Dimension Reduction for Robust Covariate Shift Correction

Fulton Wang  
MIT

Cynthia Rudin  
Duke

Abstract

In the covariate shift learning scenario, the training and test covariate distributions differ, so that a predictor’s average loss over the training and test distributions also differ. The importance weighting approach handles this shift by minimizing an estimate of test loss over predictors, obtained via a weighted sum over training sample losses. However, as the dimension of the covariates increases, this test loss estimator increases in variance. In this work, we adapt the importance weighting approach to more robustly handle higher dimensional covariates by incorporating dimension reduction into the learning process.

1 Introduction

Often, the population for which one has labelled training data differs from the population one needs to make predictions for. For example, the population that received a medical treatment likely differs from those eligible for it. In the specific case of "covariate shift", the marginal covariate distribution is assumed to differ between training and test domains ($P_{\text{train}}(x) \neq P_{\text{test}}(x)$), while the conditional outcome distributions are the same ($P_{\text{train}}(y|x) = P_{\text{test}}(y|x)$). Given labelled training data and unlabelled test data drawn from the training and test domains, respectively, the covariate shift task is to learn a model exhibiting low expected loss over the test domain. Often, a model is misspecified due to computational or interpretability considerations. Under model misspecification, a predictor naively learned from the training data may have worse performance over the test domain.

One popular approach to handling covariate shift finds a (possibly non-linear) lower dimensional space in which the training and test covariate distributions are similar $[6,28]$. A model can then be learned using the projected training data, which now more accurately represents the projected test domain. For example, $[29]$ finds a linear subspace minimizing the maximum mean discrepancy $[14]$ between the projected distributions. Such methods enjoy the general benefits of dimension reduction, such as robustness and interpretability. However, with the exception of $[8]$, such approaches are unsupervised, so that the projected covariates may not be predictive of the outcome of interest.

Another approach to handling covariate shift reweights the empirical training loss of a given predictor to emphasize training samples in regions of high test density. A popular weighing scheme is to weight a training sample $x$ by the density ratio $P_{\text{train}}(x)/P_{\text{test}}(x)$ $[32, 15, 34, 5]$. Doing so corrects the naive training loss so that it is no longer a biased estimate of expected test loss, the actual quantity of interest during training. However, this approach fails in high dimensions, where the test loss estimator has high variance due to two reasons.

Firstly, even if the true weights are known, in higher dimensions, the training and test distributions will tend to be very different, which leads to a small “effective sample size” $[11]$, where the “true” weights are concentrated on a small number of training samples. To reduce the variance of the weighted estimator, one line of work $[32, 10, 41, 16]$ uses various forms of regularization to discourage exceedingly large weights, at the cost of increased bias. Another line eschews weight estimation and builds predictors that are robust to potential shifts in the covariate $[10]$ or conditional outcome $[25, 9]$ distribution. A separate work $[30]$ reduces variance by using the predictor minimizing training loss as a prior when minimizing the reweighted loss.

Secondly, the variance of the density ratios estimates themselves increase as the dimension increases. Recognizing this, recent methods $[15, 34, 3]$ estimate the density ratios directly, without separately estimating the training and test densities explicitly. To further reduce the variance, $[35, 33]$ propose incorporating dimension reduction into the density ratio estimation procedure. Specifically, they search for a subspace in
We believe that dimension reduction is a promising way to reduce density ratio estimate variance, but when the ratios are used for covariate shift correction, the choice of subspace should be chosen according to different criteria. Specifically, the subspace should be one that is predictive of the outcome of interest, and one in which the effective sample size is sufficiently large. Then, the importance weighting method can be applied directly to the projected data, in which an accurate predictor exists, and the reweighted loss is reliably estimated due to the two respective criterion. Furthermore, if the predictive utility of subspace is simply the downstream achievable reweighted loss (instead of a surrogate measure[36, 13]), this suggests a wrapper[22] approach to dimension reduction, with the subspace and resultant predictor jointly chosen.

Thus in this work, we adapt the importance weighting approach to more robustly handle higher dimensional covariates. We present a method that jointly learns a linear covariate subspace and predictor acting on the covariate subspace that minimizes, over linear predictors, a low variance estimator of test loss. In particular, our estimator is simply the importance weighted test loss estimator, applied to the subspace. Thus, our estimator is lower variance simply by virtue of avoiding high dimensional density ratio estimation. Although our test loss estimator turns out to be biased, we believe it preferable to sacrifice bias for reduced variance when data is high dimensional and scarce. Furthermore, we can give preference to subspaces within which the training and test distributions are similar, to avoid small effective sample sizes. The effective sample size we require can be chosen via cross-validation, giving a practical way to navigate the bias-variance tradeoff, which is nontrivial in the covariate shift setting.

Because our method jointly finds the subspace and predictor it improves on a two step approach of first applying unsupervised dimension reduction methods like those aforementioned for covariate shift or simply PCA, and then an importance weighting method. Because our method evaluates the subspace and predictor based on the estimated resulting test loss, it improves on supervised dimension reduction methods that find a subspace (and possibly predictor, jointly) with high predictive utility in the training domain. In particular, our method improves upon [8], which finds a linear subspace minimizing an additive combination of maximum mean discrepancy, and the average squared loss of a linear classifier over the labelled, projected training data. However, the linear model is likely misspecified, so that their linear prediction utility measure may not be an accurate of prediction utility in the test domain. Relatedly, our method can be considered orthogonal to [17], who, not emphasizing interpretability, consider a very flexible model class via deep neural network representation learning, do not suffer from model misspecification and thus do not use importance reweighting in evaluating the representation’s predictive utility.

Our optimization routine involves gradient descent over the space of projection matrices, with the objective function for a given projection being the minimum regularized estimated test loss over linear predictors acting on the resultant subspace. The optimization routine requires a linear predictor, but can handle any convex loss function, e.g. squared and logistic loss for regression and classification. We propose to estimate the density ratios in a given subspace using unconstrained least squares importance fitting (uLSIF)[18], though other methods like kernel mean matching or kernel density estimation also fit into the optimization framework. The objective function of the routine is not analytically available, as it is implicitly defined as the solution to another optimization problem (that estimates the density ratios in the subspace to obtain the test loss estimator, and then minimizes it over all predictors). Thus, we use the gradient trick of [4] to calculate the gradient efficiently.

