ID}) \\
X^{style} &\leftarrow k_{style}(Y, ID) + \varepsilon_{style} + \kappa \cdot \varepsilon_{style}' \\
X &\leftarrow k_x(Y, ID) + BX^{style}.
\end{align*}
\]

Looking at the expected squared error in a bias-variance decomposition (with the classical roles of \(Y\) and \(\hat{Y}\) here reversed due to the nature of the causal graph),

\[
E_\kappa [(Y - \theta^t X)^2] = E_\kappa [(Y - \hat{Y})^2] = E_\kappa [(E_\kappa(\hat{Y}|Y) - Y)^2] + E_\kappa [\text{Var}_\kappa(\hat{Y}|Y)].
\]

The bias term in (23) is unaffected by a change in \(\kappa\) as we can write the structural equation for \(X\) for a suitable function \(g(Y, ID) = k_x(Y, ID) + BK_{\text{style}}(Y, ID)\) as

\[
X \leftarrow g(Y, ID) + BX^{style} + \kappa B\varepsilon_{style}^t,
\]

and hence, using that the expected values of \(\varepsilon_{style}\) and \(\varepsilon_{style}'\) vanish and both are here independent of \(Y\) and \(ID\),

\[
E_\kappa(\hat{Y}|Y) = E_\kappa(\theta^t X|Y) = E_\kappa(\theta^t g(Y, ID)|Y) = E_0(\theta^t g(Y, ID)|Y).
\]

35
The variance term in (23) can be decomposed by the law of total variance as

\[ E_\kappa \left[ \text{Var}_\kappa (\hat{Y} | Y) \right] = E_\kappa \left[ \text{Var}_\kappa (\hat{Y} | Y, \text{ID}) \right] + \text{Var}_\kappa \left[ E_\kappa (\hat{Y} | Y, \text{ID}) \right]. \] (25)

The second term is not a function of \( \kappa \), using the analogous argument as in (24). Using that \( \varepsilon_{\text{style}} \) and \( \varepsilon'_{\text{style}} \) are independent and identically distributed, the first term in (25) can be written as

\[ \text{Var}_\kappa (\hat{Y} | Y, \text{ID}) = \text{Var}_\kappa (\theta^t B \varepsilon_{\text{style}}) + \kappa^2 \text{Var}_\kappa (\theta^t B \varepsilon'_{\text{style}}) = (1 + \kappa^2) \text{Var}_\kappa (\theta^t B \varepsilon_{\text{style}}) = (1 + \kappa^2) \text{Var}_\kappa=0 (\hat{Y} | Y, \text{ID}) = (1 + \kappa^2) C_\theta. \]

The expected loss under a scaling \( \kappa \) of the noise is then

\[ E_\kappa \left[ (Y - \theta^t X)^2 \right] = E_{\kappa=0} \left[ (Y - \theta^t X)^2 \right] + \kappa^2 \cdot C_\theta, \]

where \( C_\theta = E_{\kappa=0} (\text{Var}_{\kappa=0} (f_\theta(X)|Y,\text{ID})) \) is the expected conditional variance under \( \kappa = 0 \).

If we thus have training data generated under \( \kappa = 0 \), then the CoRe estimator with \( \lambda = \kappa^2 \) is optimizing the loss function under an increased style noise level, anticipating that the multiplier \( \kappa \) will rise potentially from the current value of 1 to higher values in different domains. In other words, the population CoRe estimator (13) is

\[ \theta^{\text{core}}(\lambda) = \arg\min_{\theta} E_{\kappa=0} \left[ (Y - \theta^t X)^2 \right] + \lambda \cdot C_\theta \]

\[ = \arg\min_{\theta} E_{\kappa=\sqrt{\lambda}} \left[ (Y - \theta^t X)^2 \right] \]

\[ = \arg\min_{\theta} \sup_{\kappa \leq \sqrt{\lambda}} E_\kappa \left[ (Y - \theta^t X)^2 \right], \]

which completes the proof.

