

Fitting the Smallest Enclosing Bregman Ball

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Abstract. Finding a point which minimizes the maximal distortion with respect to a dataset is an important estimation problem that has recently received growing attentions in machine learning, with the advent of one class classification. We propose two theoretically founded generalizations to arbitrary Bregman divergences, of a recent popular smallest enclosing ball approximation algorithm for Euclidean spaces coined by Bădoiu and Clarkson in 2002.

1 Introduction

Consider the following problem: given a set of observed data \mathcal{S} , compute some accurate set of parameters, or simplified descriptions, that *summarize* (“fit well”) \mathcal{S} according to some criteria. This problem is well known in various fields of statistics and computer science. In many cases, it admits two different formulations:

- (1.) Find a point \mathbf{c}^* which minimizes an *average distortion* with respect to \mathcal{S} .
- (2.) Find a point \mathbf{c}^* which minimizes a *maximal distortion* with respect to \mathcal{S} .

These two problems are cornerstones of different subfields of applied mathematics and computer science, such as (i) parametric estimation and the computation of *exhaustive* statistics for broad classes of distributions in statistics, (ii) one class classification and clustering in machine learning, (iii) the one center problem and its generalizations in computational geometry, among others [1, 2, 5, 7]. The main unknown in both problems is what we mean by *distortion*.

In fact, many examples of distortion measures found in domains concerned by the problems above (computational geometry, machine learning, signal processing, probabilities and statistics, among others) fall into a *single* family of distortion measures known as Bregman divergences [3]. Informally, each of them is the tail of the Taylor expansion of a strictly convex function. Using a neat result in [2], it can be shown that the solution to problem (1.) above is always the average member of \mathcal{S} , *regardless of the Bregman divergence*. This means that problem (1.) can be solved in optimal linear time / space in the size of \mathcal{S} : since \mathcal{S} may be huge, this property is crucial. Unfortunately, the solution of (2.) does not seem to be as affordable; tackling the problem with quadratic programming buys an expensive time complexity cubic in the worst case, and the space complexity is quadratic [8]. Notice also that it is mostly used with L_2^2 . Instead of

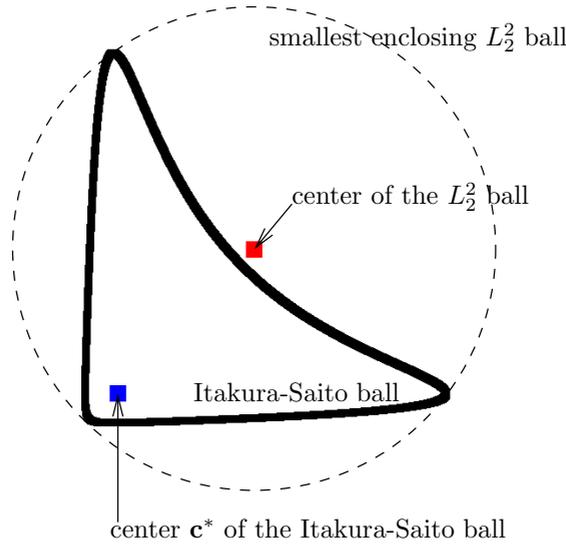


Fig. 1. An optimal Itakura-Saito ball and its smallest enclosing L_2^2 ball, for $d = 2$. Notice the poor quality of this *optimal* approximation: the center of the L_2^2 ball does not even lie inside the Itakura-Saito ball.