Conceptually, our work can be considered an extension of joint dimension reduction and learning prediction methods [31, 38, 69], adapted to the covariate shift setting in which the dimension reduction is further useful for improved weight estimation. Our optimization procedure is an application of a body of work on calculating gradients for hyperparameter learning [12, 7, 20, 26], which has recently been used to both construct[2] and understand [21] neural networks. Finally, because the output of our method is a subspace, our method can in theory be used in conjunction with aforementioned methods for robust importance weighted learning.

## 2 Background

### 2.1 Covariate Shift Problem

In the covariate shift problem, one is given \( N^{tr} \) labelled training samples \( \{x_i^{tr}, y_i^{tr}\} \), with \( x_i^{tr}, y_i^{tr} \sim P_{X,Y}^{tr} \), the training distribution, and \( N^{te} \) unlabelled test samples \( \{x_i^{te}\} \), with \( x_i^{te} \sim P_X^{te} \), the test distribution, with \( x_i^{tr}, x_i^{te} \in \mathbb{R}^D \). Importantly, one makes the covariate shift assumption, that \( P_{Y|X}^{tr} = P_{Y|X}^{te} \). But \( P_X^{tr} \neq P_X^{te} \).

Given a model class \( F \), the covariate shift problem seeks \( \text{argmin}_{f \in F} E_{P_{X,Y}^{te}}[L(f(X), Y)] \), where \( L \) is a loss function that we assume to be convex in \( f(X) \).
2.2 Importance Weighted Loss Minimization

To minimize expected test loss over predictors, noting that $E_{P_{X, Y}} [L(f(X), Y) = E_{P_{X, Y}}[P_{X}(X) L(f(X), Y)]$, past work constructs an unbiased estimator of test loss by forming the empirical expectation version of the latter expectation, and then minimizes it over predictors, adding some regularization:

$$\arg\min_{f \in \mathcal{F}} \sum \hat{w}(x_i^{tr}) L(f(x_i^{tr}), y_i^{tr}) + \Omega(f) \quad (1)$$

where $\hat{w}(x_i^{tr})$ estimates $w(x_i^{tr}) := \frac{P_{X}^{tr}(x_i^{tr})}{P_{X}^{te}(x_i^{tr})}$. We note that the “effective sample size” of the estimator is $N^{tr} / \sum_i (\hat{w}(x_i^{tr}))^2$ \cite{12}.

2.3 Density Ratio Estimation

To carry out importance weighting requires estimating the density ratios $\frac{P_{X}^{tr}(x)}{P_{X}^{te}(x)}$. A variety of methods \cite{13,14} exist for doing so, but one, least squares importance fitting (LSIF) \cite{15}, and its computationally more efficient variant, unconstrained LSIF (uLSIF) stands out because it involves only a (possibly constrained) quadratic program, and admits a cross validation scheme.

LSIF assumes the estimated ratio function can be written as $\alpha^T \phi(x)$, where $\phi(x) = \{\phi_m(x)\}$ is a set of $M$ basis functions they choose to be gaussian kernels centered at test points and $\alpha \in \mathbb{R}^K$ is a parameter they aspire to identify by minimizing the expected squared error to the true ratios: $E_{P_{X, Y}}[(\alpha^T \phi(X) - \frac{P_{X}^{tr}(X)}{P_{X}^{te}(X)})^2] = E_{P_{X, Y}}[(\alpha^T \phi(X))^2] - 2E_{P_{X, Y}}[\alpha^T \phi(X)] + C$, where $C$ is a constant. Substituting empirical expectations, dividing by 2, and regularizing, they obtain the fit value of $\alpha$ as

$$\alpha^* = \arg\min_{\alpha} \frac{1}{2} \alpha^T H \alpha - h^T \alpha + \gamma 1^T \alpha \text{ subject to } \alpha \geq 0,$$

with $H = \frac{1}{N^{tr}} \sum_k \phi(x_k^{tr}) \phi(x_k^{tr})^T$, $h = \frac{1}{N^{tr}} \sum_k \phi(x_k^{te})$, $\gamma$ is the regularization constant, and $1$ is the vector of all 1’s. The estimated ratio function is then $\hat{w}(x) = \alpha^{*T} \phi(x)$, with the element-wise positive constraint $\alpha \geq 0$ ensuring $\hat{w}(x)$ is positive. uLSIF simply removes the positivity constraint on $\alpha$ in obtaining $\alpha^*$. With $\alpha^T \phi(x)$ no longer guaranteed to be positive, under uLSIF, the learned ratio function is $\hat{w}(x) = \max(\alpha^{*T} \phi(x), 0)$.

3 Formulation

3.1 Motivation

Our approach is motivated by the following: suppose we constrain the model class to be the composition of a linear projection to a subspace, followed by a predictor acting on the projected features. That is, the model class contains functions of the form $g(A^T x)$ where $A$ is a projection matrix, and $g$ is a base model class. The fact that such a composite function only depends on a subspace opens up two opportunities to decrease the variance of the learning procedure.

Firstly, we can construct a surrogate estimator of $E_{P_{Y, X}}[L(g(A^T X), Y)]$ as

$$\frac{1}{N^{tr}} \sum \hat{w}_A(x_i^{tr}) L(g(A^T x_i^{tr}), y_i^{tr}), \quad (2)$$

where $\hat{w}_A(x_i^{tr})$ estimates $w_A(x_i^{tr}) := \frac{P_{X}^{tr}(A^T x_i^{tr})}{P_{X}^{te}(A^T x_i^{tr})}$. This estimator is lower variance than that in Equation 1 because the density ratio estimates are lower variance, being those in the lower dimensional subspace parameterized by $A$. Furthermore, as we show later, in expectation the effective sample size in any subspace is higher than that in the full space. This estimator turns out to be biased relative to $E_{P_{Y, X}}[L(g(A^T X), Y)]$, due to $P_{Y, X}^{tr} \neq P_{Y, X}^{te}$ despite $P_{X}^{tr} \neq P_{X}^{te}$. However as our experiments show, this bias can be a worthwhile tradeoff when the variance would otherwise be high.

