Abstract

$f$-divergences are a general class of divergences between probability measures which include as special cases many commonly used divergences in probability, mathematical statistics and information theory such as Kullback-Leibler divergence, chi-squared divergence, squared Hellinger distance, total variation distance etc. In this paper, we study the problem of maximizing or minimizing an $f$-divergence between two probability measures subject to a finite number of constraints on other $f$-divergences. We show that these infinite-dimensional optimization problems can all be reduced to optimization problems over small finite dimensional spaces which are tractable. Our results lead to a comprehensive and unified treatment of the problem of obtaining sharp inequalities between $f$-divergences. We demonstrate that many of the existing results on inequalities between $f$-divergences can be obtained as special cases of our results and we also improve on some existing non-sharp inequalities.

1 Introduction

Suppose that the Kullback-Leibler divergence between two probability measures is bounded from above by 2. What then is the maximum possible value of the Hellinger distance between them? Such questions naturally arise in many fields including mathematical statistics and machine learning, information theory, probability, statistical physics etc. and the goal of this paper is to provide a way of answering them. From the variational viewpoint, this problem can be posed as: maximize the Hellinger distance subject to a constraint on the Kullback-Leibler divergence over the space of all pairs of probability measures over all possible sample spaces. We shall prove in this paper that the value of this maximization problem remains unchanged if one restricts the sample space to be the three-element set \{1, 2, 3\}. In other words, in order to find the maximum Hellinger distance subject to an upper bound on the Kullback-Leibler divergence, one can just restrict attention to pairs of probability measures on \{1, 2, 3\}. Thus, the large infinite-dimensional optimization problem is reduced to an optimization problem over a small finite-dimensional space (of dimension $\leq 4$) which makes it tractable.
In this paper, we prove such results in a very general setting. The Kullback-Leibler divergence and the (square of the) Hellinger distance are special instances of a general class of divergences between probability measures called $f$-divergences (also known as $\phi$-divergences). Let $f : (0, \infty) \to \mathbb{R}$ be a convex function satisfying $f(1) = 0$. By virtue of convexity, both the limits $f(0) := \lim_{x \downarrow 0} f(x)$ and $f'(\infty) := \lim_{x \uparrow \infty} f(x)/x$ exist, although they may equal $+\infty$. For two probability measures $P$ and $Q$, the $f$-divergence (see, for example, [1, 5–7]), $D_f(P||Q)$, is defined by

$$D_f(P||Q) := \int_{q > 0} f\left(\frac{p}{q}\right) dQ + f'(\infty)P\{q = 0\}$$

where $p$ and $q$ are densities of $P$ and $Q$ with respect to a common measure $\lambda$. The definition does not depend on the choice of the dominating measure $\lambda$. Special cases of $f$ lead to, among others, Kullback-Leibler divergence, total variation distance, square of the Hellinger distance and chi-squared divergence.

We are now ready to introduce the general form of the optimization problem we described at the beginning of the paper. Given divergences $D_f$ and $D_{f_i}, i = 1, \ldots, m$ and nonnegative real numbers $D_1, \ldots, D_m$, let

$$A(D_1, \ldots, D_m) := \sup \{D_f(P||Q) : D_{f_i}(P||Q) \leq D_i \ \forall i\}$$

and

$$B(D_1, \ldots, D_m) := \inf \{D_f(P||Q) : D_{f_i}(P||Q) \geq D_i \ \forall i\}$$

where the probability measures on the right hand sides above range over all possible measurable spaces. The goal of this paper is to provide a method for computing these quantities. We show that these large infinite-dimensional optimization problems can all be reduced to optimization problems over small finite-dimensional spaces. Specifically, in Theorem 2.1, we show that in order to compute these quantities, one can restrict attention to probability measures on the set $\{1, \ldots, m + 2\}$.

One of the main reasons for studying the quantities $A(D_1, \ldots, D_m)$ and $B(D_1, \ldots, D_m)$ is that they yield sharp inequalities for the divergence $D_f$ in terms of the divergences $D_{f_1}, \ldots, D_{f_m}$. Indeed, the inequalities

$$D_f(P||Q) \leq A(D_{f_1}(P||Q), \ldots, D_{f_m}(P||Q))$$

(1)

and

$$D_f(P||Q) \geq B(D_{f_1}(P||Q), \ldots, D_{f_m}(P||Q))$$

(2)

hold for every pair of probability measures $P$ and $Q$. Further, the functions $A$ and $B$ satisfy the natural monotonicity inequalities

$$A(D_1, \ldots, D_m) \leq A(D'_1, \ldots, D'_m)$$

(3)

and

$$B(D_1, \ldots, D_m) \leq B(D'_1, \ldots, D'_m)$$

(4)

for every $(D_1, \ldots, D_m)$ and $(D'_1, \ldots, D'_m)$ such that $D_i \leq D'_i$ for all $i$.  

