Predictive Optimization
with Zero-Shot Domain Adaptation

Tomoya Sakai\textsuperscript{1,2} and Naoto Ohsaka\textsuperscript{1}

\textsuperscript{1}NEC Corporation
\textsuperscript{2}RIKEN
\{tomoya_sakai, ohsaka\}@nec.com

Abstract

Prediction in a new domain without any training sample, called zero-shot domain adaptation (ZSDA), is an important task in domain adaptation. While prediction in a new domain has gained much attention in recent years, in this paper, we investigate another potential of ZSDA. Specifically, instead of predicting responses in a new domain, we find a description of a new domain given a prediction. The task is regarded as predictive optimization, but existing predictive optimization methods have not been extended to handling multiple domains. We propose a simple framework for predictive optimization with ZSDA and analyze the condition in which the optimization problem becomes convex optimization. We also discuss how to handle the interaction of characteristics of a domain in predictive optimization. Through numerical experiments, we demonstrate the potential usefulness of our proposed framework.

Keywords— Predictive optimization, Zero-shot domain adaptation, Convex optimization

1 Introduction

Prediction in a new domain without any training samples, called zero-shot domain adaptation (ZSDA) ([Yang and Hospedales, 2015a,b]), is an important task in domain adaptation. To this end, an approach to utilize domain descriptions ([Yang and Hospedales, 2015a,b]), called domain attributes, has been developed. A goal of ZSDA is to obtain predictions in an unseen domain in which we did not observe any training samples. An application of ZSDA is the sales prediction of new products; regarding domains as products and given product attributes and sales data, we can use ZSDA to the sales prediction of a customer for a new product. Thanks to ZSDA, we can predict the response of input in an unseen domain; however, one potential aspect of ZSDA has been overlooked.

We demonstrate another potential of ZSDA; by reversing the ZSDA prediction process, we can optimize domain attributes so that an evaluation metric of responses over customers is maximized, referred to as attribute optimization as shown in Figure 1. That is, instead of predicting responses given new domain attributes as in ZSDA, our task is to find new domain attributes given a prediction. In our example of new product prediction, we optimize an average
of new product sales with respect to product attributes over a pre-specified customer group. The obtained product attributes would be useful for designing a new product.

Our attribute optimization task can be regarded as predictive optimization (Ito and Fujimaki, 2017; Donti et al., 2017; Ito et al., 2018), in which the goal is to optimize predicted outputs in terms of input variables. There are various applications of predictive optimization: water distribution management (Žliobaite and Pechenizkiy, 2010), retail price optimization (Ito and Fujimaki, 2016, 2017), and grid scheduling (Donti et al., 2017). However, existing studies of predictive optimization mainly focus on a single domain, and the case of multiple domains has yet to be considered. While we can use existing methods for each domain independently, it would not exploit the structures and similarities across multiple domains. Moreover, it is not straightforward to optimize domain attributes for finding, e.g., a promising product in existing methods.

In this paper, we propose a novel simple framework for attribute optimization. Given domain attributes, inputs, and responses, our framework first trains a prediction function and then optimizes a measure computed by predicted outputs to find a new domain attribute. Our method can handle continuous and discrete domain attributes and concave measure functions as objective functions. Moreover, it can deal with cases when two or more domain-attribute variables are dependent, i.e., the interaction of domain attributes. By regarding domains as objects, domain attributes as designs, and objective functions as sales, quality, or durability, we use attribute optimization to discover the design of new best-selling, high-quality, and durable objects. Our attribute optimization framework can be applied to the following concrete tasks:

• **New product design:** Consider that we are given sales, consumer features, and product characteristics data to design a new product by combining best-selling products’ ingredients. Our framework easily satisfies this demand by regarding domains as products, domain attributes as product characteristics, features as consumer features, and the objective function as sales.

• **New tourist spot design:** Suppose that we are given reputations of tourist spots, tourist features, and characteristics of tourist spots data to design a new tourist spot on the basis of characteristics of tourist spots. Our framework easily fits this task by regarding a domain as a tourist spot, domain attributes as characteristics of a tourist spot, features as tourist features, and the objective function is the average reputation.

Our technical contributions for achieving the above-mentioned attribute optimization framework are as follows:

• We propose a simple framework for attribute optimization. The main components of our framework are training predictors (ZSDA) and subsequent mathematical optimization (Sections 4.1 and 4.2).
• We devise conditions on objective functions and constraints whose corresponding optimization problem can be cast to convex optimization, which is quickly solvable by off-the-shelf solvers (Section 4.3).
• We provide practical examples of objective functions and constraints that meet the devised conditions (Section 5).
• We describe how to handle interactions between domain-attribute variables. We show that the second-order interaction of 0-1 domain attributes can be relaxed to semidefinite programming (Section 6).
• We establish theoretical analyses of the proposed framework, which bounds the generalization error of the prediction method and approximation factors of the optimization method (Section 7).
• We demonstrate the potential usefulness of our proposed method on synthetic and benchmark datasets (Section 8).

2 Related work

2.1 Predictive optimization

Predictive optimization has been applied to several real-world applications such as water distribution management (Žliobaite and Pechenizkiy, 2010), retail price optimization (Ito and Fujimaki, 2016, 2017), grid scheduling (Donti et al., 2017), and inventory optimization (Ohsaka et al., 2020). In existing work, a set of input-output samples is collected from a target domain; we train a prediction function and then optimize features of input to maximize a certain measure of output in the target domain. For example, in price optimization, we have sales for each item at a certain price. We first train a model to output the sales of an item from a price. We then optimize the prices of items such that the total sales is maximized. In existing work, the way of using item information, i.e., domain attributes, is not considered. In addition, prediction and optimization including features of input and domain attributes are not trivial.

In contrast, our approach optimizes domain attributes to maximize a certain measure of output for a set of fixed input samples. In other words, we can find a prospective target domain for specific input samples through the optimized domain attributes. Moreover, existing studies often consider a single domain while our study considers multiple domains. To the best of our knowledge, this is the first study of predictive optimization for multiple domains with its attribute information.

2.2 Data-driven design

An application of our method is data-driven design for new products. For this purpose, several methods based on machine learning have been proposed recently (Koutra et al., 2017; Kang et al., 2017; Vo and Soh, 2018). Among them, Koutra et al. (2017) is related to our problem setting, which considers multiple domains. They also considered optimization of a domain for fixed target users and applied their method to movie design for target users by regarding a domain as a movie. The method learns user-preferences through a tripartite graph of users, movies, and movie attributes. The movie attributes are optimized by a greedy approach, which is optimal under specific assumptions (Koutra et al., 2017).

Compared with the work of (Koutra et al., 2017), our method is not limited to data having graph structures and enables us to use various prediction models and optimization algorithms,
as shown in Section 4. In addition, we demonstrate the effectiveness of our method on various real-world datasets in Section 8.

3 Background

3.1 Problem settings

Let $x(t) \in \mathbb{R}^d$ be a feature vector and $y(t) \in \mathbb{R}$ be a response in a domain $t \in \{1, \ldots, T\}$, where $d$ is a positive integer and $T$ denotes the number of domains. We have a set of observations $\mathcal{D}(t) := \{(x_i^{(t)}, y_i^{(t)})\}_{i=1}^{n(t)}$ for each $t$, where $n(t)$ is the number of samples in $t$. For each domain, we assume that a description of a domain is available and they can be expressed as $m$ domain-attribute variables. We denote a domain-attribute vector for $t$ by $a(t) \in \mathbb{R}^m$ and a set of domain-attribute vectors by $\mathcal{A} := \{a(t)\}_{t=1}^{T}$. We define a dataset as $\mathcal{D} := \{(\mathcal{D}(t), a(t))\}_{t=1}^{T}$.