Secondly, we can explicitly refuse to consider functions $g(A^T x)$ for which the effective sample size of its loss estimate $N^{tr} \sum \hat{w}_A(x_i^{tr})^2$ is too low. Note that this constraint lower bounds the effective sample size of estimators considered even if constraining $A$ does not end up constraining the resultant model class, since the effective sample size only depends on $A$, not on $g$.

These ideas suggest finding the predictor $g(A^T x)$ minimizing test loss by minimizing over $g$ and $A$ the estimator of Equation 2 plus a regularizer $\sum_i (\hat{w}_A(x_i^{tr}))^2$. To complete the optimization problem, we still need to construct the projected density ratio estimates $\hat{w}_A(x_i^{tr})$, which notably depend on $A$. We can do so by imposing the constraint that the $\hat{w}_A(x_i^{tr})$ are equal to the projected density ratio estimates that would be returned by a ratio estimation method, i.e. LSIF or uLSIF, run on the projected covariates $\{A^T x_i^{tr}\}$, $\{A^T x_i^{te}\}$.

3.2 Joint Dimension Reduction and Importance Weighting

Given the above motivation, in this work, we propose a method for solving the covariate shift problem described in Section 2.1 for the case when the model class $\mathcal{F}$ consists of functions expressed as the composition of a linear projection followed by a function from some base model class. That is, $\mathcal{F} = \{g(A^T x) : A \in \mathbb{R}^{K \times D}, A^T A = I, g \in \mathcal{G}\}$, where $D < K$ is the specified dimension of the subspace and $\mathcal{G}$ is a specified base model class. In this exposition and in the experiments, we will restrict our attention to the case where $\mathcal{G}$ consists of linear functions of $\mathbb{R}^D$, so that $\mathcal{F}$ consists of
linear functions of original feature space \( \mathbb{R}^K \). We do so because importance weighting only helps when the model is misspecified, and misspecification is often due to a desire for interpretability, which linear models provide. However, our framework is readily applied to kernel methods and other base models where the fitting procedure is a convex problem.

To learn a model from the linear model class (over-parameterized as) \( \mathcal{F} = \{b^T(A^Tx) ; A \in \mathbb{R}^{K \times D}, A^TA = I, b \in \mathbb{R}^D \} \) for the covariate shift problem, where the loss function \( L \) is assumed convex, we propose obtaining the parameters \( A, b \) via the following optimization:

\[
\min_{A,b} \sum_i w_i^{tr} L(b^T u_i^{tr}, y_i^{tr}) + \lambda \sum_i (u_i^{tr})^2 + c\|b\|^2
\]  

(3)

subject to

\[
u_i^{tr} = A^T x_i^{tr}, \quad w_i^{tr} = A^T x_i^{te}
\]  

(4)

\[w_i^{tr} = \max(\alpha^T \phi(u_i^{tr}), 0)
\]  

(5)

\[\alpha^* = \arg\min_{\alpha} \frac{1}{2} \alpha^T H \alpha - b^T \alpha + \gamma \alpha^T \alpha
\]  

(6)

\[H = \frac{1}{N^{tr}} \sum_k \phi(u_i^{tr})\phi(u_i^{tr})^T, \quad h = \frac{1}{N^{tr}} \sum_k \phi(u_i^{tr})
\]  

(7)

\[A^T A = I,
\]  

(8)

where \( \lambda, \gamma, c \) are hyperparameters described shortly.

The first term of the objective is the surrogate test loss estimator of Equation 2; the second term is a regularizer that encourages the effective sample size of that estimator, \( N^{tr} / \sum_i (w_i(x_i^{tr}))^2 \), to be high. These terms have such an interpretation because by Equations 3, the \( w_i^{tr} \) are the estimates of \( \frac{P_{x_i^{tr}}(x_i^{te})}{P_{x_i^{tr}}(x_i^{te})} \) returned by running uLSIF on \( \{u_i^{tr}\}, \{u_i^{te}\} \), which by Equation 3 are the original training and test covariates, projected by \( A \). Again, note that the \( w_i^{tr} \) thus depend on \( A \) through an optimization problem: that of running uLSIF. We use uLSIF instead of LSIF for ratio estimation, as we found experimentally that the computational benefits of uLSIF outweighed its marginal accuracy gain in the low dimensions we apply it to. Equation 8 ensures that \( A \) is a projection matrix. Finally, \( c\|b\|^2 \) is \( L_2 \) regularization of the composite linear model \( f(x) = b^T A^T x \), whose coefficient’s squared norm is simply \( \|b\|^2 \) due to \( A \) being orthonormal. Regarding hyperparameters, \( \lambda \) controls the tradeoff between the test loss estimator and the effective sample size of it, and \( c \) controls the amount of regularization on the composite linear model.

For the sake of transforming the optimization problem to one over only \( A \) and not \( b \), we choose to rewrite it as follows: we remove \( b \) from the minimization, but add in an additional constraint so the underlying problem is unchanged, to arrive at the alternate formulation:

\[
\min_{A} \sum_i w_i^{tr} L(b^T u_i^{tr}, y_i^{tr}) + \lambda \sum_i (u_i^{tr})^2 + c\|b^*\|^2
\]  

(9)

subject to

\[
b^* = \arg\min_{b} w_i^{tr} L(b^T u_i^{tr}, y_i^{tr}) + c\|b\|^2,
\]  

(10)

and all the original constraints of Equations 4-8. Figure 1 shows the architecture of this formulation, where \( A \) is the only parameter upon which objective \( L \) depends.

