Learning Bregman Divergences

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Abstract

Metric learning is the problem of learning a task-specific distance function given supervision. Classical linear methods for this problem (known as Mahalanobis metric learning approaches) are well-studied both theoretically and empirically, but are limited to Euclidean distances after learned linear transformations of the input space. In this paper, we consider learning a Bregman divergence, a rich and important class of divergences that includes Mahalanobis metrics as a special case but also includes the KL-divergence and others. We develop a formulation and algorithm for learning arbitrary Bregman divergences based on approximating their underlying convex generating function via a piecewise linear function. We show several theoretical results of our resulting model, including a PAC guarantee that the learned Bregman divergence approximates an arbitrary Bregman divergence with error $O_p(m^{-1/(d+2)})$, where $m$ is the number of training points and $d$ is the dimension of the data. We provide empirical results on using the learned divergences for classification, semi-supervised clustering, and ranking problems.

1 Introduction

Metric learning is the task of learning a distance metric from supervised data such that the learned metric is tailored to a given task. The training data for a metric learning algorithm is typically either relative comparisons ($B$ is more similar to $A$ than to $C$) [1, 2, 3] or similar/dissimilar pairs ($B$ and $A$ are similar, $B$ and $C$ are dissimilar) [4]. This supervision may be available when underlying training labels are not directly available, such as from ranking data [5], but can also be obtained directly from class labels in a classification task. In each of these settings, the learned similarity measure can be used downstream as the distance measure in a nearest neighbor algorithm, for similarity-based clustering [6, 1], to perform ranking [7], or for other tasks.

Existing metric learning approaches are often divided into two classes, namely linear and non-linear methods. Linear methods learn linear mappings and compute distances (usually Euclidean) in the mapped space [4, 3, 8]; this approach is typically referred to as Mahalanobis metric learning. These methods generally yield simple convex optimization problems, can be analyzed theoretically [9, 10], and are applicable in many general scenarios. Non-linear methods, most notably deep metric learning algorithms, can yield superior performance but require a significant amount of data to train and have little to no associated theoretical properties [11, 12]. In this paper, our focus is on generalizing the class of linear methods to encompass a richer class of possible learned divergences, including non-linear divergences, while retaining strong theoretical guarantees. Specifically, we focus on the class of Bregman divergences, which includes Mahalanobis metrics but includes many other popular measures such as the KL-divergence, the LogDet-divergence, and the Itakura-Saito distance. Our aim is to provide a principled framework for learning an arbitrary Bregman divergence given supervision, and to prove approximation and generalization bounds under our proposed framework.

A Bregman divergence $D_\phi : X \times X \to \mathbb{R}_+$ is parametrized by a strictly convex function $\phi : X \to \mathbb{R}$ such that the divergence of $x_1$ from $x_2$ is defined as the approximation error of the linear
We empirically compare our proposed method with several existing Mahalanobis metric learning algorithms. In [2], the authors use pairwise similarity comparisons (labeled data points to be close in each neighborhood while leaving the dissimilar labeled data points far away from the local neighborhood. In [3], the authors use pairwise similarity comparisons drawn from data points in left by linear metric learning (ITML). (Right) convex function learned from pairwise similarity comparisons drawn from data points in left by PBDL algorithm. When this convex function is used to define a Bregman divergence, points within a given class have a small learned divergence, leading to clustering, k-nn, and ranking performance of 98%+ (see experimental results for details).

approximation of \( \phi(x_1) \) from \( x_2 \), i.e. \( D_\phi(x_1, x_2) = \phi(x_1) - \phi(x_2) - \nabla \phi(x_2)^T(x_1 - x_2) \). The case of linear metrics (as studied in Mahalanobis metric learning) corresponds to \( \phi(x) = x^TMx \), a quadratic function. A significant challenge when extending from Mahalanobis metric learning to learning arbitrary Bregman divergences is how to appropriately parameterize the class of convex functions; in our work, we choose to parameterize \( \phi \) via piecewise linear functions of the form \( h(x) = \max_{k=1,...,K} a_k^T x + b_k \). As we discuss later, such \textit{max-affine} functions can be shown to approximate arbitrary convex functions via precise bounds. Furthermore we prove that sub-gradients of these functions can approximate gradient of the convex function that they are approximating, making it a suitable choice for approximating arbitrary Bregman divergences.

Using max-affine functions, we set up loss functions to learn an arbitrary Bregman divergence given supervision either in the form of pairwise similarity comparisons or similarity values. We propose a model, called piecewise linear Bregman divergence learning (PBDL), which is convex and can be efficiently solved on even large-scale problems. We then provide a strong theoretical foundation for our approach. Our main theoretical results are: i) a result showing that piecewise linear functions can be used to approximate Bregman divergences arbitrarily well, ii) a bound on the Rademacher complexity of our class of Bregman divergences, iii) generalization bounds of order \( O_p(n^{-1/2}) \) for our relative constraint divergence learning problem, where \( n \) is the number of training points—this order is the same as that provided in [9,10] for the less general setting of Mahalanobis metric learning methods; iv) in the regression setting we show a bound of \( O_p(n^{-1/(d+2)}) \) for learning an underlying Bregman divergence.

We empirically compare our proposed method with several existing Mahalanobis metric learning methods on both synthetic and real data. We see the advantages of our more general model on problems in similarity search, clustering, and ranking.

2 Related work

In this section, we first briefly overview linear metric learning algorithms; then we discuss some related results on non-linear metric learning and known theoretical results in this area.

Linear metric learning methods find a linear mapping \( G \) of the input data and compute (squared) Euclidean distance in the mapped space. This is equivalent to learning a positive semi-definite matrix \( M = G^TG \) where \( d_M(x_1, x_2) = (x_1 - x_2)^TM(x_1 - x_2) = ||Gx_1 - Gx_2||_2^2 \). The literature on linear metric learning is quite large and cannot be fully summarized here; see the surveys [11,13] for an overview of several approaches. One of the prominent approaches in this class is information theoretic metric learning (ITML) [4], which places a LogDet regularizer on \( M \) while enforcing similarity/dissimilarity supervisions as hard constraints for the optimization problem. Large-margin nearest neighbor (LMNN) metric learning [3] is another popular Mahalanobis metric learning algorithm tailored for k-nn by using a local neighborhood loss function which encourages similarly labeled data points to be close in each neighborhood while leaving the dissimilar labeled data points away from the local neighborhood. In [12], the authors use pairwise similarity comparisons (\( B \) is more similar to \( A \) than to \( C \)) by minimizing a margin loss. [14] uses similarity/dissimilarity information in
the assignment step of the k-means algorithm constraining similar points to be in the same cluster and vice versa. Other popular approaches include neighbourhood components analysis [8], the online learning methods POLA [15] and LEGO [16], and the clustering-based MMC method [17].

To our knowledge, the only existing work on approximating a Bregman divergence is [18], but this work does not provide any statistical guarantees. They assume that the underlying convex function is of the form \( \phi(x) = \sum_{i=1}^{N} \alpha_i h(x^T x_i) \), \( \alpha_i \geq 0 \), where \( h(\cdot) \) is a pre-specified convex function such as \( |z|^2 \). Namely, it is a linear superposition of known convex functions \( h(\cdot) \) evaluated on all of the training data. In our preliminary experiments, we have found this assumption to be quite restrictive and falls well short of state-of-art accuracy on benchmark datasets. Different from their work, we consider a piecewise linear family of convex functions capable of approximating any convex function. Other relevant non-linear methods include the kernelization of linear methods, as discussed in [1, 4]; these methods require a particular kernel function and typically do not scale well for large data.

There is sparse literature analyzing metric learning algorithms theoretically. Regret bounds have been proven in the online setting for some formulations [4, 15, 16]. Generalization bounds for Mahalanobis metric learning from pairwise similarity comparisons of order \( O_p(n^{-1/2}) \) are found in [9, 10], which matches the rate that we find for our more general approach. As far as we are aware, there are no known statistical guarantees for convergence of the learned Mahalanobis metric to the ground truth metric. However for our learning model which includes the Mahalanobis metric as well, we provide PAC guarantees for convergence to the ground truth Bregman divergence when supervised by similarity values.

3 Problem Formulation

We now turn to the general problem formulation considered in this paper. Suppose we observe data points \( X = [x_1, \ldots, x_n] \), where each \( x_i \in \mathbb{R}^d \). The goal is to learn an appropriate divergence measure for pairs of data points \( x_i \) and \( x_j \), given appropriate supervision. The class of divergences considered here is Bregman divergences; recall that Bregman divergences are parameterized by a continuously differentiable, strictly convex function \( \phi : \Omega \rightarrow \mathbb{R} \), where \( \Omega \) is a closed convex set. The Bregman divergence associated with \( \phi \) is defined as

\[
D_\phi(x_i, x_j) = \phi(x_i) - \phi(x_j) - \nabla \phi(x_j)^T (x_i - x_j).
\]

Learning a Bregman divergence can be equivalently described as learning the underlying convex function for the divergence. In order to fully specify the learning problem, we must determine both a supervised loss function as well as a method for appropriately parameterizing the convex function to be learned. Below, we describe both of these components.