Let $g: \mathbb{R}^d \times \mathbb{R}^m \rightarrow \mathbb{R}$ be a prediction function and $\mathcal{B}$ be a set of target feature vectors. Let $f$ be an objective function that returns a gain of a domain described by $a$. That is, we measure the value in a domain through $f(a)$. An example of $f$ is a mean response: $f(a) = (1/|\mathcal{B}|) \sum_{x \in \mathcal{B}} g(x, a)$, where $|\cdot|$ denotes the size of a set.

The goal of the attribute optimization problem is to find a new domain-attribute vector optimized for a gain function.

3.2 Feature-unaware approach (FUA)

An approach to optimize domain attributes is that we first learn a function from $a(t)$ to, e.g., the mean of $\{y_i^{(t)}\}_{i=1}^{n(t)}$, and then find $a$ which maximizes the learned function. We call the above approach the feature-unaware approach (FUA). Specifically, let $\overline{y}(t)$ be the average of responses of domain $t$. As a function, we use a linear model defined as $s(a) = w^\top a$, where $w \in \mathbb{R}^m$ is the parameter vector. We then train $s$ with $\{(a(t), \overline{y}(t))\}_{t=1}^{T}$ by, say, regularized least squares, i.e., ridge regression. Let $\hat{w}$ be the estimated parameter obtained after training. To optimize domain attributes, an approach is to select a domain-attribute variable whose corresponding weight of $\hat{w}$ to satisfy the user-defined and system-derived constraints. Another approach is to formulate an optimization problem and solve it.

The FUA is simple, but it ignores dependence on features $x$. We thus cannot optimize domain-attributes for each $x$ or a group of $x$, and cannot use the measure taking a distribution of features into account, which will be introduced in Section 5.1. Moreover, since the number of training samples is $T$, the use of complex models, such as neural networks, for $s$ leads to ill-posed problems, resulting in that an inaccurate estimation of response. In contrast, our proposed approach takes features of input into account. Moreover, we can use complex models for estimating response since the number of training samples is much larger than the FUA.

4 Proposed method

Our method consists of two steps: i) a prediction step that estimates a prediction function from $\mathcal{D}$, and ii) an optimization step that solves an optimization problem under a user-preferred gain function.
4.1 Prediction step

In the prediction step, we train a parameterized prediction function, \( g \), with a training dataset \( D \). A simple example of \( g \) is \( g(x, a) = x^\top \Theta a \), where \( \Theta \in \mathbb{R}^{d \times m} \) are the parameters to be learned.

For a fixed domain-attribute vector \( a^{(t)} \), we can regard \( g \) as a prediction function for a specific domain \( t \), e.g., \( g^{(t)} : \mathbb{R}^d \to \mathbb{R} \).

Let \( \ell : \mathbb{R} \times \mathbb{R} \to \mathbb{R}_\geq \) be a loss function. By solving the following optimization problem, we obtain a learned prediction function as

\[
\hat{g} := \text{argmin}_g \frac{1}{T} \sum_{t=1}^{T} \frac{1}{n(t)} \sum_{i=1}^{n(t)} \ell(g(x^{(t)}_i, a^{(t)}_i), y^{(t)}_i) + \lambda W(g),
\]

where \( W \) is the regularization functional and \( \lambda \geq 0 \) is the regularization parameter.

With the learned prediction function, we can estimate a response of \( x \) even in a domain never seen before. Let \( a' \) be a domain-attribute vector for an unseen domain. We can obtain a prediction in a domain that did not appear in a training dataset as \( \hat{g}(x, a') \).

Our idea is to reverse the aforementioned prediction process for finding a new domain-attribute vector that is likely to get a high gain as shown in Figure 1. That is, instead of obtaining a prediction given \( a \), we find \( a \) such that a prediction-based gain function is maximized.

4.2 Optimization step

After we obtained a learned prediction function \( \hat{g} \), we move on to the optimization step. As \( B \) is a set of target feature vectors, we can regard it as a set of target users. On the basis of \( \hat{g} \), we compute an estimate of an objective function \( \hat{f} \).

For a user-preferred gain function, we can find a promising domain-attribute vector by solving the following optimization problem:

\[
\max_{a \in \mathbb{R}^m} \hat{f}(a)
\]

s. t. \( b_j(a) \leq 0, \quad j = 1, \ldots, s \) \( c_j(a) = 0, \quad j = 1, \ldots, t \),

where \( b_j \) and \( c_j \) are an inequality and equality constraint function, respectively. An example of a constraint is a budget constraint; if \( a \) is the 0-1 vector and \( \gamma \in \mathbb{R}_\geq^m \) is defined as a cost vector, a budget constraint can be expressed as \( a^\top \gamma \leq C \), where \( C \) is the user-specified constant.

By solving the optimization problem in Eq. (1), we obtain a domain-attribute vector that is potentially new and will achieve a high gain. In the subsequent section, we explain the conditions in which the optimization problem can be solved efficiently.

4.3 Linear-in-attribute model (LAM)

In this section, we reveal conditions in which an optimization problem is regarded as a convex optimization problem.

We first define a model of a prediction function:

**Definition 4.1** (Linear-in-attribute model). A linear-in-attribute model (LAM) is defined as

\[
g(x, a) = a^\top \phi(x),
\]

where \( \phi(x) := (\phi_1(x), \ldots, \phi_m(x))^\top \in \mathbb{R}^m \) is a basis function vector whose parameters are to be learned with training data and \( ^\top \) denotes the transpose of a vector or matrix.
We denote the learned basis function vector by \( \hat{\phi} \); an estimated response function is expressed as \( \hat{g}(x, a) = a^\top \hat{\phi}(x) \).

Let \( h : \mathbb{R}^d \to \mathbb{R} \) be a prediction function. We then define a functional computing gain given \( h \).

**Definition 4.2 (Aggregate functional).** An aggregate functional \( F \) computes gain from \( h \) and \( B \). That is, the computed gain is given by \( F(h; B) \). For the sake of brevity, we omit the notation \( B \) and use \( F(h) \).

Let us denote \( g(\cdot, a) \) by \( g_a : \mathbb{R}^d \to \mathbb{R} \). A gain function is expressed as \( f(a) = F(g_a) \). We then have the following proposition that characterizes a gain function:

**Proposition 4.1.** If \( F \) is a concave function and \( g \) is a LAM, the gain function \( f \) is concave.

**Proof.** Without loss of generality, we assume \( d = 1 \). The second derivative of \( f \) with respect to \( a \) is given by \( \partial^2_a f = \partial^2_a g \cdot F + \partial^2 g_a F \partial^2 g \), where \( \partial_a g = \frac{\partial}{\partial a} \) and \( \partial g_a = \frac{\partial}{\partial g_a} \). The second term becomes zero because \( g \) is linear in attributes, i.e., \( \partial^2 g \) is linear. Since \( F \) is concave, \( \partial^2_a F \leq 0 \). The first term is thus non-positive. Then, \( \partial^2_a f \leq 0 \), concluding that \( f \) is concave.

Proposition 4.1 leads to the following corollary:

**Corollary 4.1.1.** If a LAM, \( g \), and convex constraints, \( b_j \) and \( c_j \), are used and \( F \) is concave, the optimization problem in Eq. (1) is a convex optimization problem.

For convex optimization problems, we can use efficient off-the-shelf solvers to obtain a solution. In Section 5.1 and 5.2, we introduce useful candidates of \( F \), \( b_j \), and \( c_j \). Note that for higher accuracy, one can use non-convex models, rather than LAM, and use Bayesian optimization (Mockus et al., 1978), but we do not pursue that direction because non-convex optimization is often time-consuming than convex optimization.