3.3 Analysis of Surrogate Loss Estimator

We first show that in expectation, for any candidate function \( f(x) = b^T A^T x \), the effective sample size of our “ideal” surrogate loss estimator, \( N^{tr} / \sum_i (w_i(x_i^{tr})^2) \), where the density ratio estimates are replaced by the true density ratios, is larger than that of the naive “ideal” loss estimator of Equation 4:

\[N^{tr} / \sum_i (w(x_i^{tr})^2): \]

**Lemma 3.1.** For any \( A \in \mathbb{R}^{D \times K} \) such that \( A^T A = I \),

\[E_{P_X} [N^{tr} / \sum_i (w_i(x_i^{tr})^2)] \geq E_{P_X} [N^{tr} / \sum_i (w(x_i^{tr})^2)].
\]

**Pf.** Let \( C \) be a matrix whose columns span the orthogonal complement to the subspace spanned by the columns of \( A \), and let \( (U, V) = (A^T X, CT^T X) \). Then

\[E_{P_X} [N^{tr} / \sum_i (w(x_i^{tr})^2)] = E_{P_X} [(\frac{P_{x_i^{tr}}(X)}{P_{x_i^{tr}}(X)})^2]
\]  

(11)

\[= E_{P_{X|U,V}} [(\frac{P_{x_i^{tr}|U,V}(X|U,V)}{P_{x_i^{tr}|U,V}(X|U,V)})^2]
\]  

(12)

\[= E_{P_{U,V}} [(\frac{P_{x_i^{tr}|U,V}(X|U,V)}{P_{x_i^{tr}|U,V}(X|U,V)})^2]
\]  

(13)

\[\geq E_{P_{U,V}} [(\frac{P_{x_i^{tr}|U,V}(X|U,V)}{P_{x_i^{tr}|U,V}(X|U,V)})^2]
\]  

(14)

where in going from Equation 13 to 14 we have used the fact that for any fixed \( U, 1 \leq E_{P_{X|U,V}} [(\frac{P_{x_i^{tr}|U,V}(X)}{P_{x_i^{tr}|U,V}(X)})^2] := PE(P_{x_i^{tr}|U,V}(X|U,V)) + 1 \) which follows because \( PE(\|\cdot\|) \), denoting the Pearson Divergence between distributions, is always at least 0. This verifies our intuition that projecting onto a subspace can, under idealized circumstances, increase effective sample size.

Note that since the effective sample size of our surrogate loss estimator is only larger in expectation, and even so might still be too small for some \( A \), the empirical objective still needs to explicitly regularize against small effective sample sizes. We can also bound the bias of our “ideal” surrogate loss estimator relative to the true test loss, where true density ratios replace their estimates (see Supplement for proof):
Lemma 3.2. Given $A, b$, let $U, V$ be as defined in Lemma 3.1, and $(x_{i}^{tr}, y_{i}^{tr}) \sim P_{X,Y}^{tr}$. Then

$$
\left| E_{P_{X,Y}^{tr}} \left[ \frac{1}{N^{tr}} \sum_{i} w_{A}(x_{i}^{tr}) L(b^{T}(A^{T} x_{i}^{tr}), y_{i}^{tr}) \right] - E_{P_{X,Y}^{tr}} [L(b^{T} A^{T} X, Y)] \right| 
\leq E_{P_{U}^{tr}} \left[ PE(P_{V}^{tr} || P_{U}^{tr}) \right]^{1/2} E_{P_{U}^{tr}} \left[ V a r_{P_{U}^{tr}} (L(b^{T} U, Y)) \right]^{1/2}.
$$

The LHS is the absolute bias of our estimator. The first term of the bound measures, roughly speaking, how much the training and test distributions differ in the subspace orthogonal to the subspace $A$ parameterizes. The second term measures how much variance there is in $L(b^{T} U, Y)$, with $U$ fixed, averaged over the test distribution of $U$, so that it represents how well the loss can be predicted, given only $U$. In particular, this term is 0 if $Y \perp X | A^{T} X$, i.e. $A$ parameterizes a sufficient subspace of the original covariate space. The bias is high only if both terms are simultaneously high. It also allows for two extensions. Firstly, we can take the maximum of the RHS over all $A, b$ to obtain a (trivial) uniform bound in the bias of our surrogate loss estimator. Secondly, the form of the bound admits a way to construct an estimator for an upper bound of the test loss. However, we found experimentally minimizing this upper bound estimator instead of our original surrogate estimator did not help performance.

4 Solving the Optimization Problem

The objective $L$ of the optimization problem of Equations 9 and 10 depends only on projection matrix $A$, through several intermediate variables. Thus, we solve the optimization problem via gradient descent over projection matrices. The challenge is in calculating the gradient $\frac{dL}{dA}$, as intermediate variables $\alpha^{*}$ and $b^{*}$ depend on other variables not analytically, but as the solution to convex optimization problems parameterized by the dependent variables. We call them argmin variables.

Fortunately we can apply existing work [12, 20, 26] to efficiently calculate $\frac{dL}{dA}$ through reverse mode differentiation. We used Autograd[27] to calculate gradients not involving argmin variables.

4.1 Differentiation with argmin Variables

In reverse mode differentiation, the generic task is to recursively, given an objective of the form $L(v(u))$ and $\frac{dv}{du}$, to compute $\frac{dv}{du} \cdot \frac{du}{dv}$. In our problem, we use reverse mode differentiation to compute $\frac{db^{*}}{dA}$ and $\frac{d\alpha^{*}}{dA}$ given $\frac{dL}{db^{*}}$, where $w$ is the length $N^{tr}$ vector of weights $\{w_{i}^{tr}\}$ of Equation 5. We will illustrate the latter calculation; the same technique suffices for both, as both argmin variables are the solutions to unconstrained problems. Please see 2 for how to calculate $\frac{d\alpha^{*}}{dA}$ if LSIF is used, where $\alpha^{*}$ is given by a constrained optimization problem.

4.1.1 Calculating $\frac{db^{*}}{dv}$

We first describe how to explicitly form $\frac{db^{*}}{dv}$, as the naive way to calculate $\frac{dL}{dA} \cdot \frac{d\alpha^{*}}{dA}$ is simply to form $\frac{d\alpha^{*}}{dA}$ and then matrix multiply. Since $b^{*}$ minimizes the convex function $f(b) := \sum_{i} w_{i}^{tr} L(b^{T} u_{i}^{tr}, y_{i}^{tr}) + c\|b\|^{2}$, $b^{*}$ satisfies the stationarity condition

$$
\frac{df}{db}(b^{*}(w), w) = 0,
$$

where $0$ is a length $D$ vector of zeros, and the notation suggests $f$ depends on both $b^{*}$ and $w$, and $b^{*}$ further depends on $w$. Differentiating with respect to $w$ gives

$$
\frac{dL}{dv} \left( \frac{d\alpha^{*}}{dA} \right) + \frac{dL}{dv} \left( \frac{db^{*}}{dA} \right) = 0,
$$

where $\frac{d\alpha^{*}}{dA}$ is the desired $N \times K$ Jacobian matrix, $\frac{dL}{dv}$ is the $K \times K$ Hessian matrix of $f$, and $\frac{dL}{dv} \frac{d\alpha^{*}}{dA}$ is $N \times K$. Rearranging, we obtain a multiple linear system we can solve for $\frac{db^{*}}{dv}$:

$$
\left( \frac{dL}{dv} \right) \frac{db^{*}}{dv} = -\left( \frac{dL}{dv} \frac{d\alpha^{*}}{dA} \right)^{T}.
$$