3.1 Loss Functions

We can easily generalize the standard empirical risk minimization framework for metric learning, as discussed in [1], to our more general setting. In particular, suppose we have supervision in the form of \( m \) loss functions \( c_i \); these \( c_i \) depend on the learned Bregman divergence parameterized by \( \phi \) as well as the data points \( X \) and some corresponding supervision \( y \). We can express a general loss function as

\[
L(\phi) = \sum_{i=1}^{m} c_i(D_{\phi}, X, y) + \lambda r(\phi),
\]

where \( r \) is a regularizer over the convex function \( \phi \), \( \lambda \) is a hyperparameter that controls the tradeoff between the loss and the regularizer, and the supervised losses \( c_i \) are assumed to be a function of the Bregman divergence corresponding to \( \phi \). The goal in an empirical risk minimization framework is to find \( \phi \) to minimize this loss, i.e., \( \min_{\phi \in \mathcal{F}} L(\phi) \), where \( \mathcal{F} \) is the set of convex functions over which we are optimizing. For the rest of this paper, we will consider two specific examples:

**Bregman regression:** Suppose the function \( c_i \) consists of a pair of points from \( X \), say \( x_{i_1} \) and \( x_{i_2} \), and the \( y_i \) value is the target (ground truth) Bregman divergence between \( x_{i_1} \) and \( x_{i_2} \). A standard least squares loss function (with no regularization) would seek to solve

\[
\min_{\phi \in \mathcal{F}} \sum_{i=1}^{m} (D_{\phi}(x_{i_1}, x_{i_2}) - y_i)^2.
\]
We now briefly discuss algorithms for solving the underlying loss functions described in the previous section. These loss functions will model the response random variable $y$. A key question is whether piecewise linear functions can be used to approximate Bregman divergences $D_{\phi}(x_i, x_j)$ for some points $x_i, x_j$. Here the loss function would depend on the difference between the two Bregman divergences. As is common, we may put a margin loss to approximately satisfy the given supervision:

$$
\min_{\phi \in \mathcal{P}, L} \sum_{i=1}^{m} \max(0, 1 - D_{\phi}(x_i, x_i) + D_{\phi}(x_i, x_j)) + \lambda r(\phi).
$$

Note that one may consider other forms of supervision, such as pairwise similarity constraints, and these can be handled in an analogous manner.

### 3.2 Convex piecewise linear fitting

Next we must appropriately parameterize $\phi$. We choose to parameterize our Bregman divergences using piecewise linear approximations. Piecewise linear functions are used in many different applications such as global optimization [19], circuit modeling [20] and convex regression [21]. There are many methods for fitting piecewise linear functions including using neural networks [23], the Gauss-Newton method [20] and others; however, we are interested in formulating a convex optimization problem as done in [24]. We use convex piecewise linear functions of the form $F_{P,L} = \{ h : \Omega \rightarrow \mathbb{R} \mid h(x) = \max_{k=1,...,K} a_k^T x + b_k, \|a_k\|_1 \leq 1 \}$, called max-affine functions.

In the next section we will discuss how to formulate optimization over $F_{P,L}$ in order to solve the loss function described earlier. In particular, the following lemma will allow us to express appropriate optimization problems using linear inequality constraints:

**Lemma 1.** There exists a convex piecewise linear function $h : \mathbb{R}^d \rightarrow \mathbb{R}$, that satisfies the conditions

$$
h(x_i) = v_i, \quad \nabla h(x_i) = g_i \quad i = 1, \ldots, n,
$$

if and only if there exist a mutual exclusive partition of the data $C = \{C_1, \ldots, C_K \mid C_i \cap C_j = \emptyset, \forall (i, j)\}$, real values $b_1, \ldots, b_K$, and $a_1, \ldots, a_K \in \mathbb{R}^d$ s.t:

$$
\begin{cases}
v_i = b_k + a_k^T x_i \geq b_j + a_j^T x_i \quad \forall x_i \in C_k, \quad k, j = 1, \ldots, K \\
g_i = a_k
\end{cases}
$$

**Proof.** Assuming such $h$ exists, (2) holds by convexity. Conversely, assuming (2) holds, define $h$ as

$$
h(x) = \max_{k=1,...,K} a_k^T x + b_k.
$$

$h$ is convex due to the proposed function being a max of linear functions. $h(x_i) = v_i$ using (2). \qed

A key question is whether piecewise linear functions can be used to approximate Bregman divergences well enough. An existing result in [25] says that for any $L$-Lipschitz convex function $\phi$ there exists a piecewise linear function $h \in F_{P,L}$ such that $\|\phi - h\|_\infty \leq 36LRK^{-\frac{1}{2}}$, where $R$ is the radius of the input space. However, this existing result is not directly applicable to us since a Bregman divergence utilizes the gradient $\nabla \phi$ of the convex function. As a result, in section 5 we bound the gradient error $\|\nabla \phi - \nabla h\|_\infty$ of such approximators. This in turn allows us to prove a result demonstrating that we can approximate Bregman divergences with arbitrary accuracy under some regularity conditions.

### 4 Algorithms

We now briefly discuss algorithms for solving the underlying loss functions described in the previous section.

#### 4.1 Regression Setting

Suppose we observe the data $S_m = \{(x_i, x_j, y_i), i = 1, \ldots, m\}$, where $x \in \mathbb{R}^d$ and $y \in \mathbb{R}$. We will model the response random variable $y$ as a Bregman divergence $D_h(x, x)$ with $h \in F_{P,L}$. Let $h_m : \mathbb{R}^d \rightarrow \mathbb{R}$ be the empirical risk minimizer of

$$
\min_{h \in F_{P,L}} \frac{1}{n} \sum_{i=1}^{m} (D_h(x_i, x_i) - y_i)^2.
$$
Example Algorithms for piecewise linear Bregman divergence learning (PBDL)

Step 1: Given $X = \{x_1, \ldots, x_n\}$, partition $X$ to $K$ sets using farthest point clustering $\mathcal{C} = \{C_1, \ldots, C_K\}$, $C_k = \{x_{i_1}, \ldots, x_{i_{m_k}}\}$, $C_i \cap C_j = \emptyset$, $i, j = 1, \ldots, K$. Define $p_j = k$ given $x_j \in C_k$.

Step 2e: Given regression data $S_m = \{(x_{i_1}, x_{i_2}, y_i) | i = 1, \ldots, m\}$, solve the QP:

$$\min_{a_k, b_k} \sum_{k=1}^m (b_{p_1} - b_{p_2} + (a_{p_1} - a_{p_2})^T x_{i_1} - y_i)^2$$

subject to:

$$\|a_k\| \leq L, \quad k = 1, \ldots, K.$$

Step 2e: Given relative similarity data $S_m = \{(x_{i_1}, x_{i_2}, x_{i_3}, x_{i_4}, y_i) | i = 1, \ldots, m\}$, solve the LP:

$$\min_{a_k, b_k, L} \sum_{i=1}^m \lambda L$$

subject to:

$$\{\begin{align*}
y_i (b_{p_{i_3}} - b_{p_{i_4}} - b_{p_{i_1}} + b_{p_{i_2}} + (a_{p_{i_3}} - a_{p_{i_4}})^T x_{i_3} - (a_{p_{i_1}} - a_{p_{i_2}})^T x_{i_1}) &\geq 1 - \zeta_i, \quad \forall i, \\
y_i \geq 0, \quad i = 1, \ldots, m, \\
b_{p_j} + a_j^T x_j &\geq b_k + a_k^T x_j, \quad j = 1, \ldots, n, \quad k = 1, \ldots, K.
\end{align*}\}$$

Step 3: Define $h_m(x) = \max_{k=1, \ldots, K} a_k^T x + b_k$, $p(x) = \arg \max_{k=1, \ldots, K} a_k^T x + b_k$ and the learned Bregman divergence $D_{h_m}(x, y') = D_{p(x)} - D_{p(x')} + (a_{p(x)} - a_{p(x')})^T x$.

Noting $D_h(x_1, x_2) = h(x_1) - h(x_2) - \nabla h(x_2)^T (x_1 - x_2)$ and using Lemma 1, we can solve 4 for a fixed partition of the data $\mathcal{C}$ by solving a quadratic optimization problem, which is given as step 2e1 under Example Algorithms for PBDL. We note that finding the optimal partition $\mathcal{C}$ in PBDL is NP-hard and there are heuristics [24, 26] to choose a good partition. We use the Voronoi cell partition obtained by the simple greedy farthest-point clustering algorithm [27] to obtain an approximate solution to this partitioning problem. See appendix, section A5, for some further details on this partitioning algorithm and its associated guarantees.

4.2 Pairwise similarity comparisons

Now suppose we observe the data $S_m = \{(x_{i_1}, x_{i_2}, x_{i_3}, x_{i_4}, y_i) | i = 1, \ldots, m\}$ where $y_i = \text{sign}(D(x_{i_3}, x_{i_4}) - D(x_{i_1}, x_{i_2}))$. We model $D$ as a Bregman divergence parametrized by a piecewise linear function, as in the regression setting. Then we propose to learn the Bregman divergence by empirical risk minimization for mis-classification of these similarity comparisons. We use a margin loss to approximately satisfy the supervision given:

$$h_m = \arg \min_{h \in \mathcal{H}_{\text{P-L}}} L_{S_m}^{\text{hinge}}(D_{h_m}) = \frac{1}{m} \sum_{i=1}^m \max(0, 1 - y_i (D_h(x_{i_1}, x_{i_4}) - D_h(x_{i_1}, x_{i_2}))) + \lambda L.$$ (5)

Using Lemma 1 and substituting the the hinge loss with $\zeta_i$, we reformulate 3 as a linear programming problem (see Step 2e under Example Algorithms). Later we will provide a PAC generalization bound for PBDL’s misclassification of pairwise similarity comparisons $P\{\text{sign}(D_{h_m}(x_3, x_k) - D_{h_m}(x_1, x_2)) \neq y\}$ in Theorem 2.