## 5 Examples of objective functions and constraints

### 5.1 Aggregate functionals

We introduce concave aggregate functionals. Recall that \( h : \mathbb{R}^d \to \mathbb{R} \) is a prediction function.

**Mean response:** A standard choice of \( F \) is a mean response defined as

\[
F(h) = \frac{1}{|B|} \sum_{x \in B} h(x).
\]

With \( g \), the mean response with respect to \( a \) is expressed as \( f(a) = (1/|B|) \sum_{x \in B} g(x, a) \). For simplicity, we refer to the mean response aggregate functional as the mean gain function. A mean response can be interpreted easily; in our example of product sales prediction, maximization of a mean response over all users with respect to \( a \) corresponds to finding a product that is likely to be preferred by all users on average.

On the implementation side, a mean response is linear, resulting in \( f \) being concave by Proposition 4.1. It thus enables us to obtain a solution efficiently under convex constraints.
Conditional value at risk (CVaR):  A mean response is simple and a standard choice but it
does not take into account a distribution of responses. In practical applications, we are sometimes
interested in a tail of a distribution, in particular, a group of customers whose responses are
relatively lower than others. If we maximize an objective that can capture a left tail of a response
distribution, it corresponds to avoiding the situation in which users will put a lower rating on an
object.

To treat a left tail of a response distribution, we can use conditional value at risk (CVaR)
(Rockafellar and Uryasev, 2000, 2002) at a significance level $0 < \beta < 1$, defined as
\[
\text{CVaR}_\beta(h) := \max_{\tau \in \mathbb{R}} \left( \tau - \frac{1}{\beta|B|} \sum_{x \in B} \max(0, \tau - h(x)) \right).
\]

For brevity, we refer to the CVaR-based aggregate functional as the CVaR-based gain function.

A useful property of CVaR is concavity; the CVaR-based gain function with the LAM
becomes concave from Proposition 4.1.

5.2 Constraints

In this section, we introduce constraints that can be used in practical applications.

Continuous domain attributes:  If a domain-attribute variable is a continuous value and
a mean response is used as an objective function, we can maximize the objective function as
much as we can by increasing the magnitude of the domain-attribute variable; it is, however,
meaningless. To avoid such a useless solution, we normalize a domain-attribute vector and add a
constraint such that an obtained solution is also normalized.

More specifically, we first preprocess all the continuous domain-attribute vector in training
data such that $\|a\|_2^2 = 1$,\footnote{If the domain-attribute vector consists of continuous and (after-mentioned) categorical variables, we
split the vector into a continuous and a categorical domain-attribute part and apply normalization to
the continuous part.} and then add $\|a\|_2^2 = 1$ as constraints to an optimization problem. As
long as the objective function and other constraints are convex, the optimization problem with
the constraint $\|a\|_2^2 = 1$ is still a convex optimization problem. To be precise, the optimization
problem is second-order cone programming (Boyd and Vandenberghe, 2004).

Categorical domain attribute:  In a number of applications, we may want to use a categor-
tical type of variable as a domain attribute. We can encode such a categorical variable to a 0-1
vector, called the encoded domain attribute, as a binary domain attribute. However, optimization
over binary variables results in a 0-1 integer programming, which is NP-hard. We thus use a
relaxation technique to avoid solving NP-hard optimization problems.

If $m$ categories are encoded as an $m$-dimensional domain-attribute vector, choosing $k$ from
$m$ categories can be expressed as convex constraints: $0 \leq a_j \leq 1$ and $\sum_{j=1}^m a_j = k$. After
solving the optimization problem, we round the obtained solution to binary variables. By the
relaxation, we can handle categorical domain attributes under a convex optimization framework.

Budget limitation:  In practice, we may need to pay attention to the cost of a domain-
attribute variable. Suppose that a domain-attribute vector is element-wise non-negative, i.e.,
a_j \geq 0, j = 1, \ldots, m. Let $C$ be a total budget and $\gamma \in \mathbb{R}^m$ be a cost vector whose each element
is a cost of using a corresponding domain-attribute variable. To reflect budget limitation, we add
the convex constraint $a^\top \gamma \leq C$ as a budget limitation to an optimization problem.
6 Interaction of domain attributes

Interaction of domain attributes, i.e., the dependency of variables, is important, in practice. In this section, we explain the means to handle interactions of domain attributes.

LAM with domain-attribute interaction: One approach is to make an interaction term, e.g., \(a_ja_{j'}\) for \(j \neq j'\), and use the extended domain-attribute vector by concatenating these interaction terms with the original domain-attribute vector. Then, we can use the LAM, meaning that Proposition 4.1 holds. For example, if we are interested in the second-order interaction only, the extended domain-attribute vector is simply expressed as \(\bar{a} \otimes \bar{a}\), where \(\bar{a} := (\mathbf{a}^\top, 1)^\top\) and \(\otimes\) denotes the Kronecker product.\(^2\) The prediction model taking the second-order interaction into account is still linear in the extended domain-attribute vector \(a \otimes a\); by redefining \(a = \bar{a} \otimes \bar{a}\),
\[
g(x, a) = \mathbf{a}^\top \bar{\phi}(x),
\]
where \(\bar{\phi}(x) := (\phi_1(x), \ldots, \phi_{(m+1)^2}(x))^\top \in \mathbb{R}^{(m+1)^2}\). Although the LAM can be extended to handle domain-attribute interactions, we use the LAM without domain-attribute interactions in our experiments. This is because we next develop a model for handling the interaction of domain attributes efficiently.

Semidefinite programming approach: In Section 5.2, we explained the relaxation approach for a binary domain attribute, i.e., the constraint \(a \in \{0,1\}\) is relaxed to \(0 \leq a \leq 1\). While the relaxation approach is useful, if our interest is the second-order interaction of binary domain attributes, we can use the theoretically-supported algorithm (Ito and Fujimaki, 2017) inspired by the Goemans and Williamson’s MAX-CUT approximation algorithm (Goemans and Williamson, 1995).

Since the original purpose of the algorithm developed by (Ito and Fujimaki, 2017) is for price optimization, we modify it for the domain attribute optimization problem. To this end, let us first define the model taking into account the second-order binary domain-attribute interaction as

**Definition 6.1 (Quadratic-in-binary-attribute model).** A quadratic-in-binary-attribute model (QBM) is defined as
\[
g(x, a) = \sum_{j=1}^{m} \sum_{j'=1}^{m} a_j a_{j'} \left( \sum_{q=1}^{r} \phi_q^{(j)}(x) \phi_q^{(j')}(x) \right),
\]
where \(\phi_q : \mathbb{R}^d \to \mathbb{R}\) is a basis function to be learned and \(r\) is a positive integer that controls flexibility of the QBM, similarly to factorization machines (Rendle, 2010). Note that in the binary domain attribute case, a linear term, i.e., \(\mathbf{a}^\top \phi(x)\), is included in the quadratic term because of \(a_j^2 = a_j\) for any \(j \in \{1, \ldots, m\}\).

We can check that the QBM can be expressed as \(g(x, a) = \mathbf{a}^\top \Phi(x) \mathbf{a}\), where \(\Phi(x)_{j,j'} = \phi_j(x)^\top \phi_{j'}(x)\). \(\Phi(x) = (\phi_1^{(1)}(x), \ldots, \phi_r^{(r)}(x))^\top \in \mathbb{R}^r\). The QBM with linear constraints is binary quadratic programming (BQP), which is difficult to optimize in general. However, for certain special cases, we can solve BQP efficiently.

We next introduce a constraint to domain-attribute vectors:

**Definition 6.2 (Choice constraint).** For a set of indices \(\mathcal{I}\), a choice constraint is \(\sum_{j \in \mathcal{I}} a_j = 1\).