**Appendix C. Network architectures**

We implemented the considered models in TensorFlow (Abadi et al., 2015). The model architectures used are detailed in Table C.1. CoRe and the pooled estimator use the same network architecture and training procedure; merely the loss function differs by the CoRe regularization term. In all experiments we use the Adam optimizer (Kingma and Ba, 2015). All experimental results are based on training the respective model five times (using the same data) to assess the variance due to the randomness in the training procedure. In each epoch of the training, the training data \( x_i, i = 1, \ldots, n \) are randomly shuffled, keeping the grouped observations \( (x_i)_{i \in I_j} \) for \( j \in \{1, \ldots, m\} \) together to ensure that mini batches will contain grouped observations. In all experiments the mini batch size is set to 120. For small \( c \) this implies that not all mini batches contain grouped observations, making the optimization more challenging.
Table C.1: Details of the model architectures used.

| Dataset     | Optimizer | Architecture                                      |
|-------------|-----------|--------------------------------------------------|
| MNIST       | Adam      | Input: 28 × 28 × 1 CNN Conv 5 × 5 × 16, 5 × 5 × 32 |
|             |           | (same padding, strides = 2, ReLu activation),    |
|             |           | fully connected, softmax layer                   |
| Stickmen    | Adam      | Input: 64 × 64 × 1 CNN Conv 5 × 5 × 16, 5 × 5 × 32 |
|             |           | (same padding, strides = 2, leaky ReLu activation),|
|             |           | fully connected, softmax layer                   |
| CelebA      | Adam      | Input: 64 × 48 × 3 CNN Conv 5 × 5 × 16, 5 × 5 × 32 |
| (all experiments) |           | (same padding, strides = 2, leaky ReLu activation),|
|             |           | fully connected, softmax layer                   |
|             |           | using CelebA                                      |
| AwA2        | Adam      | Input: 32 × 32 × 3 CNN Conv 5 × 5 × 16, 5 × 5 × 32 |
|             |           | (same padding, strides = 2, leaky ReLu activation),|
|             |           | fully connected, softmax layer                   |

(a) Examples of misclassified observations.

\[
y \equiv \text{glasses} \\
\hat{P}_{\text{core}}(\text{gl.}) = 1.00 \\
\hat{P}_{\text{pool}}(\text{gl.}) = 0.21
\]

\[
y \equiv \text{no glasses} \\
\hat{P}_{\text{core}}(\text{no gl.}) = 0.84 \\
\hat{P}_{\text{pool}}(\text{no gl.}) = 0.13
\]

(b) Misclassification rates.

Figure D.1: CelebA eyeglasses detection with brightness interventions, grouping setting 1. (a) Misclassified examples from the test sets. (b) Misclassification rates for \( \beta = 20 \) and \( c = 2000 \). Results for different test sets, grouping settings, \( \beta \in \{5, 10, 20\} \) and \( c \in \{200, 5000\} \) can be found in Figure D.3.
Appendix D. Additional experiments

D.1 Eyeglasses detection: known and unknown brightness interventions

Here, we show additional results for the experiment discussed in §7.7. Recall that we work with the CelebA dataset and consider the problem of classifying whether the person in the image is wearing eyeglasses. We discuss two alternatives for constructing different test sets and we vary the number of grouped observations in \( c \in \{200, 2000, 5000\} \) as well as the strength of the brightness interventions in \( \beta \in \{5, 10, 20\} \), all with sample size \( n = 20000 \). Generation of training and test sets 1 and 2 were already described in §7.7. Here, we consider additionally test set 3 where all images are left unchanged (no brightness interventions at all) and in test set 4 the brightness of all images is increased.

Furthermore, we consider three different ways of grouping images. In §7.7 we used images of the same person to create a grouped observation by sampling a different value for the brightness intervention. We refer to this as ‘Grouping setting 2’ here. An alternative is to use the same image of the same person in different brightnesses (drawn from the same distribution) as a group over which the conditional variance is calculated. We call this ‘Grouping setting 1’ and it can be useful if we know that we want to protect against brightness interventions in the future. For comparison, we also evaluate grouping with an image of a different person as a baseline (‘Grouping setting 3’). Examples from the training sets using grouping settings 1, 2 and 3 can be found in Figure D.2.

Results for all grouping settings, \( \beta \in \{5, 10, 20\} \) and \( c \in \{200, 5000\} \) can be found in Figure D.3. We see that using grouping setting 1 works best since we could explicitly control that only \( X^{\text{style}} \equiv \text{brightness} \) varies between grouping examples. In grouping setting 2, different images of the same person can vary in many factors, making it more challenging to isolate brightness as the factor to be invariant against. Lastly, we see that if we group images of different persons (‘Grouping setting 3’), the difference between CoRe estimator and the pooled estimator becomes much smaller than in the previous settings.