However solving this multiple linear system is in general not feasible, as calculating $\frac{dL}{dv}$ involves solving $N$ separate linear systems, with $w$ being $N$-dimensional. Solving the multiple linear system by inverting the coefficient matrix might be feasible when that matrix is $\frac{dL}{dv} \frac{d\alpha^{*}}{dA}$, but not when calculating $\frac{dL}{dv} \frac{d\alpha^{*}}{dA}$, where the coefficient matrix in the corresponding multiple linear system would be $\frac{dL}{dv} \frac{d\alpha^{*}}{dA}$, where $g$ is the objective in Equation 5 and the dimension of $\alpha$ is the number of basis functions used, possibly large. Also, explicit construction of Hessian matrices should be avoided.

4.1.2 Efficient Calculation of $\frac{db^{*}}{dv} \frac{dL}{dv} \frac{d\alpha^{*}}{dA}$

Fortunately, two computational tricks can be applied. Firstly, we can solve a single linear system instead of $N$ of them. We can express the desired gradient as

$$
\frac{db^{*}}{dv} \frac{dL}{dv} \frac{d\alpha^{*}}{dA} = -\frac{dL}{dv} \frac{d\alpha^{*}}{dA} \frac{d\alpha^{*}}{dA}^{-1} \frac{dL}{dv} \frac{d\alpha^{*}}{dA} \frac{d\alpha^{*}}{dA}.
$$

As $\frac{dL}{dv}$ is assumed available, we can first solve

$$
\left( \frac{dL}{dv} \frac{d\alpha^{*}}{dA} \right) v = \frac{dL}{dv} \frac{d\alpha^{*}}{dA} \frac{d\alpha^{*}}{dA},
$$

for $v$, and then left multiply by $-\frac{d\alpha^{*}}{dA}$ to get $\frac{db^{*}}{dv} \frac{dL}{dv} \frac{d\alpha^{*}}{dA}$.

Secondly, solving Equation 19 still requires us to solve a linear system involving an explicitly formed Hessian matrix, which in the case of calculating $\frac{dL}{dv} \frac{d\alpha^{*}}{dA}$, is $\frac{dL}{dv} \frac{d\alpha^{*}}{dA}$, of large size. However, matrix free linear system solvers such as conjugate gradient, when solving a linear system $Cz = d$, do not require $C$ to be explicitly given, but only that the matrix vector product $Cu$ be able to
be calculated for any vector \( u \). Furthermore, Hessian-vector products can generally be calculated efficiently. Returning to the example, note that for any \( u \),

\[
\left( \frac{d}{d\theta} \frac{df}{d\theta} \right) u = \frac{d}{d\theta} (u^T \frac{df}{d\theta}).
\]  

(20)

This means the requisite Hessian vector can be computed by first analytically forming the scalar valued function \( u^T \frac{df}{d\theta} \) and then calculating its gradient with respect to \( b \), or using finite differences: \( \left( \frac{d}{d\theta} \right) (b^*(w) + ru, w) = \frac{d}{d\theta} (b^*(w) - ru, w) / 2r \), with \( r \) a small scalar.

### 4.2 Gradient Descent over Projection Matrices

We use the package Pymanopt\[37\] to perform gradient descent over projection matrices using steepest descent with backtracking line search. As the problem is not convex in \( A \), we utilize multiple random restarts.

### 5 Simulation Study

We now show a synthetic data example involving covariate shift that shows the benefit of our method compared to other baselines. We generated 13-dimensional covariates and real valued labels. The labels only depend on the first two covariates, \( X_1 \) and \( X_2 \). In particular, we let \( Y | X \sim N(\|X_1\| + 0.2 \|X_2\|, 0.01) \). Figure 2a shows samples from \( P_{Y|X_1}^{tr} \) and \( P_{Y|X_1}^{te} \), and Figure 2b shows samples from \( P_{Y|X_2}^{tr} \) and \( P_{Y|X_2}^{te} \). Training samples are in blue, test samples are in orange. Thus for \( X_1 \) and \( X_2 \), the test distribution contains only positive values. The distributions of each covariate are independent of each other, generated as follows:

\[
\begin{align*}
X_1^{tr} & \sim 0.95 \text{Uniform}(-1, 0) + 0.05 \text{Uniform}(0,1) \\
X_1^{te} & \sim \text{Uniform}(0,1) \\
X_2^{tr} & \sim \text{Uniform}(-1, 1), \ X_2^{te} \sim \text{Uniform}(0,1) \\
X_1^{tr}, \ldots, X_{12}^{tr} & \sim 0.9 \text{Uniform}(-1, 0) + 0.1 \text{Uniform}(0,1) \\
X_1^{te}, \ldots, X_{12}^{te} & \sim 0.1 \text{Uniform}(-1, 0) + 0.9 \text{Uniform}(0,1) \\
X_1^{tr}, X_1^{te} & \sim \text{Uniform}(-1, 1)
\end{align*}
\]

Note that as our model class contains only linear models, when trained and tested on \( P_{tr} \), a model that only uses \( X_1 \) will have comparable (actually slightly better) performance compared to a model that only uses \( X_2 \). This is because even though \( X_2 \) appears more informative, the model class does not contain the “v-shaped” predictor that the mean of \( P_{tr}^{Y|X_1} \) follows. Contrarily, when trained and tested on \( P_{te} \), a model that uses only \( X_2 \) will have far superior performance to one that uses only \( X_1 \), because due to the covariate shift, the test covariates only have support under one of the two “arms” of the “v”. Also, \( X_{13} \), while not predictive, is identically distributed between training and test, so that an unsupervised method would recover it.