finding an exact solution, a recent approach due to [1] *approximates* the solution of the problem for L_2^2 : the user specifies some $\varepsilon > 0$, and the algorithm returns, in time *linear* in the size of \mathcal{S} (quadratic in $1/\varepsilon$) and in space *linear* in the size of \mathcal{S} , the center \mathbf{c} of a ball which is at L_2^2 divergence no more than $\varepsilon^2 r^*$ from \mathbf{c}^* . Here, r^* is the squared radius of the so-called *smallest enclosing ball* of \mathcal{S} , whose center \mathbf{c}^* is obviously the solution to problem (2.). Let us name this algorithm the Bădoiu-Clarkson algorithm, and abbreviate it BC. The key point of the algorithm is its simplicity, which deeply contrasts with quadratic programming approaches: basically, after having initialized \mathbf{c} to a random point of \mathcal{S} , we iterate through finding the farthest point away from the current center, and then move along the line between these two points. The popularity of the algorithm, initially focused in computational geometry, has begun to spread to machine learning as well, with its adaptation to fast approximations of SVM training [8].

The applications of BC have remained so far focused on L_2^2 , yet the fact that the algorithm gives a clean and simple approach to problem (2.) for *one* Bregman divergence naturally raises the question of whether it can be tailored to approximating problem (2.) for *any* Bregman divergence as well. Figure 1 highlights the importance of this issue.

In this paper, we propose two theoretically founded generalizations of BC to arbitrary Bregman divergences, along with a bijection property that has a flavor similar to a Theorem of [2]: we show a bijection between the set of Bregman divergences and the set of the most commonly used functional averages, which yields that each element of the latter set encodes the minimax distortion solution

for a Bregman divergence. This property is the cornerstone of our modifications to BC. The next Section presents some definitions. Section 3 gives the theoretical foundations and Section 4 the experiments regarding our generalization of BC.

2 Definitions

Our notations mostly follow those of [1, 2]. Bold faced variables such as \mathbf{x} and $\boldsymbol{\alpha}$, represent column vectors. Sets are represented by calligraphic upper-case alphabets, *e.g.* \mathcal{S} , and enumerated as $\{\mathbf{s}_i : i \geq 1\}$ for vector sets, and $\{s_i : i \geq 1\}$ otherwise. The j^{th} component of vector \mathbf{s} is noted s_j , for $j \leq 1$. Vectors are supposed d -dimensional. We write $\mathbf{x} \geq \mathbf{y}$ as a shorthand for $x_i \geq y_i, \forall i$. The cardinal of a set \mathcal{S} is written $|\mathcal{S}|$, and $\langle \cdot, \cdot \rangle$ defines the inner product for real valued vectors, *i.e.* the dot product. Norms are L_2 for a vector, and Frobenius for a matrix. Bregman divergences are a parameterized family of distortion measures: let $F : \mathcal{X} \rightarrow \mathbb{R}$ be strictly convex and differentiable on the interior $int(\mathcal{X})$ of some convex set $\mathcal{X} \subseteq \mathbb{R}^d$. Its corresponding Bregman divergence is:

$$D_F(\mathbf{x}', \mathbf{x}) = F(\mathbf{x}') - F(\mathbf{x}) - \langle \mathbf{x}' - \mathbf{x}, \nabla F(\mathbf{x}) \rangle . \tag{1}$$

Here, ∇F is the gradient operator of F . A Bregman divergence has the following properties: it is convex in \mathbf{x}' , always non negative, and zero iff $\mathbf{x} = \mathbf{x}'$. Whenever $F(\mathbf{x}) = \sum_{i=1}^d x_i^2 = \|\mathbf{x}\|_2^2$, the corresponding divergence is the squared Euclidean distance (L_2^2): $D_F(\mathbf{x}', \mathbf{x}) = \|\mathbf{x} - \mathbf{x}'\|_2^2$, with which is associated the common definition of a ball in an Euclidean metric space:

$$\mathcal{B}_{\mathbf{c},r} = \{ \mathbf{x} \in \mathcal{X} : \|\mathbf{x} - \mathbf{c}\|_2^2 \leq r \} , \tag{2}$$

with $\mathbf{c} \in \mathcal{S}$ the center of the ball, and $r \geq 0$ its (squared) radius. Eq. (2) suggests a natural generalization to the definition of balls for arbitrary Bregman divergences. However, since a Bregman divergence is usually not symmetric, any $\mathbf{c} \in \mathcal{S}$ and any $r \geq 0$ define actually two dual *Bregman balls*:

$$\mathcal{B}_{\mathbf{c},r} = \{ \mathbf{x} \in \mathcal{X} : D_F(\mathbf{c}, \mathbf{x}) \leq r \} , \tag{3}$$

$$\mathcal{B}'_{\mathbf{c},r} = \{ \mathbf{x} \in \mathcal{X} : D_F(\mathbf{x}, \mathbf{c}) \leq r \} . \tag{4}$$