Regarding the results for grouping setting 1 in Figure D.1 we notice that the pooled estimator performs better than CoRe on test set 1. This can be explained by the fact that it can exploit the predictive information contained in the brightness of an image while CoRe is restricted not to do so. Second, we observe that the pooled estimator does not perform well on test sets 2 and 4 as its learned representation seems to use the image’s brightness as a predictor for the response which fails when the brightness distribution in the test set differs significantly from the training set. In contrast, the predictive performance of CoRe is hardly affected by the changing brightness distributions.

D.2 Gender classification

In §7.4 we assessed whether the results differ when (a) training a five-layer CNN (as detailed in Table C.1) end-to-end versus (b) using Inception V3 features and merely retraining the softmax layer. Here, we show some additional results for different sample sizes and number of grouped observations. Figure D.4 shows the results for varying numbers of \( n \) and \( c \)— in the left column for training a five-layer CNN; in the right column for using Inception V3 features. Overall, we see the same trends: As \( c \) increases, the performance difference between CoRe and the pooled estimator becomes smaller. This is due to the fact that...
Figure D.2: Examples from the CelebA eyeglasses detection with brightness interventions, grouping settings 1–3 with $\beta \in \{5, 10, 20\}$. In all rows, the first three images from the left have $y \equiv \text{no glasses}$; the remaining three images have $y \equiv \text{glasses}$. Connected images are grouped examples. In panels (a)–(c), row 1 shows examples from the training set, rows 2–4 contain examples from test sets 2–4, respectively. Panels (d)–(i) show examples from the respective training sets.

$X_{\text{style}}$ is binary in this example and, therefore, including grouped examples corresponds to data augmentation. Interestingly, the pooled estimator performs worse on test set 2 as $n$ becomes larger. It thus seems to exploit $X_{\text{style}}$ to a larger extent as $n$ grows.
Figure D.3: Misclassification rates for the CelebA eyeglasses detection with brightness interventions, grouping settings 1–3 with $c \in \{200, 2000, 5000\}$ and the mean of the exponential distribution $\beta \in \{5, 10, 20\}$. 
D.3 MNIST: more sample efficient data augmentation

Here, we show further results for the experiment introduced in §7.5. We vary the number of augmented training examples $c$ from 100 to 5000 for $m = 10000$ and $c \in \{100, 200, 500, 1000\}$
Figure D.5: Data augmentation setting: Misclassification rates for MNIST and $X^{\text{style}} \equiv \text{rotation}$. In test set 1 all digits are rotated by a degree randomly sampled from $[35, 70]$. Test set 2 is the usual MNIST test set.

for $m = 1000$. The degree of the rotations is sampled uniformly at random from $[35, 70]$. Figure D.5 shows the misclassification rates. Test set 1 contains rotated digits only, test set 2 is the usual MNIST test set. We see that the misclassification rates of CoRE are always lower on test set 1, showing that it makes data augmentation more efficient. For $m = 1000$, it even turns out to be beneficial for performance on test set 2.

D.4 Stickmen image-based age classification

Here, we show further results for the experiment introduced in §7.3. Figure D.6 illustrates the data generating process. Recall that test set 1 follows the same distribution as the training set. In test sets 2 and 3 large movements are associated with both children and adults, while the movements are heavier in test set 3 than in test set 2. Figure D.7b shows
(a) Examples from test sets 1–3.

(b) Misclassification rates.

Figure D.7: a) Examples from the stickmen test set 1 (row 1), test set 2 (row 2) and test sets 3 (row 3). In each row, the first three images from the left have \( y \equiv \text{child} \); the remaining three images have \( y \equiv \text{adult} \). Connected images are grouped examples. b) Misclassification rates for different numbers of grouped examples.

Results for different numbers of grouping examples. For \( c = 20 \) the misclassification rate of CoRE estimator has a large variance. For \( c \in \{50, 500, 2000\} \), the CoRE estimator shows similar results. Its performance is thus not sensitive to the number of grouped examples, once there are sufficiently many grouped observations in the training set. The pooled estimator fails to achieve good predictive performance on test sets 2 and 3 as it seems to use “movement” as a predictor for “age”.