We compare our joint projection method, denoted \( JP(D) \), \( D \) being the subspace dimension, to:

- Unweighted (UW): performing no covariate shift correction, minimizing (regularized) unweighted loss over the training data
- Naive Importance Weighting (IW): Estimating full density ratio weights using LSIF (not the less accurate uLSIF), and minimizing (regularized) weighted loss over the training data.
- Random Projection to \( D \) dimensions (RP(\( D \))): Applying a random projection to generate \( D \)-dimensional covariates, and then applying IW to the projected data.
- Sliced Inverse Regression (SIR(\( D \))): Applying sliced inverse regression \[23\] to project to \( D \) dimensions, and then applying IW.
- Cheating (CT): Projecting the data to only retain the first two covariates, the only ones upon which the outcome depends, and then applying IW.

Table 1 shows the mean and standard deviation of out-of-sample test loss over 100 replicates for the methods, as \( N \), the number of generated training and test samples changes. To elaborate, we generate \( N \) samples each from \( P_{tr}^{Y|X_1} \) and \( P_{te}^{Y|X_1} \), set aside \( \frac{1}{N} \) of the test data for evaluation, fit a model using the \( N \) labelled training

![Figure 2](image-url)

(a) \( X_1 \) is moderately predictive in both the test and training distribution.
(b) \( X_2 \) is very predictive in the test distribution, but not very predictive in the training distribution.

| Method      | 50     | 100    | 150    | 200    |
|-------------|--------|--------|--------|--------|
| JP(1)       | .85(,82) | .40(,34) | .28(,32) | .27(,25) |
| UW          | 1.00(,36) | 1.00(,20) | 1.00(,16) | 1.00(,23) |
| IW          | 1.05(,39) | 1.06(,33) | 1.01(,23) | .95(,15) |
| SIR(1)      | 1.02(,42) | 1.02(,27) | .98(,22) | .96(,17) |
| SIR(2)      | 1.10(,44) | 1.01(,27) | .99(,20) | .98(,22) |
| RP(1)       | 1.02(,35) | .99(,17) | .99(,14) | .98(,13) |
| RP(2)       | 1.10(,44) | 1.11(,27) | 1.08(,27) | 1.03(,21) |
| CT          | .59(,39) | .83(,01) | .45(,23) | .30(,11) |
samples and remaining $\frac{2N}{3}$ unlabelled test samples, and then evaluate the predictions on the set aside test data. Losses are normalized so UW has a loss of 1 for each data size. We note the performance of IW is often worse than that of UW, due to the difficulty in estimating the weights and small sample size. Furthermore, the sliced inverse regression methods, which do not account for covariate shift in estimating the projection, do not find any subspace particularly informative and thus do about the same as the random projection methods. On the other hand, our method is able to jointly find that $X_2$ is most useful in the test domain, and learn an importance weighted model in the correct single dimension. For some data sizes, our method even does better than CT, which is told the ground truth that only $X_1$ and $X_2$ are relevant. Even though $Y$ does depend on both features, the combination of weights being harder to estimate and effective sample size being smaller in 2 dimensions versus 1 illustrates the benefit of joint dimension reduction and importance weighting.

6 Experiments with Real Data

6.1 Choosing Hyperparameters

The hyperparameters in the formulation fall into two groups: those whose optimal value does not change with $A$, namely $\lambda$, and those whose optimal value does change with $A$: $c$, which prevents overfitting, and those required for density ratio estimation, namely $\gamma$ as well as the bandwidth of the Gaussian kernel basis functions, which we refer to as $\sigma$. We do not consider the latter group of hyperparameters fixed, but instead update them throughout the gradient descent over $A$. We also note that by updating these hyperparameters as the optimization runs, they are no longer hyperparameters in the conventional sense. The reduced number of hyperparameters is thus computationally convenient.

The optimal values of $\gamma$ and $\sigma$ change with $A$ because they are used to obtain estimates $\hat{\lambda}_A(x_i^{tr})$ of $P(x_i^{tr} | A) / P(x_i^{tr} | \bar{A})$, which changes with $A$. Certainly, the hyperparameters of a density ratio estimation procedure should change as the true density ratios change. To choose $\gamma, \sigma$ for a given $A$, we use the cross validation procedure [13] suggest. As part of the procedure, a training holdout set $\{A_i x_i^{(h)tr}\}$ and test holdout set $\{A_i x_i^{(h)te}\}$ are removed from the projected training and test covariates $\{A_i x_i^{tr}\}, \{A_i x_i^{te}\}$, respectively. Given $\gamma, \sigma$, a density ratio function $\hat{\lambda}_A(x)$ is estimated using the remaining projected training and test data based on the uLSIF procedure (Equations 19 and 17), and the out of sample error is measured as

$$\frac{1}{2N^{(h)tr}} \sum_i \hat{\lambda}_A(x_i^{(h)tr})^2 - \frac{1}{N^{(h)tr}} \sum_i \hat{\lambda}_A(x_i^{(h)te}),$$

where $N^{(h)tr}, N^{(h)te}$ are the size of the holdout training and test sets, respectively. Note that this is simply the objective that LSIF and uLSIF minimize, without regularization, computed over the holdout set. This process can be repeated for the distinct holdout sets as given by K-fold cross validation, and the average error over the holdout sets can be minimized using grid search.

The optimal value of $c$ is presumed to change with $A$ for more practical reasons. Ideally, we would choose $c$ in order to minimize the expected test loss of the predictor, $f(x) = b^T A^T x$, obtained after solving the optimization problem. As labelled samples from the test distribution are not available in the problem setup, one can use a holdout set $\{x_i^{(h)tr}, y_i^{(h)tr}\}$ from the training data and compute an importance weighted loss, $\sum_i \hat{w}(x_i^{(h)tr}) L(b^T A^T x_i^{(h)tr}, y_i^{(h)tr})$, to approximate the expected test loss of the predictor obtained using the data not in the holdout set. However, this estimate, involving density ratios of the full covariate space, is exactly the high variance estimate our work seeks to avoid using. Instead, we measure the error on the holdout set as $\sum_i \hat{w}(x_i^{(h)tr}) L(b^T A^T x_i^{(h)tr}, y_i^{(h)tr})$, where the ratios are now those of the densities projected by $A$. As before, this measure of error can be averaged over distinct holdout sets, and minimized using grid search. Of course, as $A$ changes, the $\hat{\lambda}_A(x_i^{(h)tr})$ change, so that the optimal value of $c$ according to this criteria also changes, which is why we update $c$ as $A$ changes.