Remark that $D_F(\mathbf{c}, \mathbf{x})$ is always convex in \mathbf{c} while $D_F(\mathbf{x}, \mathbf{c})$ is not always, but the *boundary* $\partial \mathcal{B}_{\mathbf{c},r}$ is not always convex (it depends on \mathbf{x} , given \mathbf{c}), while $\partial \mathcal{B}'_{\mathbf{c},r}$ is always convex. In this paper, we are mainly interested in $\mathcal{B}_{\mathbf{c},r}$ because of the convexity of D_F in \mathbf{c} . The conclusion of the paper extends some results to build $\mathcal{B}'_{\mathbf{c},r}$ as well. Let $\mathcal{S} \subseteq \mathcal{X}$ be a set of m points that were sampled from \mathcal{X} . A *smallest enclosing Bregman ball* (SEBB) for \mathcal{S} is a Bregman ball $\mathcal{B}_{\mathbf{c}^*,r^*}$ with r^* the minimal real such that $\mathcal{S} \subseteq \mathcal{B}_{\mathbf{c}^*,r^*}$. With a slight abuse of language, we will refer to r^* as the *radius* of the ball. Our objective is to approximate as best as possible the SEBB of \mathcal{S} , which amounts to minimizing the radius of the enclosing ball we build. As a simple matter of fact indeed, the SEBB is unique.

Lemma 1. *The smallest enclosing Bregman ball $\mathcal{B}_{\mathbf{c}^*,r^*}$ of \mathcal{S} is unique.*

(proof omitted due to the lack of space) Algorithm 1 presents Bădoiu-Clarkson’s algorithm for the SEBB approximation problem with the L_2^2 divergence [1].

Algorithm 1: BC(\mathcal{S}, T)

Input: Data $\mathcal{S} = \{\mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_m\}$;
Output: Center \mathbf{c} ;
 Choose at random $\mathbf{c} \in \mathcal{S}$;
for $t = 1, 2, \dots, T - 1$ **do**
 $\mathbf{s} \leftarrow \arg \max_{\mathbf{s}' \in \mathcal{S}} \|\mathbf{c} - \mathbf{s}'\|_2^2$;
 $\mathbf{c} \leftarrow \frac{t}{t+1} \mathbf{c} + \frac{1}{t+1} \mathbf{s}$;

3 Extending BC

The primal SEBB problem is to find:

$$\arg \min_{\mathbf{c}^*, r^*} r^* \quad \text{s.t.} \quad D_F(\mathbf{c}^*, \mathbf{s}_i) \leq r^*, \forall 1 \leq i \leq m . \tag{5}$$

Its Lagrangian is $L(\mathcal{S}, \boldsymbol{\alpha}) = r^* - \sum_{i=1}^m \alpha_i (r^* - D_F(\mathbf{c}^*, \mathbf{s}_i))$, with the additional Karush-Kuhn-Tucker condition $\boldsymbol{\alpha} \geq \mathbf{0}$. The solution to (5) is obtained by minimizing $L(\mathcal{S}, \boldsymbol{\alpha})$ for the parameters \mathbf{c}^* and r^* , and then maximize the resulting dual for the Lagrange multipliers. We obtain $\partial L(\mathcal{S}, \boldsymbol{\alpha}) / \partial \mathbf{c}^* = \nabla_F(\mathbf{c}^*) \sum_{i=1}^m \alpha_i - \sum_{i=1}^m \alpha_i \nabla_F(\mathbf{s}_i)$ and $\partial L(\mathcal{S}, \boldsymbol{\alpha}) / \partial r^* = 1 - \sum_{i=1}^m \alpha_i$. Setting $\partial L(\mathcal{S}, \boldsymbol{\alpha}) / \partial \mathbf{c}^* = \mathbf{0}$ and $\partial L(\mathcal{S}, \boldsymbol{\alpha}) / \partial r^* = 0$ yields $\sum_{i=1}^m \alpha_i = 1$ and:

$$\mathbf{c}^* = \nabla_F^{-1} \left(\sum_{i=1}^m \alpha_i \nabla_F(\mathbf{s}_i) \right) . \tag{6}$$

Table 1. Some common Bregman divergences and their associated functional averages. The second row depicts the general I (information) divergence, also known as Kullback-Leibler (KL) divergence on the d -dimensional probability simplex. On the fourth row, A is the inverse of the covariance matrix [2].

domain	$F(\mathbf{s})$	$D_F(\mathbf{c}, \mathbf{s})$	$c_j \ (1 \leq j \leq d)$
		L_2^2 norm	arithmetic mean
\mathbb{R}^d	$\sum_{j=1}^d s_j^2$	$\sum_{j=1}^d (c_j - s_j)^2$	$\sum_{i=1}^m \alpha_i s_{i,j}$
$(\mathbb{R}^{+,*})^d$		(1/KL)-divergence	geometric mean
$/ d$ -simplex	$\sum_{j=1}^d s_j \log s_j - s_j$	$\sum_{j=1}^d c_j \log(c_j/s_j) - c_j + s_j$	$\prod_{i=1}^m s_{i,j}^{\alpha_i}$
$(\mathbb{R}^{+,*})^d$	$-\sum_{j=1}^d \log s_j$	Itakura-Saito distance	harmonic mean
		$\sum_{j=1}^d (c_j/s_j) - \log(c_j/s_j) - 1$	$1 / \sum_{i=1}^m (\alpha_i / s_{i,j})$
\mathbb{R}^d	$\mathbf{s}^T A \mathbf{s}$	Mahalanobis distance	arithmetic mean
		$(\mathbf{c} - \mathbf{s})^T A (\mathbf{c} - \mathbf{s})$	$\sum_{i=1}^m \alpha_i s_{i,j}$
	$p \in \mathbb{N} \setminus \{0, 1\}$		weighted power mean
$\mathbb{R}^d / \mathbb{R}^{+d}$	$(1/p) \sum_{j=1}^d s_j^p$	$\sum_{j=1}^d \frac{c_j^p}{p} + \frac{(p-1)s_j^p}{p} - c_j s_j^{p-1}$	$(\sum_{i=1}^m \alpha_i s_{i,j}^{p-1})^{1/(p-1)}$

Because F is strictly convex, ∇_F is bijective, and \mathbf{c}^* lies in the convex closure of \mathcal{S} . Finally, we are left with finding:

$$\arg \max_{\boldsymbol{\alpha}} \sum_{i=1}^m \alpha_i D_F \left(\nabla_F^{-1} \left(\sum_{j=1}^m \alpha_j \nabla_F(\mathbf{s}_j) \right), \mathbf{s}_i \right) \text{ s.t. } \boldsymbol{\alpha} \geq \mathbf{0}, \sum_{i=1}^m \alpha_i = 1 . (7)$$

This problem generalizes the dual of support vector machines: whenever $F(\mathbf{s}) = \sum_{i=1}^d s_i^2 = \langle \mathbf{s}, \mathbf{s} \rangle$ (Table 1), we return to their kernel-based formulation [4]. There are essentially two categories of Lagrange multipliers in vector $\boldsymbol{\alpha}$. Those corresponding to points of \mathcal{S} lying on the interior of $\mathcal{B}_{\mathbf{c}^*, r^*}$ are zero, since these points satisfy their respective constraints. The others, corresponding to the *support* points of the ball, are strictly positive. Each $\alpha_i > 0$ represents the contribution of its support point to the computation of the circumcenter of the ball. Eq. (6) is thus some *functional average* of the support points of the ball, to compute \mathbf{c}^* .