\(^2\)For vectors \(\mathbf{a} \in \mathbb{R}^{m_1}\) and \(\mathbf{b} \in \mathbb{R}^{m_2}\), \(\mathbf{a} \otimes \mathbf{b} = (a_1 \mathbf{b}^\top, a_2 \mathbf{b}^\top, \ldots, a_{m_1} \mathbf{b}^\top)^\top \in \mathbb{R}^{m_1m_2}\).
Hereafter, if we use the choice constraints, we assume that the index sets for the choice constraints satisfies the following condition: The index sets \( \{I_p\}_{p=1}^m \) satisfies \( \sum_{p=1}^m |I_p| = m \), where \(|\cdot|\) denotes the size of a set.

For the mean response and the QBM with the choice constraints, the BQP optimization problem can be relaxed to the following semidefinite programming (SDP):

\[
\begin{align*}
\text{max.} \quad & \text{tr}(C^T Y) \\
\text{s.t.} \quad & Y_{j,j} = 1, \quad j = 1, \ldots, m + 1 \\
& \sum_{j \in I_p} Y_{j,m+1} = 2 - |I_p|, \quad p = 1, \ldots, m \\
& \sum_{j \in I_p} \sum_{j' \in I_p'} Y_{j,j'} = (2 - |I_p|)(2 - |I_p'|), \\
& p, p' = 1, \ldots, m,
\end{align*}
\]

where \( S_m^{m+1} \) is the set of real symmetric semidefinite matrices of size \( m + 1 \) (Boyd and Vandenberghe, 2004),

\[
C := \frac{1}{4} \begin{pmatrix}
\bar{C} & \bar{C} 1_m \\
1_m^T & 1_m^T 1_m
\end{pmatrix} \in S_m^{m+1},
\]

\( \bar{C} := (1/|B|) \sum_{x \in B} \sum_{t=1}^{r_x} \phi(t)(x) \phi(t')(x) \), and \( 1_m \) is the \( m \)-dimensional all-ones vector. We round the obtained solution to the binary domain-attribute vector on the basis of the randomized search algorithm proposed in (Ito and Fujimaki, 2017).

An advantage of the SDP formulation is that if we further add convex constraints to the optimization problem in Eq. (3), the optimization problem is still SDP. Thus, thanks to the SDP formulation, we can obtain the solution efficiently rather than solving the BQP.

7 Theoretical analyses

In this section, we present two theoretical properties of our proposed algorithm. Specifically, in Section 7.1, we show generalization error bounds of the prediction method used in Section 4.1. In Section 7.2, we present approximation factors of the optimization method used in Section 4.2. All the proofs are given in Appendix A.

7.1 Generalization error bound

In this analysis, we consider the case where the feature mapping function can be expressed as \( \phi(x) = W \psi(x) \), where \( W \in \mathbb{R}^{m \times b} \) is the parameter matrix, \( \phi: \mathbb{R}^d \to \mathbb{R}^b \) is the vector of basis functions, i.e., \( \psi(x) = (\psi_1(x), \ldots, \psi_b(x))^T \), and \( \{\psi \in \mathbb{R}^d \to \mathbb{R}^b\} \) is fixed in advance. Then, LAM can be expressed as the bilinear function model \( g(x, a) = a^T W \psi(x) \).

The key idea is to reformulate the prediction model \( g \) into

\[ h(\bar{x}) = \bar{w}^T \bar{x}, \]

where \( \bar{w} := \text{vec}(W^T) \in \mathbb{R}^{dm}, \bar{x}_i := \text{vec}(\psi(x_i^{(t)})(a^{(t)})^T) \in \mathbb{R}^{dm} \), and \( i' = i + \sum_{t'=1}^{t-1} n(t') \). Accordingly, we express a set of training samples drawn from a distribution \( Q \) as \( \{(x_i, y_i)\}_{i=1}^n \).
where $n = \sum_{t=1}^{T} n^{(t)}$. We assume that there exists the target labeling function $f_{Q}: \mathbb{R}^{dm} \rightarrow \mathbb{R}$, $y_{i} = f_{Q}(\bar{x}_{i})$. We next respectively define the expected and empirical risks as $J_{Q}(h) := E_{Q} [\ell(h(\bar{x}), f_{Q}(\bar{x}))]$ and $\hat{J}_{Q}(h) := \frac{1}{n} \sum_{i=1}^{n} \ell(h(\bar{x}_{i}), f_{Q}(\bar{x}_{i}))$, where $E_{Q}$ is the expectation over $Q$.

We also assume the $\ell_{q}$ loss function $\ell_{q}(y, y') = |y - y'|^{q}$ for a real number $q \geq 1$. Besides, we assume that there exists a $M > 0$ such that $|h(\bar{x}) - f_{Q}(\bar{x})| \leq M$ for all $\bar{x}$ and $h \in \mathcal{H}$, and there exists $B_{\bar{w}} > 0$ such that $\|\bar{w}\| \leq B_{\bar{w}}$. Similarly, we assume that $\|\bar{a}\| \leq B_{\bar{a}}$, leading to $\|\bar{a}\| \leq B_{\bar{a}}B_{\bar{w}}$. We denote a function class of $g$ by $\mathcal{H} := \{h(\bar{x}) = \bar{w}^{\top} \bar{a} \mid \|\bar{w}\| \leq B_{\bar{w}}, \|\bar{a}\| \leq B_{\bar{a}}\}$.

Fix $\bar{a}$, then, we have the following proposition:

**Proposition 7.1.** Fix $\bar{a}$, then, for any $\delta > 0$, the following inequality holds with probability at least $1 - \delta$ for any $h \in \mathcal{H}$:

$$J_{Q}(h) \leq \hat{J}_{Q}(h) + \frac{2qM^{q-1}B}{\sqrt{n}} + M^{q} \sqrt{\frac{\ln(1/\delta)}{2n}},$$

where $B := B_{\bar{w}}B_{\bar{a}}$.

This result shows that for the same domain, i.e., the domain characterized by the training attributes, the generalization error bound converges with the order $O(1/\sqrt{n})$, which is the optimal without any additional assumption (Mendelson, 2008).

Next, we consider generalization error bounds on the domain characterized by the optimized attribute vectors. Compared with the above analysis, it requires to measure the difference between the source (training attribute vectors) and target (optimized attribute vectors) domains. Let $P$ and $Q$ be distributions of the target and source domains, respectively. We regard that $\bar{x}_{i}' = \text{vec}(\psi(x_{i}^{(t)})\hat{a}^{(t)})^{\top}$ and $\bar{x}_{i} = \text{vec}(\psi(x_{i}^{(t)})a^{(t)})^{\top}$ are independently drawn from distributions $Q$ and $P$, respectively, where $a^{(t)}$ is an test/optimized domain-attribute vector. We then analyze the generalization error bounds of ZSDA on the basis of a tool for domain adaptation. More specifically, we have training samples from the source domain with distribution $Q$ and evaluate the performance on the target domain with distribution $P$.