5 Analysis

Now we present an analysis of our approach. Due to space considerations, our proofs appear in the appendix. Briefly, our results: i) show that a Bregman divergence parameterized by a piecewise linear convex function can approximate an arbitrary Bregman divergence with error $O_p(K^{-\frac{1}{2}})$, where $K$ is the number of affine functions; ii) bound the Rademacher complexity of the class of Bregman divergences parameterized by piecewise linear generating functions; iii) provide a generalization error for the regression scenario that shows that the error grows as $O_p(m^{-\frac{1}{2}})$; iv) provide a generalization error for the relative similarity classification scenario that shows that the generalization error gap grows as $O_p(m^{-\frac{1}{2}})$.

Approximation Guarantees for Bregman Divergences using Piecewise Linear Functions: First we would like to bound how well one can approximate an arbitrary Bregman divergence when using...
Furthermore, the generalization error of the empirical risk minimizer is bounded by:
\[ \|\phi(x) - h(x)\|_\infty \leq 4R^2L_\phi K^{-\frac{1}{2}}, \]
\[ \|\nabla \phi(x) - \nabla h(x)\|_1 \leq 16RL_\phi K^{-\frac{1}{2}}, \]
and
\[ \phi(x) - h(x) \geq 0, \forall x \]
where \( \Omega_R = \Omega \cap B(0, R) \), where \( B(x_0, R) \) is the q-norm ball of radius \( R \) centered at \( x_0 \) and \( \epsilon = 2RK^{-1/d} \).

By combing the approximators constructed \( h \) and its sub-gradient \( \nabla h \) in theorem 1, we can prove that the Bregman divergence \( D_h \) can approximate \( D_\phi \) with arbitrary accuracy (see Appendix 3).

**Corollary 1** For each Bregman divergence \( D_\phi \) with \( \phi \in C_{L,1} \), there exists \( h \in F_{P,L} \) such that:
\[ \sup_{x_1, x_2 \in \Omega_R} |D_\phi(x_1, x_2) - D_h(x_1, x_2)| \leq 36R^2L_\phi K^{-\frac{1}{2}}. \]

**Rademacher Complexity of Bregman Divergences with Piecewise Linear Functions:** Another result we require for proving generalization error is the Rademacher complexity of the class of Bregman divergences using our choice of generating functions. We have the following result:

**Lemma 2.** The Rademacher complexity of Bregman divergences parameterized by a max-affine functions \( R_m(D_{P,L}) \leq 4KLR\sqrt{\frac{2\ln(2d+2)}{m}} \).

**Generalization Error for Bregman Regression:** Next we consider the regression scenario. Here we are interested in the expected squared loss between the Bregman divergence obtained from the minimizer of the regression loss and the true divergence value, on unseen (test) data. We have the following result:

**Theorem 2.** Consider \( S_m = \{(x_1, x_2, y_i), i = 1, \ldots, m\} \sim \mu^n \). Let \( \|\|_\mu^2 = E[\|\cdot\|_\mu^2] \) and assume,

- \( A_1: E[y|x_1, x_2] = D_\phi(x_1, x_2) \), with \( \phi \in C_{L,1} \)
- \( A_2: \|x\|_\infty \leq R \) and \( \sup |y - E[y|x_1, x_2]| \leq \sigma \) i.e. both the input and noise are bounded.

The generalization error of the empirical risk minimizer \( D_{h_m} \) of the regression loss on \( S_m \) is bounded by
\[ \|D_{h_m} - y\|_\mu^2 \leq \|D_{h_m} - y\|_{S_m}^2 + 16MKLR\sqrt{\frac{2\ln(2d+2)}{m}} + M^2 \sqrt{\ln(1/\delta)/m} \text{ w.p. } 1 - \delta. \]

Furthermore, \( D_{h_m} \) converges to the ground truth Bregman divergence \( D_\phi \) and the approximation error is bounded by
\[ \|D_{h_m} - D_\phi\|_\mu^2 \leq 36R^2L_\phi K^{-\frac{1}{2}} + 16MKLR\sqrt{\frac{2\ln(2d+2)}{m}} + M^2 \sqrt{\frac{2\ln 2/\delta}{m}} \text{ w.p. } 1 - \delta \]
where \( M = 4LR + \sigma \). By choosing \( K = \lceil m^{\frac{d}{2d+2}} \rceil \) we get: \( \|D_{h_m} - D_\phi\|_\mu^2 = O_p(m^{-\frac{d}{2d+2}}) \).

**Generalization Error for Relative Constraint Divergence Learning:** Finally, we consider the case of classification error when learning a Bregman divergence under relative similarity constraints. As with the regression case, our result bounds the loss on unseen data based on the loss on the training data.

**Theorem 3.** Consider \( S_m = \{(x_1, x_2, x_3, y_i), i = 1, \ldots, m\} \sim \mu^n \). Assume \( \|x\|_\infty \leq R \).

The generalization error of \( D_{h_m} \) the solution to PBDL learned from \( S_m \) satisfies
\[ L_{\mu}^{\text{hinge}}(D_{h_m}) \leq L_{S_m}^{\text{hinge}}(D_{h_m}) + \frac{32KL\sqrt{2\ln(2d+2)}}{\sqrt{m}} + \sqrt{\frac{4\ln(4\log_2 L) + \ln(1/\delta)}} \sqrt{m}, \]
with probability at least \( 1 - \delta \). Note: \( P(\text{sign}(D_{h_m}(x_3, x_4) - D_{h_m}(x_1, x_2)) \neq y) \leq L_{\mu}^{\text{hinge}}(D_{h_m}). \)
6 Experiments

In the following, all results are represented using 95% confidence intervals, computed using 50 runs. Our optimization problems are solved using Gurobi solvers. We compared against several existing Mahalanobis metric learning methods, as well as some baselines. Note that we also compared to ITML but found its performance in general to be much worse than the other metric learning methods. Code of our approach is available on our github page.

6.1 Bregman divergence regression on synthetic data

Data: We generate 100 synthetic data points in three ways: i) discrete probability distributions \( \{(p_1, p_2) \} \) such that \( p_1 + p_2 = 1, p_1, p_2 \geq 0 \) sampled from a Dirichlet probability distribution \( \text{Dir}(\{1\}_{1 \times 2}) \), with a target value \( y \) computed as the KL divergence between pairs of distributions; ii) symmetric 2-2 matrices sampled from a Wishart distribution \( W_2([1]_{1 \times 2}, 10) \) with target value \( y \) computed as the LogDet divergence between pairs; iii) data points are sampled uniformly from a unit-ball \( B_{\infty}([0, 1]_{1 \times 2}, 1) \) with target value \( y \) computed as the Itakura-Saito distance between pairs. In each case we add Gaussian noise with std\( \begin{pmatrix} 0.05 \end{pmatrix} \) to the ground truth divergences. For training, we provide all pairs of an increasing set of points \( \{(x_i, x_1, y_i) \} \) for \( (i_1, i_2) \) in the power set of \( \{x_1, \ldots, x_m\} \) and the target values \( y_i \) as noisy Bregman divergence of those pairs. For testing, we generate 1000 data points from the same distribution and use noiseless Bregman divergences as targets.

Details and observations: For Bregman regression, we choose the Lipschitz constraint of PBDL for regression to be \( \infty \) since the result was not sensitive to the choice of \( L \). For Mahalanobis regression we do gradient descent for optimizing the least-square fit of a general Mahalanobis metric with the observed data which is done until convergence (as the problem is convex). We see from Figure 6.1 that Mahalanobis metric learning is not flexible enough to model the data coming from these three Bregman divergences, whereas the proposed divergence learning framework PBDL is shown to drastically improve the fit and seems to be a consistent estimator as motivated earlier in Theorem 2.

6.2 Bregman clustering, similarity ranking and k-nn from relative similarity comparisons

In this experiment we implement PBDL on five UCI classification data sets that have previously been used for metric learning, as well as the synthetic data provided in Figure 1. We apply the learned divergences to the tasks of k-nn, semi-supervised clustering, and similarity ranking. To learn a Bregman divergence we use a cross-validation scheme with 3 folds. From two folds we learn the Bregman-divergence/Mahalanobis-distance and then test it for the specified task on the other fold. The results are summarized in Table 6.1.

Data: The pairwise inequalities are generated by choosing two random samples \( x_1, x_2 \) from a random class and another random sample \( x_3 \) from a different class. Since we want the data points within a class be close together we provide as supervision \( D(x_1, x_2) \leq D(x_1, x_3) \). The number of inequalities provided was 15000 for each case.