3.1 The Modified Bădoiu-Clarkson Algorithm, MBC

There is more on eq. (6). A Bregman divergence is not affected by linear terms: $D_{F+q} = D_F$ for any constant q [6]. Thus, the partial derivatives of F in $\nabla_F(\cdot)$ determine entirely the Bregman divergence. The following Lemma is then immediate.

Lemma 2. *The set of functional averages (6) is in bijection with the set of Bregman divergences (1).*

The connection between the functional averages and divergences is much interesting because the classical means commonly used in many domains, such as convex analysis, parametric estimation, signal processing, are valid examples of functional averages. A nontrivial consequence of Lemma 2 is that each of them encodes the SEBB solution for an associated Bregman divergence. Apart from the SEBB problem, this is interesting because means are popular statistics, and we give a way to favor the choice of a mean against another one depending on the *domain* of the data and its “natural” distortion measure. Table 1 presents some Bregman divergences and their associated functional averages, for the most commonly encountered.

Speaking of bijections, previous results showed the existence of a bijection between Bregman divergences and the family of exponential distributions [2]. This has helped the authors to devise a generalization of the k -means algorithm. In our case, Lemma 2 is also of some help to generalize BC. Clearly, the dual problem in eq. (7) does not admit the convenient representation of SVMs, and it seems somehow hard to use a kernel trick replacing the elements of \mathcal{S} by local transformations involving F prior to solving problem (7). However, the dual suggests a very simple algorithm to approximate \mathbf{c}^* , which consists in making the parallel between $\nabla(\mathbf{c}^*) = \sum_{i=1}^m \alpha_i \nabla_F(\mathbf{s}_i)$ (6) and the arithmetic mean in Table 1, and consider (6) as the solution to a minimum distortion problem involving gradients into a L_2^2 space. We can thus seek:

$$\arg \min_{\mathbf{g}^*, r'^*} r'^* \text{ s.t. } \|\mathbf{g}^* - \nabla_F(\mathbf{s}_i)\|_2^2 \leq r'^*, \forall 1 \leq i \leq m . (8)$$

Finally, approximating (5) amounts to running the so-called Modified Bădoiu-Clarkson algorithm in the gradient space, MBC . Because ∇_F is bijective, this is guaranteed to yield a solution. The remaining question is whether $\nabla_F^{-1}(\mathbf{g}) = \mathbf{c}$ is close enough from the solution \mathbf{c}^* of (5). The following Lemma upperbounds the sum of the two divergences between \mathbf{c} and any point of \mathcal{S} , as a function of r'^* . It shows that the two centers can be very close to each other; in fact, they can be *much* closer than with a naive application of Bădoiu-Clarkson directly in \mathcal{S} . The Lemma makes the hypothesis that the Hessian of F , H_F , is non singular. As a matter of fact, it is diagonal (without zero in the diagonal) for all classical examples of Bregman divergences, see Table 1, so this is not a restriction either. In the Lemma, we let f denote the minimal non zero value of the Hessian norm inside the convex closure of \mathcal{S} : $f = \min_{\mathbf{x} \in \text{co}(\mathcal{S}): \|\nabla F(\mathbf{x})\|_2 > 0} \|\nabla F(\mathbf{x})\|_2$.