We first define $L_{Q}(h, h') := E_{Q} [\ell(h(\bar{x}), h'(\bar{x}))]$ and $L_{P}(h, h') := E_{P} [\ell(h(\bar{x}), h'(\bar{x}))]$, and denote the corresponding empirical approximators by $\tilde{L}_{Q}(h, h')$ and $\tilde{L}_{P}(h, h')$, respectively. By definition, we have $J_{Q}(h) = L_{Q}(h, f_{Q})$ and $\hat{J}_{Q}(h) = \tilde{L}_{Q}(h, f_{Q})$. Similarly, $J_{P}(h) := E_{P} [\ell(h(\bar{x}), f_{P}(\bar{x}))]$ and $\hat{J}_{P}(h) := \frac{1}{n'} \sum_{i=1}^{n'} \ell(h(\bar{x}_{i}), f_{P}(\bar{x}_{i}))$, where $n'$ is the number of samples in the domain $P$ and $f_{P}$ is the target labeling function in $P$. To measure the difference between two distributions $P$ and $Q$, we use the *discrepancy distance* (Mansour et al., 2009) defined as

$$\text{disc}(P, Q) = \sup_{h, h' \in \mathcal{H}} |L_{P}(h, h') - L_{Q}(h, h')|.$$

Let $h_{Q}^*$ and $h_{P}^*$ be the minimizers of $J_{Q}(h)$ and $J_{P}(h)$, respectively. We assume that $|h(\bar{x}) - h'(\bar{x})| \leq M$ for all $\bar{x}$ and $h, h' \in \mathcal{H}$. Under the above assumptions, we have the following proposition:

**Proposition 7.2.** For any $\delta > 0$, the following inequality holds with probability at least $1 - \delta$ for any $h \in \mathcal{H}$:

$$L_{P}(h, f_{P}) \leq \tilde{L}_{Q}(h, h_{Q}^*) + \text{disc}(\tilde{P}, \tilde{Q}) + L_{P}(h_{Q}^*, h_{P}^*) + L_{P}(h_{P}^*, f_{P}) + \frac{10qM^{q-1}B}{\sqrt{n}} + 3M^{q} \sqrt{\frac{\ln(3/\delta)}{2n}}.$$
This result shows that the target expected error \( L_P \) in the left-hand side is upper-bounded by the source empirical error \( \hat{L}_Q \) plus additional constants and confidence terms.

Note that the same transformation was used in (Romera-Paredes and Torr, 2015) to analyze generalization error bounds, but they considered classification while our focus is regression. Moreover, the subsequent analyses differ from (Romera-Paredes and Torr, 2015), e.g., a measure for domains.

### 7.2 Approximation factor

We here analyze the attribute optimization step in our framework from a complexity-theoretic point of view. In a nutshell, we show that the non-negative linear counterpart of attribute optimization is a generalization of packing integer programs (Raghavan, 1988), and it is \( \text{NP} \)-hard in general but approximable if the vectors representing constraints are “sparse.” For the sake of simplicity of analysis, we make the following assumptions:

- The objective function is given by \( f(\mathbf{a}) = F(g_{\mathbf{a}}) \), where \( F \) is a mean response and \( g_{\mathbf{a}} \) follows a LAM model; i.e., \( f(\mathbf{a}) = \frac{1}{|B|} \sum_{x \in B} \mathbf{a}^T \phi(x) \) for a non-negative vector function \( \phi(\cdot) \).

- Constraint functions \( b_j \) and \( c_j \) are non-negative and linear; i.e., for each \( j \in [s] \), there exists a vector \( b_j \in \mathbb{R}_{\geq 0}^n \) and a scalar \( d_j \geq 0 \) such that \( b_j(\mathbf{a}) = b_j^T \mathbf{a} - d_j \), and for each \( j \in [t] \), there exists a vector \( c_j \in \mathbb{R}_{\geq 0}^n \) and a scalar \( e_j \geq 0 \) such that \( c_j(\mathbf{a}) = c_j^T \mathbf{a} - e_j \).

The attribute optimization problem under the above assumptions (hereafter called non-negative attribute optimization; NAO) can be written as follows:

\[
\max_{\mathbf{a}} \left\{ \frac{1}{|B|} \sum_{x \in B} \mathbf{a}^T \phi(x) \mid \mathbf{b}_j^T \mathbf{a} \leq d_j, \forall j \in [s]; \mathbf{c}_j^T \mathbf{a} \leq e_j, \forall j \in [t] \right\}.
\]

Hereafter, Eq. (4) is referred to as NAO\(_\text{mix}\) if \( \mathbf{a} \) contains both binary and real-valued variables, and NAO\(_01\) if \( \mathbf{a} \) contains only binary variables. NAO\(_01\) is a special case of NAO\(_\text{mix}\).

We will discuss the relation between NAO and a discrete optimization problem called packing integer programs (PIPs) (Raghavan, 1988). Our first result is that NAO\(_01\) includes PIPs as a special case, implying a hardness-of-approximation result of NAO\(_01\).

**Theorem 7.1.** There exists a polynomial-time reduction from PIPs to NAO\(_01\). It is thus \( \text{NP} \)-hard to approximate NAO\(_01\) within a factor of \( n^{1-\epsilon} \) for any \( \epsilon > 0 \), where \( n \) is the dimension of a domain-attribute vector.

Having known that NAO\(_01\) is hard in general, we restrict the class of input structures to study the approximability of NAO\(_\text{mix}\). For each \( i \in [n] \), let \( S(i) \) be the number of constraints that \( i \) appears in; i.e.,

\[
S(i) := |\{j \in [s] : c_{j,i} > 0\}| + |\{j \in [t] : d_{j,i} > 0\}|.
\]

The column sparsity is then defined as \( S := \max_{i \in [n]} S(i) \). Our second result states that we can approximate NAO\(_\text{mix}\) accurately if \( S \) is bounded.

**Theorem 7.2.** There exists a polynomial-time \( 8S \)-factor approximation algorithm for NAO\(_\text{mix}\), where \( S \) is the column sparsity of an input instance.
We first describe the common settings between both toy and real-world datasets. For QBM, we used a three-layer neural network (the CVaR-based gain function in the same way as our proposed method. For each test set of features \(a^{(t') \in T_{te}}\), we computed the average and relative standard deviation\(^3\) over \(\{g^*(x_i^{(t')}, \tilde{a}^{(t')})\}_{i=1}^{n(t')}\), denoted by \(\bar{g}(t')\) and \(\tilde{g}(t')\), respectively. As evaluation metrics, we used \(g_{te} = (1/T_{te}) \sum_{t'=1}^{T_{te}} \bar{g}^{(\kappa(T_{tr}+t'))}\) and \(\tilde{g}_{te} = (1/T_{te}) \sum_{t'=1}^{T_{te}} \tilde{g}^{(\kappa(T_{tr}+t'))}\).

\[\hat{a}^{(t')}\] is the estimated parameter. We refer to this method as FUA-Mean. The above attribute optimization can be regarded as the use of the mean gain function in our proposed method, but it does not take the dependency of features into account in both the prediction and optimization steps. Due to the FUA’s nature, we cannot use the CVaR-based gain function in the same way as our proposed method.

For comparison, we used the FUA with linear ridge regression. Specifically, we trained \(s = w^T a + b\) with \(\{(a^{(t')}, \bar{y}^{(t')})\}_{t'=1}^{T_{te}}\), where \(b \in \mathbb{R}\) is the intercept. We then maximized \(\hat{a}^T \hat{w}\) in a feasible domain, where \(\hat{w}\) is the estimated parameter. We refer to this method as FUA-Mean. The above attribute optimization can be regarded as the use of the mean gain function in our proposed method, but it does not take the dependency of features into account in both the prediction and optimization steps. Due to the FUA’s nature, we cannot use the CVaR-based gain function in the same way as our proposed method.