Divergence learning details: The number of hyperplanes \( K \) and value of \( \lambda \) in our algorithm (PBDL) were both chosen by 3-fold cross validation on training data on a grid \( K = 40 : 20 : 120 \) and \( \lambda = 10^{-3.1 : -1} \). For implementing ITML we used the original code and the hyper-parameters were optimized by a similar cross-validation using their tuner for each different task. We used the code provided in Matlab statistical and machine learning toolbox for a diagonal version of NCA and the hyper-parameter tuning was done the same way as was done for ITML. For LMNN we used their

https://github.com/Siahkamari/Learning-Bregman-Divergences

Figure 2: Regression with KL-div (left), LogDet-div (middle) and Itakura-Saito distance (right).
Table 1: Learning Bregman divergence from pairwise inequalities. Bold values indicate where our proposed method outperforms competing algorithms.

| Data-set  | Algorithm | Clustering |  |  | K-NN |  |  | Ranking |  |  |
|-----------|-----------|------------|---|---|-----|---|---|---------|---|---|
|           |           | Rand-Ind % | Purity | Accuracy | Ave-P | AUC |
| Iris      | PBDL      | 95.1 ± 0.6 | 95.9 ± 0.5 | 95.9 ± 0.5 | 94.7 ± 0.5 | 97.2 ± 0.3 |
|           | ITML      | 95.6 ± 0.5 | 96.6 ± 0.4 | 96.6 ± 0.4 | 94.8 ± 0.3 | 97.2 ± 0.2 |
|           | LMNN      | 94.5 ± 0.6 | 95.5 ± 0.5 | 96.3 ± 0.3 | 93.3 ± 0.4 | 96.4 ± 0.2 |
|           | NCA       | 93.5 ± 0.6 | 94.6 ± 0.6 | 95.9 ± 0.4 | 92.4 ± 0.3 | 95.8 ± 0.2 |
|           | Euclidean | 88.1 ± 0.6 | 89.3 ± 0.6 | 96.2 ± 0.4 | 88.4 ± 0.4 | 93.2 ± 0.3 |
|           |           | 76.4 ± 0.7 | 86.3 ± 0.5 | 87.7 ± 0.5 | 79.9 ± 0.5 | 78.8 ± 0.5 |
|           | ITML      | 71.9 ± 0.9 | 83.1 ± 0.7 | 86.4 ± 0.6 | 74.9 ± 0.4 | 71.7 ± 0.5 |
|           | LMNN      | 57.0 ± 0.6 | 69.6 ± 0.6 | 84.6 ± 0.6 | 69.2 ± 0.4 | 63.2 ± 0.4 |
|           | NCA       | 70.3 ± 0.7 | 81.3 ± 0.7 | 90.0 ± 0.4 | 74.5 ± 0.4 | 70.3 ± 0.4 |
|           | Euclidean | 58.1 ± 0.5 | 70.5 ± 0.6 | 83.5 ± 0.5 | 67.4 ± 0.4 | 60.7 ± 0.4 |
| Balance Scale | PBDL | 73.6 ± 0.7 | 80.5 ± 0.7 | 85.1 ± 0.5 | 77.2 ± 0.4 | 84.1 ± 0.3 |
|           | ITML      | 69.8 ± 0.5 | 77.8 ± 0.6 | 90.6 ± 0.4 | 74.9 ± 0.8 | 80.5 ± 0.7 |
|           | LMNN      | 70.7 ± 0.4 | 78.4 ± 0.4 | 90.1 ± 0.3 | 74.2 ± 0.3 | 80.4 ± 0.2 |
|           | NCA       | 58.9 ± 0.5 | 65.9 ± 0.8 | 84.6 ± 0.3 | 61.7 ± 0.3 | 66.7 ± 0.2 |
|           | Euclidean | 59.2 ± 0.4 | 66.4 ± 0.7 | 85.1 ± 0.3 | 61.8 ± 0.3 | 66.8 ± 0.2 |
| Wine      | PBDL      | 84.9 ± 1.6 | 85.4 ± 1.9 | 94.0 ± 0.7 | 91.0 ± 0.7 | 94.2 ± 0.5 |
|           | ITML      | 82.9 ± 1.5 | 84.2 ± 1.7 | 93.1 ± 0.6 | 83.9 ± 0.9 | 88.9 ± 0.7 |
|           | LMNN      | 82.6 ± 1.5 | 83.8 ± 1.7 | 95.9 ± 0.4 | 88.2 ± 0.5 | 91.5 ± 0.4 |
|           | NCA       | 71.0 ± 0.5 | 70.1 ± 0.7 | 86.8 ± 0.9 | 65.6 ± 0.6 | 77.6 ± 0.5 |
|           | Euclidean | 70.7 ± 0.5 | 69.7 ± 0.8 | 69.5 ± 0.8 | 65.8 ± 0.7 | 77.6 ± 0.6 |
| Transfusion | PBDL | 58.3 ± 0.5 | 76.3 ± 0.3 | 75.0 ± 0.5 | 68.9 ± 0.4 | 55.9 ± 0.3 |
|           | ITML      | 59.7 ± 0.7 | 76.4 ± 0.3 | 74.7 ± 0.4 | 67.3 ± 0.4 | 54.2 ± 0.3 |
|           | LMNN      | 57.0 ± 0.7 | 76.3 ± 0.3 | 75.9 ± 0.4 | 67.1 ± 0.3 | 53.5 ± 0.3 |
|           | NCA       | 60.4 ± 0.5 | 76.3 ± 0.4 | 74.5 ± 0.4 | 66.8 ± 0.4 | 54.3 ± 0.2 |
|           | Euclidean | 60.3 ± 0.5 | 76.3 ± 0.3 | 74.7 ± 0.4 | 66.9 ± 0.3 | 54.3 ± 0.2 |
| Figure 1 data | PBDL | 98.2 ± 0.6 | 98.4 ± 0.7 | 98.6 ± 0.2 | 98.4 ± 0.2 | 99.1 ± 0.1 |
|           | ITML      | 74.0 ± 0.9 | 71.3 ± 1.6 | 98.9 ± 0.1 | 84.0 ± 0.2 | 91.3 ± 0.1 |
|           | LMNN      | 74.5 ± 1.1 | 71.5 ± 1.7 | 98.9 ± 0.1 | 83.4 ± 0.2 | 90.1 ± 0.3 |
|           | NCA       | 74.0 ± 0.9 | 71.5 ± 1.5 | 99.0 ± 0.1 | 84.0 ± 0.2 | 91.2 ± 0.1 |
|           | Euclidean | 74.7 ± 0.9 | 72.8 ± 1.5 | 98.9 ± 0.1 | 84.1 ± 0.2 | 91.3 ± 0.1 |

most recent code provided to date (LMNN3.0.0). Hyper-parameter tuning for LMNN was done using their provided tuner.

For the clustering task, it was shown in [5] that one can do clustering similarly to k-means for any Bregman divergence. We use the learned Bregman divergence to do Bregman clustering and measure the performance under Rand-Index and Purity. For k-nn, we use the learned Bregman divergence between a query point \( x \) as the first input and other training data as the second argument of the Bregman divergence to do k-nn classification with \( k = 5 \). For the ranking task, for each test data point \( x \) we rank all other test data points according to their Bregman divergence. The ground truth ranking is one where for any data point \( x \) all similarly labeled data points are ranked earlier than any data from other classes. We evaluate the performance by computing average-precision (Ave-P) and Area under ROC curve (AUC) on test data as in [7].

Observations: We perform comparably to Mahalanobis metric learning method for the k-nn problem, but clearly outperform the linear methods on the clustering and ranking tasks. This suggests that Bregman divergences may be most useful for downstream clustering and ranking tasks.

Conclusions: We developed a framework for learning arbitrary Bregman divergences by using max-affine generating functions. We precisely bounded approximation error of such functions as well as provided generalization guarantees in the regression and relative similarity setting. As part of our future work, we would like to explore integration of this approach with deep learning methods to compete with existing deep metric learning methods.

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References

[1] Brian Kulis. Metric learning: A survey. *Foundations and Trends® in Machine Learning*, 5(4):287–364, 2013.

[2] Matthew Schultz and Thorsten Joachims. Learning a distance metric from relative comparisons. In *Advances in neural information processing systems*, pages 41–48, 2004.

[3] Kilian Q Weinberger and Lawrence K Saul. Distance metric learning for large margin nearest neighbor classification. *Journal of Machine Learning Research*, 10(Feb):207–244, 2009.

[4] Jason V Davis, Brian Kulis, Prateek Jain, Suvrit Sra, and Inderjit S Dhillon. Information-theoretic metric learning. In *Proceedings of the 24th international conference on Machine learning*, pages 209–216. ACM, 2007.

[5] Tie-Yan Liu et al. Learning to rank for information retrieval. *Foundations and Trends® in Information Retrieval*, 3(3):225–331, 2009.

[6] Arindam Banerjee, Srujana Merugu, Inderjit S Dhillon, and Joydeep Ghosh. Clustering with bregman divergences. *Journal of machine learning research*, 6(Oct):1705–1749, 2005.

[7] Brian McFee and Gert R Lanckriet. Metric learning to rank. In *Proceedings of the 27th International Conference on Machine Learning (ICML-10)*, pages 775–782, 2010.

[8] Jacob Goldberger, Geoffrey E Hinton, Sam T Roweis, and Ruslan R Salakhutdinov. Neighbourhood components analysis. In *Advances in neural information processing systems*, pages 513–520, 2005.