Lemma 3. $\forall \mathbf{s} \in \mathcal{S}$, we have:

$$D_F(\mathbf{s}, \nabla_F^{-1}(\mathbf{g})) + D_F(\nabla_F^{-1}(\mathbf{g}), \mathbf{s}) \leq (1 + \varepsilon)^2 r'^* / f \quad (9)$$

where $\mathbf{g} = \text{BC}(\{\nabla_F(\mathbf{s}_i) : \mathbf{s}_i \in \mathcal{S}\}, T)$, r'^* is defined in eq. (8), and ε is the error parameter of BC.

(proof omitted due to the lack of space) Remark that Lemma 3 is optimal, in the sense that if we consider $D_F = L_2^2$, then each point $\mathbf{s}_i \in \mathcal{S}$ becomes $2\mathbf{s}_i$ in \mathcal{S}' . The optimal radii in (5) and (8) satisfy $r'^* = 4r^*$, and we have $f = 2$. Plugging this altogether in eq. (9) yields $2\|\mathbf{c} - \mathbf{s}\|_2^2 \leq (1 + \varepsilon)^2 \times 4r^* / 2$, i.e. $\|\mathbf{c} - \mathbf{s}\|_2 \leq (1 + \varepsilon)\sqrt{r^*}$, which is exactly Bădoiu-Clarkson’s bound [1] (here, we have fixed $\mathbf{c} = \nabla_F^{-1}(\mathbf{g})$, like in Lemma 3). Remark also that Lemma 3 upperbounds the sum of both possible divergences, which is very convenient given the possible asymmetry of D_F .

3.2 The Bregman-Bădoiu-Clarkson Algorithm, BBC

It is straightforward to check that at the end of BC (algorithm 1), the following holds true:

$$\begin{cases} \mathbf{c} = \sum_{i=1}^m \hat{\alpha}_i \mathbf{s}_i \quad , \quad \sum_{i=1}^m \hat{\alpha}_i = 1 \quad , \quad \hat{\alpha} \geq \mathbf{0} \quad , \\ \forall 1 \leq i \leq m, \hat{\alpha}_i \neq 0 \text{ iff } \mathbf{s}_i \text{ is chosen at least once in BC} \quad . \end{cases}$$

Since the furthest points chosen by BC ideally belong to $\partial \mathcal{B}_{\mathbf{c}^*, r^*}$, and the final expression of \mathbf{c} matches the arithmetic average of Table 1, it comes that BC *directly* tackles an iterative approximation of eq. (6) for the L_2^2 Bregman divergence. If we replace L_2^2 by an arbitrary Bregman divergence, then BC can be generalized in a quite natural way to algorithm BBC (for Bregman-Bădoiu-Clarkson) below.

Again, it is straightforward to check that at the end of BBC, we have generalized the iterative approximation of BC to eq. (6) for any Bregman divergence, as we have:

$$\begin{cases} \mathbf{c} = \nabla_F^{-1}(\sum_{i=1}^m \hat{\alpha}_i \nabla_F(\mathbf{s}_i)) \quad , \quad \sum_{i=1}^m \hat{\alpha}_i = 1 \quad , \quad \hat{\alpha} \geq \mathbf{0} \quad , \\ \forall 1 \leq i \leq m, \hat{\alpha}_i \neq 0 \text{ iff } \mathbf{s}_i \text{ is chosen at least once in BC} \quad . \end{cases}$$

Algorithm 2: BBC(\mathcal{S})

Input: Data $\mathcal{S} = \{\mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_m\}$;
Output: Center \mathbf{c} ;
 Choose at random $\mathbf{c} \in \mathcal{S}$;
for $t = 1, 2, \dots, T - 1$ **do**
 $\mathbf{s} \leftarrow \arg \max_{\mathbf{s}' \in \mathcal{S}} D_F(\mathbf{c}, \mathbf{s}')$;
 $\mathbf{c} \leftarrow \nabla_F^{-1} \left(\frac{t}{t+1} \nabla_F(\mathbf{c}) + \frac{1}{t+1} \nabla_F(\mathbf{s}) \right)$;

The main point is whether $\hat{\alpha}$ is a good approximation to the true vector of Lagrange multipliers α . From the theoretical standpoint, the proof of BC’s approximation ratio becomes tricky when lifted from L_2^2 to an arbitrary Bregman divergence, but it can be shown that many of the key properties of the initial proof remain true in this more general setting. An experimental hint that speaks for itself for the existence of such a good approximation ratio is given in the next Section.