We used a four-layer neural network (\(d=100-100-100-m\)) for the feature mapping function \(\phi\) of the LAM. For QBM, we used a three-layer neural network (\(d=100-m\)) for \(\phi_q\) and set \(r = 3\). For

\[^3\]The relative standard deviation is the standard deviation over \(\{g^*(x_i^{(t')}, \tilde{a}^{(t')})\}_{i=1}^{n(t')}\) divided by the mean \(\bar{g}(t')\).
Table 1: Average of $\bar{g}_{te}$ over 10 trials. The number in parentheses is average of $\tilde{g}_{te}$. In terms of the average response, the mean gain function was better than the CVaR-based gain function. The CVaR-based gain function was stable in terms of the relative standard deviation of obtained responses (see also Figure 2). The boldface denotes the best method in terms of the average gain.

|          | FUA-Mean | LAM-Mean | LAM-CVaR |
|----------|----------|----------|----------|
|          | 3.24 (0.54) | 3.28 (0.52) | 2.86 (0.46) |

the hidden layers of neural networks, we used the ReLU activation function (Glorot et al., 2011) and batch normalization (Ioffe and Szegedy, 2015). We further split the training data into 80% training and 20% validation data. We then trained the neural network with the Adadelta optimizer (Zeiler, 2012) until 200 epochs, and we used the model that achieved the lowest validation error for inference. We refer to LAM/QBM with the mean gain function as $LAM$-$Mean$/$QBM$-$Mean$ and refer to LAM with the CVaR gain function and $\beta = 0.05$ as $LAM$-$CVaR$.

8.2 Mean vs. CVaR-based gain function

We here show the effect of the mean and CVaR-based gain functions.

**Data:** We considered an attribute vector to consist of continuous $(a_1, a_2, a_3)$ and binary $(a_4, a_5, a_6)$ variables, i.e., $m = 6$. Each element of the continuous variables was drawn from the standard Gaussian distribution, denoted by $\mathcal{N}(0, 1^2)$, and the continuous variables were then normalized such that $\sum_{i=1,2,3} a_i^2 = 1$. For the categorical variables, one of the elements was chosen uniformly at random.

For a response function, we used $g^*(x, a) = x^\top W a$, where each element of $W \in \mathbb{R}^{d \times m}$ was drawn from $\mathcal{N}(0, 1^2)$. The response $y$ was then observed by $y = g^*(x, a) + \epsilon$, where $\epsilon$ was drawn from $\mathcal{N}(0, 0.1^2)$. We drew 15 attribute vectors and 50 samples for each object, i.e., we had $\{(D^{(t)}, a^{(t)})\}_{t=1}^{15}$, where $D^{(t)} = \{(x_i^{(t)}, y_i^{(t)})\}_{i=1}^{30}$. We set $d$ as 10 and drew each element of $x$ from $U(0, 1)$, where $U(a, b)$ denotes a uniform distribution with the range $[0, 1]$.

**Results:** Table 1 summarizes the averages of $\bar{g}_{te}$ and $\tilde{g}_{te}$ over 10 trials, showing that the mean gain function was better than the CVaR-based gain function in terms of the average response, while the latter gain function was stable in terms of standard deviation.

To visualize why the standard deviation of the CVaR-based gain function was lower than that of the mean gain function, we plotted two histograms of the obtained responses of the attributes obtained by the mean and CVaR-based gain functions, respectively, in Figure 2, which illustrates that the response distribution obtained by the CVaR-based gain function was narrower than that obtained by the mean gain function. This is because the CVaR-based gain function took into account the response distribution, in particular, the left-tail of the distribution, resulting in the relative standard deviation of the obtained responses being smaller while the average response remained high, almost comparable to that obtained by the mean gain function in this synthetic data experiment.
Table 2: Averages of $\overline{g}_{te}$ over 10 trials. The number in parentheses is the average of relative standard deviation $\tilde{g}_{te}$. Unlike LAM, QBM attained much higher gain. The boldface denotes the best method in terms of the average gain.

|        | FUA-Mean | LAM-Mean | QBM-Mean |
|--------|----------|----------|----------|
| g_{te} | 2.06 (0.94) | 2.08 (0.93) | 2.20 (0.97) |

8.3 Effect of interaction of domain attributes

**Data:** We considered a 10-dimensional attribute vector to consist of binary variables with $\sum_{j=1}^{3} a_j = 1$, $\sum_{j=4}^{6} a_j = 1$, and $\sum_{j=7}^{10} a_j = 1$. The categorical attribute was chosen from each group uniformly at random. For a response function, we used $g^*(x,a) = (1/30)a^T(\sum_{q=1}^{3} \phi_q(x)\phi_q(x)^T)a$, where $\phi_q(x) := W_q x$, and each element of $W_q \in \mathbb{R}^{m \times d}$ was drawn from $\mathcal{N}(0, 1^2)$. The response $y$ was then observed by $y = g^*(x,a) + \varepsilon$, where $\varepsilon$ was drawn from $\mathcal{N}(0, 0.1^2)$. We drew 15 attribute vectors and 50 samples for each object, i.e., we had $\{(D^{(t)}, a^{(t)})\}_{t=1}^{10}$, where $D^{(t)} = \{(x_i^{(t)}, y_i^{(t)})\}_{i=1}^{50}$. We set $d$ as 10 and drew each element of $x$ from $U(0, 1)$, where $U(a, b)$ denotes a uniform distribution with the range $[0, 1]$. We set $d$ as 10 and drew each element of $x$ from $U(0, 1)$.

**Results:** Table 2 summarizes the averages of $\overline{g}_{te}$ and $\tilde{g}_{te}$ over 10 trials, showing that the obtained gain of QBM was larger than that of FUA and LAM. This result shows that when there is a dependency between domain-attribute variables, models incorporating such a domain-attribute interaction attain higher performance for attribute optimization.
8.4 Real-world datasets

We next evaluate the performance on benchmark datasets. The statistics of the datasets are summarized in Table 3, and the details are given below.

**Sushi:** The SUSHI\(^4\) Preference (Sushi) Dataset (Kamishima, 2003) consists of consumer ratings for sushi, features of consumers, and domain attributes of each kind of sushi.\(^5\) The rating of sushi is done by five-grade evaluation (from 0 to 4), the mean rating is 2.73, and the median rating is 3.00. For the description (domain attributes) of sushi, we used the style of sushi, the type of sushi, the oiliness, and the normalized price. In this dataset, the type and style of sushi are categorical domain-attributes, and the oiliness and normalized price are continuous domain-attributes. The task was to find better combinations of domain attributes of sushi.

For the consumer features, we used gender, range of ages, the prefecture in which until 15 years the consumer had lived longest, the prefecture in which the consumer currently lives, and the total time taken for stating their preference of sushi. We then converted the characteristics introduced above into numerical vectors and finally obtained 12-dimensional feature vectors and 16-dimensional domain-attribute vectors.

**Coffee:** The coffee quality dataset contains 1338 reviews.\(^6\) Reviews are given for beans and farms. We used the information for a farm as features and that for a bean as domain attributes. Specifically, the “Country of Origin,” “Certification Body,” and “Altitude”\(^7\) in the dataset were used as features, and the “Species,” “Processing Method,” and “Variety” were used as domain attributes. The “Total Cup Points” were used as the score (reward). The full score is 100, the minimum and maximum scores in the dataset are 59.8 and 90.6, respectively, the mean score is 82.1, and the median score is 82.5. The number of possible choices of domain attributes is 2 species, 5 processing methods, and 29 varieties. The goal was to find a combination of a processing method, species, and variety of coffee for a specific farm.

**Book:** We used goodbooks-10k (Book).\(^8\) The Book dataset collects ratings of books from readers. The range of ratings is from 1 to 10, the mean rating is 4.68, and the median rating is 3.0. Since there were items without ratings, we used mean imputation to focus on the effect of our method for simplicity.

We used “Age” and “Country“ as the features of readers, and we used tags of books annotated by users in the book-rating platform as domain attributes. We manually extracted book tags that were likely to be relevant to ratings. Examples of extracted tags are “biography,” “comedy,” and “fiction.” After preprocessing, that is, one-hot encoding, we had 7,121 ratings of 147 books \((m = 77)\) from readers \((d = 74)\).