[9] Aurélien Bellet and Amaury Habrard. Robustness and generalization for metric learning. *Neurocomputing*, 151:259–267, 2015.

[10] Qiong Cao, Zheng-Chu Guo, and Yiming Ying. Generalization bounds for metric and similarity learning. *Machine Learning*, 102(1):115–132, 2016.

[11] Dong Yi, Zhen Lei, Shengcai Liao, and Stan Z Li. Deep metric learning for person re-identification. In *2014 22nd International Conference on Pattern Recognition*, pages 34–39. IEEE, 2014.

[12] Elad Hoffer and Nir Ailon. Deep metric learning using triplet network. In *International Workshop on Similarity-Based Pattern Recognition*, pages 84–92. Springer, 2015.

[13] Aurélien Bellet, Amaury Habrard, and Marc Sebban. Metric learning. *Synthesis Lectures on Artificial Intelligence and Machine Learning*, 9(1):1–151, 2015.

[14] Kiri Wagstaff, Claire Cardie, Seth Rogers, Stefan Schrödl, et al. Constrained k-means clustering with background knowledge. In *ICML*, volume 1, pages 577–584, 2001.

[15] Shai Shalev-Shwartz, Yoram Singer, and Andrew Y Ng. Online and batch learning of pseudometrics. In *Proceedings of the twenty-first international conference on Machine learning*, page 94. ACM, 2004.

[16] Prateek Jain, Brian Kulis, Inderjit S Dhillon, and Kristen Grauman. Online metric learning and fast similarity search. In *Advances in neural information processing systems*, pages 761–768, 2009.

[17] Eric P Xing, Michael I Jordan, Stuart J Russell, and Andrew Y Ng. Distance metric learning with application to clustering with side-information. In *Advances in neural information processing systems*, pages 521–528, 2003.

[18] Lei Wu, Rong Jin, Steven C Hoi, Jianke Zhu, and Nenghai Yu. Learning bregman distance functions and its application for semi-supervised clustering. In *Advances in neural information processing systems*, pages 2089–2097, 2009.

[19] Olvi L Mangasarian, J Ben Rosen, and ME Thompson. Global minimization via piecewise-linear underestimation. *Journal of Global Optimization*, 32(1):1–9, 2005.

[20] Pedro Julián, Mario Jordán, and Alfredo Desages. Canonical piecewise-linear approximation of smooth functions. *IEEE Transactions on Circuits and Systems I: Fundamental Theory and Applications*, 45(5):567–571, 1998.

[21] Stephen Boyd and Lieven Vandenberghe. *Convex optimization*. Cambridge university press, 2004.
[22] Gábor Balázs, András György, and Csaba Szepesvári. Near-optimal max-affine estimators for convex regression. In AISTATS, 2015.

[23] Gaurav Gothoskar, Alex Doboli, and Simona Doboli. Piecewise-linear modeling of analog circuits based on model extraction from trained neural networks. In Proceedings of the 2002 IEEE International Workshop on Behavioral Modeling and Simulation, 2002. BMAS 2002., pages 41–46. IEEE, 2002.

[24] Alessandro Magnani and Stephen P Boyd. Convex piecewise-linear fitting. Optimization and Engineering, 10(1):1–17, 2009.

[25] Gábor Balázs. Convex Regression: Theory, Practice, and Applications. PhD thesis, University of Alberta, 2016.

[26] Lauren A Hannah and David B Dunson. Multivariate convex regression with adaptive partitioning. The Journal of Machine Learning Research, 14(1):3261–3294, 2013.

[27] Teofilo F Gonzalez. Clustering to minimize the maximum intercluster distance. Theoretical Computer Science, 38:293–306, 1985.

[28] LLC Gurobi Optimization. Gurobi optimizer reference manual, 2018.

[29] Martin Anthony and Peter L Bartlett. Neural network learning: Theoretical foundations. Cambridge university press, 2009.

[30] Shai Shalev-Shwartz and Shai Ben-David. Understanding machine learning: From theory to algorithms. Cambridge university press, 2014.

[31] Mehryar Mohri, Afshin Rostamizadeh, and Ameet Talwalkar. Foundations of machine learning. MIT press, 2018.
Appendix

In this appendix, we provide full proofs of the theoretical claims given in the main paper, as well as some additional details about our algorithms.

A1 Covering and Packing

This is a brief overview of covering and packing numbers from [29]. Let $(\Omega, || \cdot ||)$ be a metric space and $\Omega \subset U$. For any $\epsilon > 0$, $x_{\epsilon} \subset U$ is an $\epsilon$-covering of $\Omega$ if:

$$\min_{x \in x_{\epsilon}} ||x - \hat{x}|| \leq \epsilon \ \forall x \in \Omega.$$ 

An $\epsilon$-packing of $\Omega$ is a set $U_{\epsilon} \subset \Omega$ such that:

$$\min_{\hat{x} \in U_{\epsilon}, \forall x} ||x - \hat{x}|| > \epsilon \ \forall x \in U_{\epsilon}.$$ 

The covering number $N(\Omega, \epsilon, || \cdot ||)$ is defined as the minimum cardinality of an $\epsilon$-covering of $\Omega$. The packing number $M(\Omega, \epsilon, || \cdot ||)$ is defined as the maximum cardinality of an $\epsilon$-packing of $\Omega$. There exist the following relation between covering and packing numbers:

$$M(\Omega, 2\epsilon, || \cdot ||) \leq N(\Omega, \epsilon, || \cdot ||) \leq M(\Omega, \epsilon, || \cdot ||).$$

Furthermore by some volumetric arguments, the covering number of the norm ball of radius $R$ in $d$-dimension $B_{\parallel \cdot \parallel}(R)$ is bounded:

$$\left( \frac{R}{\epsilon} \right)^d \leq N(B_{\parallel \cdot \parallel}(R), \epsilon, || \cdot ||) \leq \left( \frac{2R}{\epsilon} + 1 \right)^d.$$ 

A2 Rademacher complexity of piecewise linear Bergman divergences

The Rademacher complexity $R_m(\mathcal{F})$ of a function class $\mathcal{F}$ is defined as the expected maximum correlation of a function class with binary noise: $\frac{1}{m} \mathbb{E}_{\sigma \in \{-1,1\}} \left[ \sup_{f \in \mathcal{F}} \sum_{i=1}^{m} \sigma_i f(x_i) \right]$ [30]. Bounding the Rademacher complexity of a function class provides us with a measure of how complex the class is, in the sense used in [31][30] for computing probably approximately correct (PAC) generalization bounds for learning tasks such as classification, regression, and ranking. Let

$$\mathcal{F}_{P,L} = \{ h : \Omega \to \mathbb{R} : h(x) = \max_{k=1,...,K} a_k^T x + b_k, \ ||a_k||_1 \leq L \}$$

be the class of convex $L$-Lipschitz max-affine functions. Also let

$$\mathcal{D}_{P,L} = \{ h(x) - h(y) - \nabla h(y)^T (x - y) : \Omega_R \times \Omega_R \to \mathbb{R}^+ : h \in \mathcal{F}_{P,L} \}$$

be the class of Bregman divergences parameterized by a max-affine functions, where $\Omega_R = \Omega \cap B_{\infty}(x_0, R)$, and $B_{\infty}(x_0, R)$ is the $\infty$-norm ball of radius $R$ centered at $x_0$.

**Lemma 2.** The Rademacher complexity of Bregman divergences parameterized by a max-affine functions $R_m(\mathcal{D}_{P,L}) \leq 4KLR \sqrt{\frac{\ln(2d+2)}{m}}$.

**Proof.**

$$\mathcal{D}_{P,L} = \{ h(x) - h(y) - \nabla h(y)^T (x - y) \ | \ h \in \mathcal{F}_{P,L} \}$$

$$= \{ a_{p(x)}^T x + b_{p(x)} - (a_{p(y)}^T x + b_{p(y)}) \ | \ p(t) = \arg \max_k a_k^T t + b_k \}$$

$$= \{ a_{p(x)}^T x + b_{p(x)} - b_{p(0)} + LR - (a_{p(y)}^T x + b_{p(y)} - b_{p(0)} + LR) \ | \ p(t) = \arg \max_k a_k^T t + b_k \}$$

$$= \{ a_{p(x)}^T x + c_{p(x)} - (a_{p(y)}^T x + c_{p(y)}) \ | \ p(t) = \arg \max_k a_k^T t + b_k, c_i = b_i - b_{p(0)} + LR \}.$$ 

Note that $|c_1| \leq LR$:

$$-c_i = b_{p(0)} - b_i - LR = \max_k b_k - b_i - LR \geq -LR.$$
For the other side,
\[-c_i = b_p(0) - b_i - LR = \max_k b_k - b_i - LR \leq h(0) - h(x) + a_i^T x - LR \leq L\|0 - x\|_\infty + \|a_i\|_\infty x - LR \leq LR.\]