4 Experimental Results

Due to the lack of space, we only present results on BBC . To evaluate the quality of the approximation of BBC for the SEBB, we have ran the algorithm for three popular representative Bregman divergences. For each of them, averages over a hundred runs were performed for $T = 200$ center updates (see algorithm 2). In each run, a random Bregman ball is generated, and \mathcal{S} is sampled uniformly at random in the ball. Since we know the SEBB, we have a precise idea of the quality of the approximation found by BBC on the SEBB. Figure 2 gives a synthesis of the results for $d = 2$. [1]’s bound is plotted for each divergence,

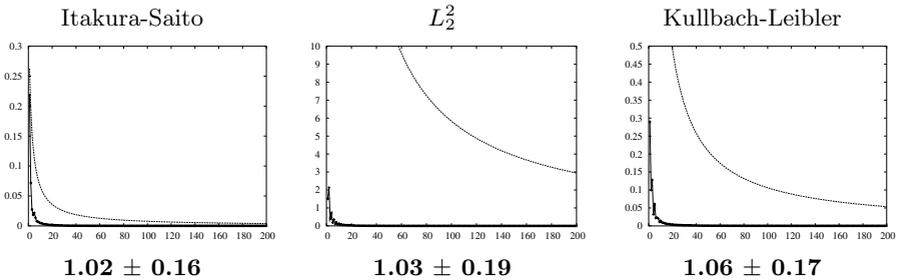


Fig. 2. Average approximation curves for 100 runs of BBC algorithm for three Bregman divergences: Itakura-Saito, L_2^2 and KL ($d = 2, m = 1000, T = 200$). The dashed curves are Bădoiu-Clarkson’s error bound as a function of the iteration number t , and the bottom, plain curves, depict $(D_F(\mathbf{c}^*, \mathbf{c}) + D_F(\mathbf{c}, \mathbf{c}^*))/2$ as a function of t for each divergence, where \mathbf{c} is the output of BBC and \mathbf{c}^* is the optimal center. The bottom number depict the estimated error (%) ± standard deviation.

Table 2. Estimated errors for the SEBB problem for data generated using a mixture of u gaussians, for $u = 1, 3, 5, 10, 20$. Conventions and parameters follow Figure 2.

u	Itakura-Saito	L_2^2	Kullbach-Leibler
1	0.37 ± 0.06	0.43 ± 0.09	0.39 ± 0.08
3	0.40 ± 0.04	0.41 ± 0.10	0.41 ± 0.06
5	0.41 ± 0.04	0.43 ± 0.10	0.41 ± 0.04
10	0.40 ± 0.02	0.44 ± 0.09	0.42 ± 0.05
20	0.41 ± 0.02	0.43 ± 0.08	0.41 ± 0.04

even when it holds formally only for L_2^2 . The other two curves give an indication of the way this bound behaves with respect to the experimental results. It is easy to see that for each divergence, there is a very fast convergence of the center found, \mathbf{c} , to the optimal center \mathbf{c}^* . Furthermore, the experimental divergences are always much smaller than [1]’s bound, *for each divergence* (very often by a factor 100 or more). We have checked this phenomenon for higher dimensions, up to $d = 20$. Following [7], the errors given are the ratio of the number of support points over the whole number of points. A good method would typically select a very small number of points, regardless of the domain. While this is clearly displayed in Figure 2, Table 2 goes deeper in this phenomenon, as it displays the errors when the points are drawn from random mixtures of Gaussians. Even in this case, where the Gaussians may be very distant from each other, MBC with the three Bregman divergences of Figure 2 still displays a very low error.

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