**Results:** Table 4 summarizes the averages of \(\bar{g}_{te}\) and \(\bar{g}_{te}\) over 10 trials, showing that i) LAM with the mean gain function achieved a higher response than the other methods, and ii) LAM with the CVaR gain function tended to produce results with smaller variances among them.

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\(^4\)Sushi is a Japanese dish containing vinegared rice.

\(^5\)http://www.kamishima.net/sushi/

\(^6\)The dataset was downloaded from https://github.com/jldbc/coffee-quality-database. Note that we deleted samples that have missing entries.

\(^7\)If the altitude is given as a range, e.g., 1200-1300, we used the mean value.

\(^8\)https://github.com/zygmuntz/goodbooks-10k.
Table 3: Statistics of real-world datasets.

| Dataset | n   | d  | m  | T  |
|---------|-----|----|----|----|
| Sushi   | 50,000 | 31 | 15 | 100 |
| Coffee  | 1,161  | 63 | 36 | 23 |
| Book    | 7,282  | 64 | 77 | 169 |

Table 4: Averages of $\tilde{g}_{te}$ over 10 trials. The Number in parentheses is the average of $\tilde{g}_{te}$ over 10 trials. The boldface denotes the best method in terms of the average gain.

| Dataset | FUA-Mean | LAM-Mean | LAM-CVaR |
|---------|----------|----------|----------|
| Sushi   | 3.79 (0.11) | **3.85 (0.11)** | 3.76 (0.10) |
| Coffee  | 74.7 (0.09)  | **99.4 (0.05)** | 98.2 (0.04) |
| Book    | 4.76 (0.18)  | **7.00 (0.16)** | 6.17 (0.10) |

In the real-world datasets, the obtained performance difference between the FUA and the proposed method was larger, compared with the artificial datasets. Since the difference between the different sets of features in the real-world datasets was larger than that in the artificial datasets, the proposed method, taking features into account to optimize attributes, returned more suitable domain attributes than the FUA. These results imply that attribute optimization is a promising means of cooperating with humans in designing new products. On the basis of the results presented by our method, humans can continue further trial and error to find a better description of new products. Another aspect of using our method is that it reduces the cost of designing products and services for each customer because our method is aware of customers’ features. The proposed method will allow us to provide products and services tailored to each customer, which will improve customer satisfaction.

9 Conclusion

Zero-shot domain adaptation is useful in real-world applications, e.g., predicting the sales of a new product for which labeled data are not available. While existing studies focus on improving the prediction accuracy, we considered a reverse process for prediction that can be categorized as predictive optimization. To this end, we proposed a simple framework for predictive optimization with zero-shot domain adaptation and analyzed the conditions in which optimization problems become convex. Furthermore, we discussed the way of handling interactions of variables representing a domain description. Through numerical experiments, we demonstrated the potential effectiveness of the proposed framework.

Finding a promising combination of characteristics of existing products is an important task for manufacturers. While the amount of available data on existing products and consumer reactions is increasing day by day, handling a large amount of data is often difficult for humans without support from computer systems. Our simple formulation could be a guideline for investigating bottlenecks in data-driven design systems and unlock further possibilities in this direction of research.
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A Proofs

A.1 Proofs of generalization error bound

Recall the notations and assumptions:

- $f_P$ and $f_Q$ are the labeling functions on the target and source domains, respectively.
- $\ell_q(y, y') = |y - y'|^q$ for a real number $q \geq 1$.
- $|h(\bar{x}) - f(\bar{x})| \leq M$ for all $\bar{x}$ and $h \in \mathcal{H}$.
- $|h(\bar{x}) - h'(\bar{x})| \leq M$ for all $\bar{x}$ and $h, h' \in \mathcal{H}$.
- $\|\bar{w}\| \leq B_{\bar{w}}, \|\bar{x}\| \leq B_{\bar{x}}, \|x\| \leq B_x$, and $\|a\| \leq B_a$.
- $S := \{((\bar{x}_i, y_i))_{i=1}^n \sim P, S' := \{(\bar{x}_i', y_i')\}_{i=1}^{n'} \sim Q, and n = n'$.

Proof. From the assumptions, $L_Q(h, h') = E_Q[\ell(h(\bar{x}), h'(\bar{x}))] \leq M^q$. Let $L: \bar{x} \mapsto \ell(h(\bar{x}), h'(\bar{x}))$. Based on the standard Rademacher analysis (see, e.g., Mohri et al. (2012)), we have for any $\delta > 0$, the following inequality with probability at least $1 - \delta$ for any $h, h' \in \mathcal{H}$:

$$L_Q(h, h') - \hat{L}_Q(h, h') \leq 2\mathcal{R}_n(\mathcal{L}) + M^q \sqrt{\frac{\ln(1/\delta)}{2n}},$$

(5)

where $\hat{\mathcal{R}}_S(\mathcal{H}) := \frac{1}{n} E_{\sigma}[\sup_{h \in \mathcal{H}} \sum_{i=1}^n \sigma_i h(\bar{x}_i)]$ and $\mathcal{R}_n(\mathcal{H}) := E_S[\hat{\mathcal{R}}_S(\mathcal{H})]$ are the empirical and expected Rademacher complexity, $\sigma_i$ is an independent uniform random variables taking values in $\{+1, -1\}$, and $\sigma := (\sigma_1, \ldots, \sigma_n)^\top$. Let $\mathcal{L}_f = \{\bar{x} \mapsto h(\bar{x}) - f(\bar{x}) \mid h \in \mathcal{H}\}$. Then, $\mathcal{L}$ can be rewritten as $\mathcal{L} = \{\ell_q \circ h_f \mid h_f \in \mathcal{H}_f\}$. Since $\ell_q$ is $qM^{q-1}$-Lipschitz over $[-M, M]$, we can use Talagrand’s lemma (Ledoux and Talagrand, 1991): $\hat{\mathcal{R}}_S(\mathcal{H}_f) \leq qM^{q-1}\mathcal{R}_S(\mathcal{H}_f)$. Furthermore, $\hat{\mathcal{R}}_S(\mathcal{H}_f) = \hat{\mathcal{R}}_S(\mathcal{H})$. For the linear model, the Rademacher complexity can be bounded (see, e.g., Mohri et al. (2012)) as $\mathcal{R}_n(\mathcal{H}) \leq \frac{B_{\bar{w}} B_{\bar{x}} B_a}{\sqrt{n}}$. Replacing $h'$ with $f_Q$ in Eq. (5), we have Proposition 7.1. That is, for any $\delta > 0$, the following inequality holds with probability at least $1 - \delta$ for any $h \in \mathcal{H}$: $L_P(h, f_P) - \hat{L}_P(h, f_P) \leq 2qM^{q-1}B_{\sqrt{n}} + M^q \sqrt{\frac{\ln(1/\delta)}{2n}}$.