D.5 Eyeglasses detection: image quality intervention

Here, we show further results for the experiments introduced in §7.2. Specifically, we consider interventions of different strengths by varying the mean of the quality intervention in \( \mu \in \{30, 40, 50\} \). Recall that we use ImageMagick to modify the image quality. In the training set and in test set 1, we sample the image quality value as \( q_{ij} \sim \mathcal{N}(\mu, \sigma = 10) \) and apply the command `convert -quality q_{ij} input.jpg output.jpg` if \( y_i \equiv \text{glasses} \). If \( y_i \equiv \text{no glasses} \), the image is not modified. In test set 2, the above command is applied if \( y_i \equiv \text{no glasses} \) while images with \( y_i \equiv \text{glasses} \) are not changed. In test set 3 all images are left unchanged and in test set 4 the command is applied to all images, i.e. the quality of all images is reduced.

We run experiments for grouping settings 1–3 and for \( c = 5000 \), where the definition of the grouping settings 1–3 is identical to §D.1. Figure D.8 shows examples from the respective training and test sets and Figure D.9 shows the corresponding misclassification rates. Again, we observe that grouping setting 1 works best, followed by grouping setting 2. Interestingly, there is a large performance difference between \( \mu = 40 \) and \( \mu = 50 \) for the pooled estimator. Possibly, with \( \mu = 50 \) the image quality is not sufficiently predictive for the target.
Figure D.8: Examples from the CelebA image quality datasets, grouping settings 1–3 with $\mu \in \{30, 40, 50\}$. In all rows, the first three images from the left have $y \equiv \text{no glasses}$; the remaining three images have $y \equiv \text{glasses}$. Connected images are grouped observations over which we calculate the conditional variance. In panels (a)–(c), row 1 shows examples from the training set, rows 2–4 contain examples from test sets 2–4, respectively. Panels (d)–(i) show examples from the respective training sets.

Figure D.9: Misclassification rates for the CelebA eyeglasses detection with image quality interventions, grouping settings 1–3 with $c = 5000$ and the mean of the Gaussian distribution $\mu \in \{30, 40, 50\}$.
Figure D.10: Examples from the subsampled and augmented AwA2 dataset (Elmer-the-Elephant dataset). Row 1 shows examples from the training set, rows 2–5 show examples from test sets 1–4, respectively.

D.6 Elmer the Elephant

The color interventions for the experiment introduced in §7.6 were created as follows. In the training set, if $y_i \equiv \text{elephant}$ we apply the following ImageMagick command for the grouped examples:

\[
\text{convert -modulate 100,0,100 input.jpg output.jpg}
\]

Test sets 1 and 2 were already discussed in §7.6: in test set 1, all images are left unchanged. In test set 2, the above command is applied if $y_i \equiv \text{horse}$. If $y_i \equiv \text{elephant}$, we sample $c_{i,j} \sim \mathcal{N}(\mu = 20, \sigma = 1)$ and apply:

\[
\text{convert -modulate 100,100,100-c_{i,j} input.jpg output.jpg}
\]

to the image.

Here, we consider again some more test sets than in §7.6. In test set 4, the latter command is applied to all images. It rotates the colors of the image, in a cyclic manner\(^9\). In test set 3, all images are changed to grayscale. The causal graph for the data generating process is shown in Figure D.12. Examples from all four test sets are shown in Figure D.10 and classification results are shown in Figure D.11.

The value of the penalty parameter $\lambda$ in Eq. (10) is chosen depending on the expected strength of future interventions. Figure D.13 shows the misclassification rates of CoRe on the subsampled and augmented AwA2 dataset (Elmer-the-Elephant dataset) as a function of the penalty $\lambda$. We see that performance is not very sensitive to the choice of the penalty parameter in a reasonable range.

---

\(^9\) For more details, see http://www.imagemagick.org/Usage/color_mods/#color_mods
Figure D.11: Elmer-the-Elephant dataset. (a) Misclassified examples from the test sets. (b) Misclassification rates on test sets 1 to 4.

Figure D.12: Data generating process for the Elmer-the-Elephant example.

Figure D.13: Misclassification rates of CoRe on the subsampled and augmented AwA2 dataset (Elmer-the-Elephant dataset) as a function of the penalty $\lambda$. The outcome does not depend strongly on the chosen value.