Now we are ready to compute the Radamacher complexity:

\[R_m(D_{P,L}) = \frac{1}{m} \mathbb{E}_\sigma \sup \sum_{i=1}^m \sigma_i D_h(x_i, y_i)\]
\[= \frac{1}{m} \mathbb{E}_\sigma \sup_{\|a_k\|_1 \leq L} \sum_{i=1}^m \sigma_i (a_p(x_i) x_i + c_p(x_i) - a_p(y_i) x_i - c_p(y_i))\]
\[\leq \frac{2}{m} \mathbb{E}_\sigma \sup_{\|a_k\|_1 \leq L} \sum_{i=1}^m \sum_{k=1}^K \sigma_i (a_k^T x_i + c_k)\]
\[= \frac{2K}{m} \mathbb{E}_\sigma \sup_{\|a_k\|_1 \leq L} \sum_{i=1}^m \sigma_i \left[ \frac{c_i/R}{a_1} \right]^T [R] \left[ x_i \right].\]

The last expression is \(2K\) times the complexity of a Lipschitz linear function which is computed in [30, Sec. 26.2]. Therefore:

\[R_m(D_{P,L}) \leq 2K \left\| \left[ \frac{c_i/R}{a_1} \right] \right\|_1 \times \sup_{i} \left\| \left[ R \right] \right\|_\infty \sqrt{\frac{2 \ln (2d + 2)}{m}}\]
\[\leq 2K \times 2L \times R \times \sqrt{\frac{2 \ln (2d + 2)}{m}}.\]

\[\square\]

**A3 Approximation results for Max-affine functions**

**Lemma 3.** For \(r_1, r_2 \in \mathbb{R}^d\), and \(\frac{1}{p} + \frac{1}{q} = 1\), \(p, q \in \mathbb{R}_+\), we have \(\|r_1 - r_2\|_p \leq \delta\) if and only if:
\[r_1^T u \geq r_2^T u - \delta, \quad \forall u \in \mathbb{R}^d, \|u\|_q = 1.\]

**Proof.** For one side consider \(\|r_1 - r_2\|_p \leq \delta\). By using Hölder’s inequality we have:
\[(r_2 - r_1)^T u \leq \|r_2 - r_1\|_p \|u\|_q = \|r_2 - r_1\|_p \leq \delta\]
\[\Rightarrow r_1^T u \geq r_2^T u - \delta.\]

For the other side by using extremal equality we have:
\[\|r_1 - r_2\|_p = \max_u \{(r_2 - r_1)^T u \|u\|_q = 1\} \leq \delta\]

\[\square\]

**Lemma 4.** Consider the piecewise linear function
\[h(x) = \max_{k=1,\ldots,K} \phi(\hat{x}_k) + \nabla \phi(\hat{x}_k)^T (x - \hat{x}_k),\]
where \(\phi(x)\) is a convex function. All sub-gradients of \(h(x)\) are lower bounded at \(K\) directions:
\[\nabla h(x)^T u_k \geq \nabla \phi(\hat{x}_k)^T u_k, \quad \forall u_k = \frac{x - \hat{x}_k}{\|x - \hat{x}_k\|}, \quad k = 1, \ldots, K.\]

(8)
Proof. We start the proof by the definition of sub-gradients of \( h(x) \):
\[
\nabla h(x)^T (x - z) \geq h(x) - h(z) \quad \forall z
\]
\[
\Rightarrow \nabla h(x)^T (x - \hat{x}_k) \geq h(x) - h(\hat{x}_k) \quad (z \leftarrow \hat{x}_k)
\]
\[
\nabla h(x)^T (x - \hat{x}_k) \geq h(x) - \phi(\hat{x}_k) \quad (h(\hat{x}_k) = \phi(\hat{x}_k) \text{ due to convexity})
\]
\[
\geq \phi(\hat{x}_k) + \nabla \phi(\hat{x}_k)^T (x - \hat{x}_k) - \phi(\hat{x}_k) \quad \forall \hat{x}_k
\]
\[
= \nabla \phi(\hat{x}_k)^T (x - \hat{x}_k) \quad \forall \hat{x}_k.
\]
By dividing the both side of the above by \( \|x - \hat{x}_k\| \), we’ll get the proposition of the lemma.  

Define \( F_{\mathcal{C},L,L_g} \) to be the class of \( L \)-Lipschitz convex function with a \( L_g \)-Lipschitz gradient:
\[
F_{\mathcal{C},L,L_g} \doteq \{ \phi : \Omega \to \mathbb{R} \mid \phi \text{ is convex}, \|\phi(x_1) - \phi(x_2)\| \leq L \|x_1 - x_2\|_\infty, \|\nabla \phi(x_1) - \nabla \phi(x_2)\|_1 \leq L \|x_1 - x_2\|_\infty \}.
\]

**Theorem 1.** For each \( \phi : \Omega \to \mathbb{R} \), \( \phi \in F_{\mathcal{C},L,L_g} \) one can construct \( h \in F_{P,L} \) such that:
\[
\sup_{x \in \Omega_R} |\phi(x) - h(x)| \leq 4R^2L_gK\frac{\epsilon^2}{d},
\]
\[
\sup_{x \in \Omega_R} \|\nabla \phi(x) - \nabla h(x)\|_1 \leq 16RL_gK\frac{\epsilon^2}{d}, \text{ and}
\]
\[
\phi(x) - h(x) \geq 0, \forall x
\]
where \( \Omega_R = \Omega \cap B_\infty(x_0, R) \), where \( B_\epsilon(x_0, R) \) is the \( q \)-norm ball of radius \( R \) centered at \( x_0 \) and \( \epsilon = 2RK^{-1/d} \).

**Proof.** The proof of (9) and (11) is based on ideas in [25]; however, they do not make the Lipschitz gradient assumption and derive a slightly different bound with a more involved proof.

Let \( X_e \subset \Omega_R \) be a \((2\epsilon)^d\)-grid over \( B_\infty(x_0, R) \) This set provides an \( \epsilon \)-cover for \( \Omega_R \) over \( \| \cdot \|_\infty \) of size
\[
\mathcal{N}(\epsilon, \| \cdot \|_\infty) \leq |X_e| \leq \left( \frac{2R}{2\epsilon} + 1 \right)^d \leq \left( \frac{2R}{\epsilon} \right)^d, \quad \forall \epsilon \leq R,
\]
Choose \( \epsilon = 2RK^{-1/d} \) and therefore \( |X_e| \leq K \). Let \( X_e = \{ \hat{x}_1, \ldots, \hat{x}_K \} \) and \( \hat{x} = \arg \min_{\hat{x}_k \in X_e} \|x - \hat{x}_k\|_\infty \). We know that \( \|x - \hat{x}\|_\infty \leq \epsilon \) due to construction of \( X_e \). Consider the piecewise linear function,
\[
h(x) \doteq \max_{k=1,\ldots,K} \phi(\hat{x}_k) + \nabla \phi(\hat{x}_k)^T (x - \hat{x}_k).
\]
Then we have:
\[
0 \leq \phi(x) - h(x) \leq \phi(x) - \phi(\hat{x}) + \nabla \phi(\hat{x})^T (x - \hat{x}) \quad (h \text{ is max-affine})
\]
\[
\leq \nabla \phi(x)^T (x - \hat{x}) - \nabla \phi(\hat{x})^T (x - \hat{x}) = (\nabla \phi(x) - \nabla \phi(\hat{x}))^T (x - \hat{x}) \quad (\text{convexity of } \phi)
\]
\[
\leq \|\nabla \phi(x) - \nabla \phi(\hat{x})\|_1 \|x - \hat{x}\|_\infty \quad (\text{Hölder’s inequality})
\]
\[
\leq L_g\|x - \hat{x}\|_\infty^2 \leq L_g \epsilon^2 = 4R^2L_gK\frac{\epsilon^2}{d}. \quad (\nabla \phi \text{ is } L_g\text{-Lipschitz})
\]
Therefore the (9) and (11) are shown. Now we show all sub-gradient of the piecewise linear approximator \( h(x) \) introduced in (12) provides a good approximation for \( \nabla \phi \). From Lemma3 it is sufficient to show that:
\[
\nabla h(x)^T u \geq \nabla \phi(x)^T u - \delta, \quad \forall u \in \mathbb{R}^d, \|u\|_1 = 1,
\]
(13)
since this is sufficient and necessary for \( \|\nabla \phi(x) - \nabla h(x)\|_1 \leq \delta \). Now consider the covering points \( \hat{x}_k \) such that \( \|x - \hat{x}_k\|_\infty \leq \delta \); therefore:
\[
\|\nabla \phi(x) - \nabla \phi(\hat{x}_k)\|_1 \leq L_g\|x - \hat{x}_k\|_\infty \leq L_g\delta.
\]
(14)
Using Lemma3 we have for all unit vectors \( u \):
\[
\nabla \phi(\hat{x}_k)^T u \geq \nabla \phi(x)^T u - \delta L_g, \quad \forall \{\hat{x}_k \in X_e \mid \hat{x}_k \in X_e \cap B_\infty(x, \delta)\}.
\]
(15)
Further from Lemma 4 we know that:

\[ \nabla h(x)^T u_k \geq \nabla \phi(\hat{x}_k)^T u_k, \quad \forall u_k = \frac{x - \hat{x}_k}{\|x - \hat{x}_k\|}, \quad k = 1, \ldots, K. \]  

(16)

Therefore by combining (16) and (15) we have:

\[ \nabla h(x)^T u_k \geq \nabla \phi(x)^T u_k - \delta L_g, \quad \forall \{u_k = \frac{x - \hat{x}_k}{\|x - \hat{x}_k\|} \mid \hat{x}_k \in \Omega \cap B_\infty(x, \delta)\}. \]  