While $\sigma, \gamma$ are updated throughout a single optimization run, $\lambda$ is held fixed, and thus chosen by “traditional” out-of-sample validation. In particular, given training and test data to apply our model to, we first set aside a portion of $\{x_i^{tr}, y_i^{tr}\}$ to form a validation set $\{x_i^{(v)tr}, y_i^{(v)tr}\}$. We then evaluate a given $\lambda$ by fitting our model to obtain $A,b$, then examining the weighted loss $\sum_i \hat{w}(x_i^{(v)tr}) L(b^T A^T x_i^{(v)tr}, y_i^{(v)tr})$. This is the same weighted loss used in selecting $c$, used once again due to the naive test loss estimator being unreliable.

In summary, a validation portion of the labelled training data is set aside, and $\lambda$, the only “conventional” hyperparameter, is chosen to be the value whose resultant predictor has the lowest value of a loss estimate computed using the validation set and estimates of projected density ratios. The remaining hyperparameters $\gamma, \sigma, c$ are updated throughout the optimization procedure for a fixed $\lambda$ using grid search cross-validation.

6.2 Data Preprocessing

We took several datasets from [23, 1], and for each, introduced covariate shift by creating a sampling scheme that can repeatedly generate training and test data samples. For each dataset, we first identify a single predictive vector in covariate space by generating 100
random vectors, and measuring the predictive utility of a vector by projecting the covariates onto it, running kernel density regression, and examining the negative in-sample squared error. We first sample the dataset to form the training data. Then to generate the test data, we subsample from the remaining dataset according to the projections along the vector. Let \( t_1, t_0 \) denote the max and min projected covariate value in the dataset, and \( \sigma \) be the standard deviation of the projected values. We select data with probability proportional to the density of a \( N(\alpha(t_1 - t_0), \sigma^2) \) distribution based on their \( \alpha \) values. The effective sample size \( N_c \) is given by: \( N_c = \frac{1}{\alpha(1 - \alpha)} \). Table 2 shows the estimate of the test loss based on the 100 replicates; regression and classification datasets are on the top and bottom, respectively. We use squared and zero-one loss to evaluate regression and classification performance, respectively. The model parameters are the same as those used in Section 5 and performances are normalized for each dataset such that the unweighted baseline has a performance of 1.

### 6.3 Experimental Results

For each dataset, we generated 100 training and test data pairs. For each pair, we set aside \( \frac{1}{5} \) of the test data to evaluate out-of-sample performance on the test distribution, and train the model with the remaining data. For our method, \( \frac{1}{5} \) of the training data was used to tune \( \lambda \). Table 2 shows the estimate of the test loss based on the 100 replicates; regression and classification datasets are on the top and bottom, respectively. We use squared and zero-one loss to evaluate regression and classification performance, respectively. The model abbreviations are the same as those used in Section 5 and performances are normalized for each dataset such that the unweighted baseline has a performance of 1.

We see the trend is when naive importance weighting (IW) helps relative to the unweighted baseline (UW), indicating the necessity of covariate shift adjustment, our method tends to improve over IW, and has lower variance, reflecting the benefit of our method’s lower variance estimator. In particular, when our method helps a lot, the variance is reduced significantly, as in the splice, diabetes, abalone, and kin-8fm datasets. When IW does not improve over UW, IW tends to have higher variance. In those situations, our method does not always help, but tends to still have lower variance. In general, our method uses a biased estimator in return for reduced variance. Here we see that in many real data, this tradeoff is worthwhile to make both in terms of average performance and the variance thereof.

### 7 Conclusion

To address the high variance of importance weighting approaches to handling covariate shift, we have presented a method that jointly learns a subspace upon which predictions depend, and within which density ratios are estimated. Our method lowers variance through estimating ratios in a reduced space, as well as a regularizer discouraging subspaces with low effective sample sizes whose tradeoff parameter can be cross-validated. To fit our model, we leverage past work on hyperparameter selection via gradient descent. We explain through lemmas why the variance is reduced and the extent of our test loss estimator’s bias, and then show empirically that in many real data, sacrificing bias for reduced variance helps performance. Finally, we believe our work has implications for causal inference, which can be formulated as a covariate shift problem, and where the propensity score, essentially a density ratio, is used widely yet unreliably estimated in higher dimensions.
References

[1] Libsvm datasets. http://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/

[2] Brandon Amos and J Zico Kolter. Optnet: Differentiable optimization as a layer in neural networks. arXiv preprint arXiv:1703.00443, 2017.

[3] Peter C Austin. An introduction to propensity score methods for reducing the effects of confounding in observational studies. Multivariate behavioral research, 46(3):399–424, 2011.

[4] Yoshua Bengio. Gradient-based optimization of hyperparameters. Neural computation, 12(8):1889–1900, 2000.

[5] Steffen Bickel, Michael Brückner, and Tobias Scheffer. Discriminative learning under covariate shift. Journal of Machine Learning Research, 10(Sep):2137–2155, 2009.

[6] John Blitzer, Ryan McDonald, and Fernando Pereira. Domain adaptation with structural correspondence learning. In Proceedings of the 2006 conference on empirical methods in natural language processing, pages 120–128. Association for Computational Linguistics, 2006.

[7] Olivier Chapelle, Vladimir Vapnik, Olivier Bousquet, and Sayan Mukherjee. Choosing multiple parameters for support vector machines. Machine learning, 46(1):131–159, 2002.

[8] Bo Chen, Wai Lam, Ivor Tsang, and Tak-Lam Wong. Extracting discriminative concepts for domain adaptation in text mining. In Proceedings of the 15th ACM SIGKDD international conference on Knowledge discovery and data mining, pages 179–188. ACM, 2009.

[9] Xiangli Chen, Mathew Monfort, Anqi Liu, and Brian D Ziebart. Robust covariate shift regression. In Artificial Intelligence and Statistics, pages 1270–1279, 2016.

[10] Corinna Cortes, Yishay Mansour, and Mehryar Mohri. Learning bounds for importance weighting. In Advances in neural information processing systems, pages 442–450, 2010.

[11] Arnaud Doucet, Nando De Freitas, and NJ Gordon. Sequential monte carlo methods in practice. series statistics for engineering and information science, 2001.