Let $\mathcal{H}_h = \{h(\bar{x}) - h'(\bar{x}) \mid h, h' \in \mathcal{H}\}$. $\mathcal{L}$ can be rewritten as $\mathcal{L} = \{\ell_q \circ h \mid h \in \mathcal{H}\}$. We then have $\hat{\mathcal{R}}_S(\mathcal{L}) \leq qM^{q-1}\mathcal{R}_S(\mathcal{H}_h) \leq 2qM^{q-1}\mathcal{R}_S(\mathcal{H})$. From Eq. (5), we have $\text{disc}(P, \hat{P}) \leq 4qM^{q-1}\mathcal{R}_n(\mathcal{H}) + M^q \sqrt{\frac{\ln(1/\delta)}{2n}}$. Based on the triangle inequality, we have $\text{disc}(P, Q) \leq \text{disc}(P, \hat{P}) + \text{disc}(Q, \hat{Q}) + \text{disc}(\hat{P}, \hat{Q})$. For any $\delta > 0$, the following inequality holds with probability at least $1 - \delta$:

$$\text{disc}(P, Q) \leq \text{disc}(\hat{P}, \hat{Q}) + 8qM^{q-1}\mathcal{R}_n(\mathcal{H}) + 2M^q \sqrt{\frac{\ln(1/\delta)}{2n}}.$$

Applying the triangle inequality, we have,

$$L_P(h, f_P) \leq L_P(h, h_Q^*) + L_P(h_Q^*, h_P^*) + L_P(h_P^*, f_P) \leq L_Q(h, h_Q^*) + \text{disc}(P, Q) + L_P(h_Q^*, h_P^*) + L_P(h_P^*, f_P).$$

We have, for any $\delta > 0$, the following inequality holds with probability at least $1 - \delta$ for any $h \in \mathcal{H}$:

$$L_P(h, f_P) \leq \hat{L}_Q(h, h_Q^*) + L_P(h_Q^*, h_P^*) + L_P(h_P^*, f_P) + \text{disc}(\hat{P}, \hat{Q}) + 10qM^{q-1}\mathcal{R}_n(\mathcal{H}) + 3M^q \sqrt{\frac{\ln(3/\delta)}{2n}}.$$

Replacing $\mathcal{R}_n(\mathcal{H})$ with the upper bound, we obtain Proposition 7.2. \qed
A.2 Proofs of approximability

Before going into the proof of the two results above, we define PIPs as follows (Raghavan, 1988).

Definition A.1 (Packing integer program). Given m vectors \( A_1, \ldots, A_m \in \mathbb{R}_{\geq 0}^n \), a capacity vector \( B \in \mathbb{R}_{\geq 0}^m \), and a weight vector \( w \in \mathbb{R}_n^m \), the packing integer program (PIP) is defined as the following problem:

\[
\max_{a \in \{0,1\}^m} \left\{ w^T a \mid A_j^T a \leq B_j, \forall j \in [m] \right\}.
\]

We define the column sparsity as \( S := \max_{i \in [n]} \{ j \in [m] : A_{j,i} > 0 \} \).

Proof of Theorem 7.1. Let \( A_1, \ldots, A_m \in \mathbb{R}_n^m \), \( B \in \mathbb{R}_{\geq 0}^m \), and \( w \in \mathbb{R}_n^m \) be an instance of PIP. We can construct an instance of \( \text{NAO}_{0.1} \) in polynomial time such that the following conditions are satisfied:

- \( \phi \) and \( B \) satisfy that \( \frac{1}{|B|} \sum_{x \in B} \phi(x) = w \),
- the number of inequality constraints is \( s = m \), the number of equality constraints is \( t = 0 \), and
- for each \( j \in [s] \), it holds that \( b_j = A_j \) and \( d_j = B_j \).

It is easy to verify that the resulting instance of \( \text{NAO}_{0.1} \) is exactly equivalent to a given instance of PIP; the inapproximability result is thus obvious (see, Bansal et al. (2012); Zuckerman (2007)).

\[ \square \]

Proof of Theorem 7.2. Fix an \( \text{NAO}_{\text{mix}} \) instance \( \phi(\cdot), B, \{b_j\}_{j \in [s]}, \{d_j\}_{j \in [s]}, \{c_j\}_{j \in [t]}, \{e_j\}_{j \in [t]} \).

We first partition an \( n \)-dimensional domain-attribute vector \( a \) into continuous domain attributes and binary domain-attributes. Let \( I_{re} \) and \( I_{bi} \) be the set of indices for continuous variables and binary variables, respectively. Let us denote \( a_{re} = (a_i)_{i \in I_{re}} \) and \( a_{bi} = (a_i)_{i \in I_{bi}} \), and denote \( w = \frac{1}{|B|} \sum_{x \in B} \phi(x) \), \( w_{re} = (w_i)_{i \in I_{re}} \), and \( w_{bi} = (w_i)_{i \in I_{bi}} \); note that \( w^T a = w_{re}^T a_{re} + w_{bi}^T a_{bi} \).

The original \( \text{NAO}_{\text{mix}} \) (denoted P1) can be rewritten as

\[
\max_{a_{re} \in \mathbb{R}_{\geq 0}^{|I_{re}|}, a_{bi} \in \{0,1\}^{|I_{bi}|}} \left\{ w^T a \mid b_j^T a \leq d_j, \forall j \in [s]; c_j^T a = e_j, \forall j \in [t] \right\}.
\]

We now describe the approximation algorithm for P1. We first consider the linear programming (LP) relaxation of P1 (denoted LP1) that relaxes “\( a_{bi} \in \{0,1\}^{|I_{bi}|} \)” to “\( a_{bi} \in \mathbb{R}_{\geq 0}^{|I_{bi}|} \)” Since LP1 is an LP instance, we can solve it exactly in polynomial time, e.g., by the ellipsoid method, and denote its optimal solution by \( \bar{a} \in \mathbb{R}_{\geq 0}^m \). We then create a new instance of \( \text{NAO}_{0.1} \) (denoted P2) where entries of \( a_{re} \) are fixed to entries of \( \bar{a}_{re} \), and relax each equality constraint “\( c_j^T a = e_j \)” to “\( c_j^T a \leq e_j \)” the resulting \( \text{NAO}_{0.1} \) instance (denoted P2’) by which is an instance of PIP whose column sparsity is at most \( S \). We thus can use Bansal et al. (2012)’s algorithm to find an \( 8S \)-factor approximate solution \( \tilde{a}_{bi} \in \{0,1\}^{|I_{bi}|} \), \( \tilde{a} \) for P2’.

We can increase some of the entries of \( \tilde{a}_{bi} \) until the equality constraints are satisfied, which does not decrease the objective value. Finally, we return a domain-attribute vector \( a \) defined as follows:

\[
a_i = \begin{cases} 
\tilde{a}_i & \text{if } i \in I_{re}, \\
\bar{a}_i & \text{if } i \in I_{bi}.
\end{cases}
\]

(6)

Since the feasibility of \( a \) is obvious, we analyze its approximation ratio. Let \( a^* \) be an optimal solution for P1. Observe that \( w^T \tilde{a} \geq w^T a^* \) as \( \tilde{a} \) is an optimal solution for LP1. We
then show that $w_{bi}^\top \bar{a}_{bi} \geq \frac{1}{8S} w_{bi}^\top \bar{a}_{bi}$. Recall that Bansal et al. (2012)’s algorithm returns a feasible solution for a PIP instance that has an objective value at least $\frac{1}{8S}$ times the optimum value of its LP relaxation. If $\bar{a}_{bi}'$ is an optimal solution for the LP relaxation of P2’, it holds that $w_{bi}^\top \bar{a}_{bi}' \geq w_{bi}^\top \bar{a}_{bi}$; hence, we have that $w_{bi}^\top \bar{a}_{bi} \geq \frac{1}{8S} w_{bi}^\top \bar{a}_{bi}' \geq \frac{1}{8S} w_{bi}^\top \bar{a}_{bi}$. Consequently,

$$w^\top a = \frac{1}{8S}(w_{re}^\top \bar{a}_{re} + w_{bi}^\top \bar{a}_{bi}) \geq \frac{1}{8S}w_{bi}^\top \bar{a}_{bi} \geq \frac{1}{8S}w_{bi}^\top \bar{a}_{bi}' \geq \frac{1}{8S}w_{bi}^\top \bar{a}_{bi} \geq \frac{1}{8S}(w_{re}^\top \bar{a}_{re} + w_{bi}^\top \bar{a}_{bi}) \geq \frac{1}{8S}w^\top \bar{a}^*.$$

$a$ is an $8S$-factor approximate solution to NAO\textsubscript{mix}, which completes the proof. □