(17)

If (17) was true for all unit vectors \( u \), immediately we had (13) and we were done, but (17) holds only for unit directions connecting \( x \) to covering points \( \hat{x}_k \) nearby. Next we prove that if we set \( \delta = 4\epsilon \), by combining linear combinations of (17) we can get for any unit direction \( u \),

\[ \nabla h(x)^T u \geq \nabla \phi(x)^T u - 8\epsilon L_g, \quad \forall u \in \mathbb{R}^d, \quad \|u\|_\infty = 1. \]  

(18)

By using a convex combination of inequalities (17) such that \( \sum_{k=1}^K \alpha_k = 1 \), \( \alpha_k \geq 0 \) we get:

\[ \nabla h(x)^T \sum_{k=1}^K \alpha_k(x - \hat{x}_k) \geq \nabla \phi(x)^T \sum_{k=1}^K \alpha_k(x - \hat{x}_k) - \delta^2 L_g, \quad \hat{x}_k \in \Omega \cap B_\infty(x, \delta). \]  

(19)

Next we show that if we set \( \delta \geq 2\epsilon \), then \( \sum_{k=1}^K \alpha_k(x - \hat{x}_k) \) can represent any vector of size \( \delta - 2\epsilon \). From there using (13) we have \( \|\nabla \phi(x) - \nabla h(x)\|_1 \leq \delta^2/(\delta - 2\epsilon) L_g \) and by choosing \( \delta = 4\epsilon \) we would get the result and the proof would be complete. Consider hyper-cubes of \( B_\infty(0, \epsilon) \) fitted to each corner of \( B_\infty(x, \delta) \) as in the 2-dimensional case depicted by Figure 1. There has to be covering points \( \bar{S}_\epsilon = \{\hat{x}_1, \ldots, \hat{x}_K\} \subseteq \Omega \) in each of these \( \epsilon \)-hyper-cubes, otherwise the center of these hyper-cubes is further away from all covering points by more than \( \epsilon \), which contradicts the existence of the \( \epsilon \)-cover. As depicted by Figure 1, \( B_\infty(x, \delta - 2\epsilon) \subset \text{Convex-hull}(\bar{S}_\epsilon) \). Therefore any vector of size \( \delta - 2\epsilon \) can be represented by \( \sum_{k=1}^K \alpha_k(x - \hat{x}_k) \). We note that correctness of this proof relies on existence of \( B_\infty(x, \delta) \) in \( \Omega_R \). Therefore the proof is valid only for inputs \( x \) interior to \( \Omega_R \), i.e. \( \forall x \in \Omega \cap B_\infty(x_0, R - \delta) \).

![Figure 3: The 2-dimensional sketch of \( B_\infty(x, \delta) \). Four solid green vectors represent \( x - \hat{x}_k \). Using convex combination of these vectors we can represent any vector \( r \) (red solid vector) of size \( \|r\|_\infty = \delta - 2\epsilon \).](image)

Next by combing the approximators constructed \( h \) and \( \nabla h \) in theorem 1 we can prove that the Bregman divergence \( D_h \) can approximate \( D_\phi \) with arbitrary accuracy.

**Corollary 1** For each Bregman divergence \( D_\phi \) with \( \phi \in \mathcal{F}_{C,L,h_\phi} \), there exists \( h \in \mathcal{F}_{P,L} \) such that:

\[
\sup_{x_1,x_2 \in \Omega_R - 4\epsilon} |D_\phi(x_1, x_2) - D_h(x_1, x_2)| \leq 36R^2L_\phi K^{-\frac{1}{2}}.
\]
Furthermore,

\[ |D_\phi(x_1, x_2) - D_h(x_1, x_2)| = |\phi(x_1) - h(x_1) + h(x_2) - \phi(x_2) - (\nabla \phi(x_2) - \nabla h(x_2))^T (x_1 - x_2)| \]

\[ \leq \max\{|\phi(x_1) - h(x_2)|, |h(x_2) - \phi(x_2)|\} \quad (\text{since } h(x) - \phi(x) \leq 0) \]

\[ + \|\nabla \phi(x_2) - \nabla h(x_2)\|_1 \|x_1 - x_2\|_\infty \]

\[ \leq 4R^2 L_g K \frac{\sigma^2}{\delta} + 16RL_g K \frac{\sigma^2}{\delta} 2R \leq 36R^2 L_g K \frac{\sigma^2}{\delta}. \]

\[ \square \]

**A4 PAC bounds for piecewise Bregman divergence learning**

Here we are interested in the expected squared loss between our learned Bregman divergence over pairs of points and the true divergence value, on unseen (test) data. We have the following result:

**Theorem 2.** Consider \( S_m = \{(x_{i1}, x_{i2}, y_i), i = 1, \ldots, m\} \sim \mu^m \). Let \( \|\cdot\|_\mu = \mathbb{E}[|\cdot|^2] \) and assume,

\[ A_1: E[y|x_1, x_2] = D_\phi(x_1, x_2), \text{ where } \phi : \Omega \to \mathbb{R} \text{ is } L\text{-Lipschitz and convex. Furthermore, the gradient of } \phi \text{ is } L_g\text{-Lipschitz, i.e., } \|\nabla \phi(x) - \nabla \phi(x')\|_1 \leq L_g \|x - x'\|_\infty. \]

\[ A_2: \|x\|_\infty \leq R \& \sup |y - E[y|x_1, x_2]| \leq \sigma, \text{ i.e. the input and noise of observation are both bounded, then the generalization error of the } \alpha\text{-empirical risk minimizer } D_{h_m} \text{ of the regression loss on } S_m \text{ (i.e. } m \sum_{i=1}^m (D_{h_m}(x_{i1}, x_{i2}) - y_i)^2 \leq \min_{h \in \mathcal{F}_{P,L}} \frac{1}{m} \sum_{i=1}^m (D_h(x_{i1}, x_{i2}) - y_i)^2 + \alpha)\).

Then

\[ \|D_{h_m} - y\|_\mu^2 \leq \|D_{h_m} - y\|_{S_m}^2 + 16MKLR \sqrt{\frac{2 \ln(2d + 2)}{m}} + M^2 \sqrt{\frac{\ln 1/\delta}{2m}} \quad \text{w.p. } \geq 1 - \delta. \]

Furthermore, \( D_{h_m} \) converges to the ground truth Bregman divergence \( D_\phi \) and the approximation error is bounded by

\[ \|D_{h_m} - D_\phi\|_\mu^2 \leq 36R^2 L_g^2 K \frac{\sigma^2}{\delta} + 16MKLR \sqrt{\frac{2 \ln(2d + 2)}{m}} + M^2 \sqrt{\frac{2 \ln 2/\delta}{m}} + \alpha \quad \text{w.p. } \geq 1 - \delta \]

where \( M = 4LR + \sigma \). By choosing \( K = \lceil m^{\frac{\sigma^2}{2L^2 R^2}} \rceil \) we get:

\[ \|D_{h_m} - D_\phi\|_\mu^2 = O_p(m^{-\frac{\sigma^2}{2L^2 R^2}}) + \alpha. \]

**Proof.** If \( |f(x) - y| \leq M \) for all \( f \in \mathcal{F}, x \) and \( y \) from \( 31 \) we have that:

\[ \|f(x) - y\|_\mu^2 \leq \|f(x) - y\|_{S_m}^2 + 2MR_{m}(\mathcal{F}) + M^2 \sqrt{\frac{\ln 1/\delta}{2m}} \quad \text{w.p. } \geq 1 - \delta. \]

By substituting \( f = D_{h_m}, \) \( \mathcal{F} = \mathcal{D}_{P,L} \) in the above we immediately get the first line of the proposition.

Further we have that for all \( \hat{f} \in \mathcal{F} \) that doesn’t depend on the training data \( S_m \):

\[ \|f_m(x) - y\|_\mu^2 \leq \|\hat{f}(x) - y\|_{S_m}^2 + 2MR_{m}(\mathcal{F}) + 2M^2 \sqrt{\frac{\ln 2/\delta}{2m}} + \alpha \quad \text{w.p. } \geq 1 - \delta. \]  \[ (20) \]

Also from \( 22 \) we have for all \( f \):

\[ \|f(x) - y\|_\mu^2 - ||f_\ast(x) - y||_\mu^2 = \|f(x) - f_\ast(x)\|_\mu^2, \]

\[ (21) \]

for \( f_\ast(x) = \mathbb{E}[y|x] \). Now, by substituting \( f_m = D_{h_m}, f_\ast = D_\phi, \hat{f} = D_h = \arg\inf_{h \in \mathcal{F}_{P,L}} ||D_\phi - D_h||_\infty \) and \( \mathcal{F} = \mathcal{D}_{P,L} \) in \( 20 \) with probability at least \( 1 - \delta \) we have:
The generalization error of $D$ is given by Theorem 3.