[12] Chuan-sheng Foo, Chuong B Do, and Andrew Y Ng. Efficient multiple hyperparameter learning for log-linear models. In Advances in neural information processing systems, pages 377–384, 2008.

[13] Kenji Fukumizu, Francis R Bach, and Michael I Jordan. Kernel dimension reduction in regression. The Annals of Statistics, pages 1871–1905, 2009.

[14] Arthur Gretton, Karsten M Borgwardt, Malte Rasch, Bernhard Schölkopf, and Alex J Smola. A kernel method for the two-sample-problem. In Advances in neural information processing systems, pages 513–520, 2006.

[15] Arthur Gretton, Alex Smola, Jiayuan Huang, Marcel Schmittfull, Karsten Borgwardt, and Bernhard Schölkopf. Covariate shift by kernel mean matching. 2009.

[16] Weihua Hu, Issei Sato, and Masashi Sugiyama. Robust supervised learning under uncertainty in dataset shift. arXiv preprint arXiv:1611.02041, 2016.

[17] Fredrik Johansson, Uri Shalit, and David Sontag. Learning representations for counterfactual inference. In International Conference on Machine Learning, pages 3020–3029, 2016.

[18] Takafumi Kanamori, Shohei Hido, and Masashi Sugiyama. A least-squares approach to direct importance estimation. Journal of Machine Learning Research, 10(Jul):1391–1445, 2009.

[19] Joseph DY Kang and Joseph L Schafer. Demystifying double robustness: A comparison of alternative strategies for estimating a population mean from incomplete data. Statistical science, pages 523–539, 2007.

[20] S Sathiya Keerthi, Vikas Sindhwani, and Olivier Chapelle. An efficient method for gradient-based adaptation of hyperparameters in svm models. In Advances in neural information processing systems, pages 673–680, 2007.

[21] Pang Wei Koh and Percy Liang. Understanding black-box predictions via influence functions. arXiv preprint arXiv:1703.04730, 2017.

[22] Ron Kohavi and George H John. Wrappers for feature subset selection.

[23] Ker-Chau Li. Sliced inverse regression for dimension reduction. Journal of the American Statistical Association, 86(414):316–327, 1991.

[24] M. Lichman. UCI machine learning repository, 2013.

[25] Anqi Liu and Brian Ziebart. Robust classification under sample selection bias. In Advances in neural information processing systems, pages 37–45, 2014.
[26] Dougal Maclaurin, David Duvenaud, and Ryan Adams. Gradient-based hyperparameter optimization through reversible learning. In *International Conference on Machine Learning*, pages 2113–2122, 2015.

[27] Dougal Maclaurin, David Duvenaud, and Ryan P Adams. Autograd: Reverse-mode differentiation of native python. In *ICML workshop on Automatic Machine Learning*, 2015.

[28] Sinno Jialin Pan, Ivor W Tsang, James T Kwok, and Qiang Yang. Domain adaptation via transfer component analysis. *IEEE Transactions on Neural Networks*, 22(2):199–210, 2011.

[29] Christian Pölitz, Wouter Duivesteijn, and Katharina Morik. Interpretable domain adaptation via optimization over the stiefel manifold. *Machine Learning*, 104(2-3):315–336, 2016.

[30] Sashank Jakkam Reddi, Barnabas Poczos, and Alexander J Smola. Doubly robust covariate shift correction. 2015.

[31] Irina Rish, Genady Grabarnik, Guillermo Cecchi, Francisco Pereira, and Geoffrey J Gordon. Closed-form supervised dimensionality reduction with generalized linear models. In *Proceedings of the 25th international conference on Machine learning*, pages 832–839. ACM, 2008.

[32] Hidetoshi Shimodaira. Improving predictive inference under covariate shift by weighting the log-likelihood function. *Journal of statistical planning and inference*, 90(2):227–244, 2000.

[33] Masashi Sugiyama, Satoshi Hara, Paul Von Bünau, Taiji Suzuki, Takafumi Kanamori, and Motoaki Kawanabe. Direct density ratio estimation with dimensionality reduction. In *Proceedings of the 2010 SIAM International Conference on Data Mining*, pages 595–606. SIAM, 2010.

[34] Masashi Sugiyama, Shinichi Nakajima, Hisashi Kashima, Paul V Buenau, and Motoaki Kawanabe. Direct importance estimation with model selection and its application to covariate shift adaptation. In *Advances in neural information processing systems*, pages 1433–1440, 2008.

[35] Masashi Sugiyama, Makoto Yamada, Paul Von Buenau, Taiji Suzuki, Takafumi Kanamori, and Motoaki Kawanabe. Direct density-ratio estimation with dimensionality reduction via least-squares hetero-distributional subspace search. *Neural Networks*, 24(2):183–198, 2011.

[36] Taiji Suzuki and Masashi Sugiyama. Sufficient dimension reduction via squared-loss mutual information estimation. In *Proceedings of the Thirteenth International Conference on Artificial Intelligence and Statistics*, pages 804–811, 2010.

[37] James Townsend, Niklas Koep, and SebastianWiechwald. Pymanopt: A python toolbox for optimization on manifolds using automatic differentiation. *Journal of Machine Learning Research*, 17(137):1–5, 2016.

[38] Kush R Varshney and Alan S Willsky. Learning dimensionality-reduced classifiers for information fusion. In *Information Fusion, 2009. FUSION’09. 12th International Conference on*, pages 1881–1888. IEEE, 2009.

[39] Weiran Wang and Miguel Á Carreira-Perpiñán. The role of dimensionality reduction in classification. In *Proceedings of the Twenty-Eighth AAAI Conference on Artificial Intelligence*, pages 2128–2134. AAAI Press, 2014.

[40] Junfeng Wen, Chun-nam Yu, and Russell Greiner. Robust learning under uncertain test distributions: Relating covariate shift to model misspecification. In *Proceedings of the 31st International Conference on Machine Learning (ICML-14)*, pages 631–639, 2014.

[41] Makoto Yamada, Taiji Suzuki, Takafumi Kanamori, Hirotaka Hachiya, and Masashi Sugiyama. Relative density-ratio estimation for robust distribution comparison. In *Advances in neural information processing systems*, pages 594–602, 2011.