Now note that the hinge loss is $\frac{1}{2}$-Lipschitz. First from Theorem 26.12 in [30] we have for a $f$ such that

$$\|D_{h_m} - y\|_F^2 \leq \|D_h - y\|_F^2 + 2M R_m(D_{P,L}) + 2M^2 \sqrt{\frac{\ln 2/\delta}{2m}}$$

⇒ $\|D_{h_m} - y\|_F^2 - \|D_h - y\|_F^2 \leq \|D_h - y\|_F^2 - 2M R_m(D_{P,L}) + 2M^2 \sqrt{\frac{\ln 2/\delta}{2m}} + \alpha$

⇒ $\|D_{h_m} - y\|_F^2 - \|D_h - y\|_F^2 \leq \|D_h - D_\phi\|_F^2 + 2M R_m(D_{P,L}) + 2M^2 \sqrt{\frac{\ln 2/\delta}{2m}} + \alpha$

$$\leq \|D_h - D_\phi\|_F^2 + 2M R_m(D_{P,L}) + 2M^2 \sqrt{\frac{\ln 2/\delta}{2m}} + \alpha$$

Let $\alpha = 4R + \sigma$.

Now by substituting $M = 4LR + \sigma$ and $R_m(D_{P,L})$ from the value given by Lemma we get the proposition. The only thing left to prove is to show $\forall h \in F_{P,L}$ and $\forall (x, y) \in S_m$ that the error is bounded, i.e., $|y - D_h(x, y)| \leq 4LR + \sigma$: $\|D_{h_m} - y\|_F^2 \leq \|D_h - y\|_F^2 + 2M R_m(D_{P,L}) + 2M^2 \sqrt{\frac{\ln 2/\delta}{2m}} + \alpha$.

Now we observe the data $S_m = \{(x_i, x_2, x_3, x_4, y_i) \mid y_i = \text{sign}(D(x_3, x_4) - D(x_1, x_2))\}$. We propose an ERM for mis-classification of these similarity comparisons.

We use a margin loss to approximately satisfy the supervisions given:

$$h_m = \arg\min_{h \in F_{P,L}} L_{S_m}^{\text{hinge}}(D_{h_m}) = \frac{1}{m} \sum_{i=1}^{m} \max(0, 1 - y_i (D_h(x_i, x_i) - D_h(x_i, x_i))) + \lambda L.$$  

(22)

We provide a PAC generalization bound for $D_{h_m}$ mis-classification of pairwise similarity comparisons $P\{\text{sign}(D_{h_m}(x, y) - D_{h_m}(x, x)) \neq y\}$.

**Theorem 3.** Consider $S_m = \{(x_i, x_2, x_3, x_4, y_i) \mid y_i = \text{sign}(D(x_3, x_4) - D(x_1, x_2))\} \sim \mu^m$. Assume $\|x\|_\infty \leq R$. The generalization error of $D_{h_m}$,

$$L_{\mu}^{\text{hinge}}(D_{h_m}) \leq L_{S_m}^{\text{hinge}}(D_{h_m}) + \frac{32 K LR \sqrt{2 \ln (2d + 2)}}{\sqrt{m}} + \frac{4 \ln (4 \log_2 L + \ln (1/\delta))}{\sqrt{m}},$$

with probability at least $1/2$. Note: $P\{\text{sign}(D_{h_m}(x, y) - D_{h_m}(x, x)) \neq y\} \leq L_{\mu}^{\text{hinge}}(D_{h_m})$.

**Proof.** The proof is very similar to that of Radamacher complexity bounds for soft-SVM given in [30]. First from Theorem 26.12 in [30] we have for a $\rho$-Lipschitz loss function $L(f, z) \leq c$ with probability of at least $1 - \delta$ we have for all $f \in F$:

$$L_{\mu}(f) \leq L_{S_m}(f) + 2\rho R_m(F) + c \sqrt{\frac{2 \ln (2/\delta)}{m}}$$

Now note that the hinge loss is 1-Lipschitz, bounded by 1. By substituting $F = D_{P,L}, f = h_m$ and $L = L_{\mu}^{\text{hinge}}$ we get:

$$L_{\mu}^{\text{hinge}}(D_{h_m}) \leq L_{S_m}^{\text{hinge}}(D_{h_m}) + 4R_m(D_{P,L}) + \sqrt{\frac{2 \ln (2/\delta)}{m}} w.p. \geq 1 - \delta,$$
By replacing $R_m(D_{p,L})$ with the value computed in Lemma 2 we get:

$$L^\text{hinge}_{\mu}(D_{h_m}) \leq L^\text{hinge}_{\mu}(D_{h_m}) + 16KL R \sqrt{\frac{2\ln(2d+2)}{m}} + \sqrt{\frac{2\ln (2\delta)}{m}} \quad w.p. \geq 1 - \delta. \quad (23)$$

Since we are also learning the Lipschitz constant $L$, for having a generalization bound we should express a uniform result for all $L$. We use the trick used in [30] for providing the union bound. To proceed for any integer $i$ take $L_i = 2^i$ and take $\delta_i = \frac{\delta}{2^{7i}}$. then using (23) we have for any $L \leq L_i$,

$$L^\text{hinge}_{\mu}(D_{h_m}) \leq L^\text{hinge}_{\mu}(D_{h_m}) + 16KL_i R \sqrt{\frac{2\ln(2d+2)}{m}} + \sqrt{\frac{2\ln (2\delta_i)}{m}} \quad w.p. \geq 1 - \delta_i. \quad (24)$$

Applying the union bound and noting $\sum_{i=1}^{\infty} \delta_i \leq \delta$ this holds for all $i$ with probability at least $1 - \delta$.

Now take $i = \lceil \log_2 L \rceil \leq \log_2 L + 1$ then $\lambda_i = \frac{(2i)^2}{\delta} \leq \frac{4\log_2 L}{\delta}$. Therefore:

$$L^\text{hinge}_{\mu}(D_{h_m}) \leq L^\text{hinge}_{\mu}(D_{h_m}) + 16KL R \sqrt{\frac{2\ln(2d+2)}{m}} + \sqrt{\frac{2\ln (2\delta)}{m}} \quad w.p. \geq 1 - \delta$$

$$\leq L^\text{hinge}_{\mu}(D_{h_m}) + 32KL R \sqrt{\frac{2\ln(2d+2)}{m}} + \sqrt{\frac{4\ln(4\log_2 L) + \ln (1/\delta)}{m}} \quad w.p. \geq 1 - \delta_i.$$  

Further hinge loss is an upper bound on $0/1$ loss.

\[ \square \]

A5 Farthest-point clustering

Farthest-point clustering is a simple greedy algorithm for a K-center problem, where the objective is to divide the space into $K$ partitions such that the farthest distance between a data point and its closest partition center $\mu_i$ is minimized. This problem can be formulated as: given a set of $n$ points $x_1, \ldots, x_n$ a distance metric $\| \cdot \|$ and a predefined partition size $K$, find a partition of data $C_1, \ldots, C_K$ and partition centers $\mu_1, \ldots, \mu_K$ to minimize the maximum radius of the clusters:

$$\max_i \max_{x \in C_i} \| x - \mu_i \|.$$  

The farthest point clustering introduced in [27] initially picks a random point $x_{00}$ as the center of the first cluster and adds it to the center set $C$. Then for iterations $t = 2 \to K$ does the following: at iteration $t$, computes the distance of all points from the center set $d(x, C) = \min_{\mu \in C} \| x - \mu \|$. Add the point that has the largest distance from the center set (say $x_{t0}$) to the center set. Report $x_{00}, \ldots, x_{K0}$ as the partition centers and assign each data point to its closest center.

Authors of [27] proved that farthest-point clustering is a 2-approximation algorithm (i.e., it computes a partition with maximum radius at most twice the optimum) for any metric. Therefore there is a relation between the partition found by farthest-point clustering and covering set. Assume a set $\{x_1, \ldots, x_n\} \subset \Omega$ has a $\epsilon$-cover of size $K$ over a metric $\| \cdot \|$. The partition found by farthest point clustering of size $K$ is a $2\epsilon$-cover for $\{x_1, \ldots, x_n\}$.

A6 Parameterizing Bregman divergences by piecewise linear functions

We parameterize the Bregman divergence using max-affine functions $h(x) = \max_{k=1, \ldots, K} a_k^T x + b_k$. Using Lemma 1 from our paper with a predefined partition of the training data points $x_1, \ldots, x_n$ to $C = \{C_1, \ldots, C_K\}$ and defining the mapping $p_i \doteq k$ given $x_i \in C_k$, we can write any pairwise divergence on training set as

$$D_h(x_i, x_j) = h(x_i) - h(x_j) - \nabla h(x_j)^T (x_i - x_j)$$

$$= (a_{p_i} x_i + b_{p_i}) - (a_{p_j} x_j + b_{p_j}) - a_{p_j}^T (x_i - x_j)$$

$$= b_{p_i} - b_{p_j} + (a_{p_i} - a_{p_j})^T x_i,$$

which is linear in terms of the parameters $a_k, b_k, k = 1, \ldots, K$. Therefore if the loss function

$$\mathcal{L}(\phi) = \sum_{i=1}^m c_i (D_{\phi}, X, y) + \lambda r(\phi),$$

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is a convex function of pairwise divergences, it will be a convex loss in terms of parameters. Furthermore one needs to satisfy the constraints given by Lemma 1 in our paper to make sure \( h(x) \) remains convex, i.e:

\[
b_{p_j} + a_{p_j}^T x_j \geq b_k + a_k^T x_j, \quad j = 1, \ldots, n, \quad k = 1, \ldots, K,
\]

which are linear inequality constraints. Therefore one can minimize the loss \( \mathcal{L}(\phi) \) as a convex optimization problem.