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The inequalities (1) and (2) are sharp in the sense that $A$ is the smallest function satisfying (3) for which (1) holds for all probability measures $P$ and $Q$. Likewise, $B$ is the largest function satisfying (4) for which (2) holds for all probability measures $P$ and $Q$.

Inequalities between $f$-divergences are useful in many areas. For example, in mathematical statistics, they are crucial in problems of obtaining minimax bounds [12, 13, 32, 34]. In probability, such inequalities are often used for converting limit theorems proved under a convenient divergence into limit theorems for other divergences [3, 14, 30]. They are also helpful for proving results in measure concentration [21–23]. Some applications in machine learning are described in [27]. Further, inequalities involving $f$-divergences are fundamental to the field of information theory [4, 8].

Because of their widespread use, many papers deal with inequalities between $f$-divergences (some references being [5, 9–12, 16, 17, 26, 28, 31, 33]). However, many of the inequalities presented in previous treatments are not sharp. The few papers which provide sharp inequalities [9, 11, 28, 33] only deal with certain special $f$-divergences as opposed to working in full generality. A popular such special case is $m = 1$ and $D_{f_1}$ corresponding to the total variation distance. In this case, sharp inequalities have been derived in [9] for the case when $D_f$ is the Kullback-Leibler divergence and in [11] for the case of general $D_f$. The case $m > 1$ is comparatively less studied although this has potential applications in the statistical problem of obtaining lower bounds for the minimax risk (see Section 6.1 for details). The only paper which deals with sharp inequalities for $m > 1$ is [28] but there the authors only study the case when $D_{f_1}, \ldots, D_{f_m}$ are all primitive divergences (see Remark 3.1 below for the definition of primitive divergences).

In contrast with all previous papers in the area, we study the problem of obtaining sharp inequalities between $f$-divergences in full generality. In particular, our main results allow $m$ to be an arbitrary positive integer and all the divergences $D_f$ and $D_{f_1}, \ldots, D_{f_m}$ to be arbitrary $f$-divergences. We show that the underlying optimization problems can all be reduced to low-dimensional optimization problems and we outline methods for solving them. We also show that many of the existing results on inequalities between $f$-divergences can be obtained as special cases of our results and we also improve on some existing non-sharp inequalities.

The rest of this paper is structured as follows. Our main result is stated in Theorem 2.1. Its three-part proof is given in Section 3. The first part is based on a recent representation theorem for $f$-divergences which implies that the optimization problems for computing $A(D_1, \ldots, D_m)$ and $B(D_1, \ldots, D_m)$ can be thought of as maximizing or minimizing an integral functional over a certain class of concave functions satisfying a finite number of integral constraints. In the second part of the proof, we use Choquet’s theorem to restrict attention only to the extreme points of the constraint set. Finally, in the third part, we characterize these extreme points and show that they correspond to probability measures over small finite sets.
One possible approach to compute $A(D_1, \ldots, D_m)$ and $B(D_1, \ldots, D_m)$ is via joint ranges of $f$-divergences. Specifically, for $m \geq 1$ and divergences $D_{f_1}, \ldots, D_{f_m}$, their joint range, denoted by $\mathcal{R}(f_1, \ldots, f_m)$ is defined as the set of all vectors in $\mathbb{R}^m$ that equal $(D_{f_1}(P||Q), \ldots, D_{f_m}(P||Q))$ for some pair of probability measures $P$ and $Q$. If the joint range $\mathcal{R}(f, f_1, \ldots, f_m)$ can be determined, then one can easily calculate the values $A(D_1, \ldots, D_m)$ and $B(D_1, \ldots, D_m)$ for every $D_1, \ldots, D_m$. The problem of determining the joint range $\mathcal{R}(f_1, \ldots, f_m)$ was solved for the case $m = 2$ in [15]. We extend their result to general $m \geq 2$ in Section 4.2 by a very simple proof which was communicated to us by an anonymous referee. Unfortunately, it turns out that this approach based on the joint range does not quite prove Theorem 2.1. It gives a slightly weaker result. We discuss this in Section 4.2.

Also in Section 4, we collect some remarks and extensions of our main theorem and, in particular, we show that the theorem is tight in general. In Section 5, we consider various special cases and show that many well-known results in the literature can be obtained as simple instances of our main theorem. In Section 6, we describe numerical methods for solving the low-dimensional optimization problems that come out of our main theorem. We solve an important subclass of these problems by convex optimization and we also describe heuristic methods for the general case.

2 Main Result

For each $n \geq 1$, let $\mathcal{P}_n$ denote the space of all probability measures defined on the finite set $\{1, \ldots, n\}$. Let us define $A_n(D_1, \ldots, D_m)$ to be

\[
\sup \{D_f(P||Q) : P, Q \in \mathcal{P}_n \text{ and } D_{f_i}(P||Q) \leq D_i \ \forall i\}
\]

and, analogously, $B_n(D_1, \ldots, D_m)$ to be

\[
\inf \{D_f(P||Q) : P, Q \in \mathcal{P}_n \text{ and } D_{f_i}(P||Q) \geq D_i \ \forall i\}.
\]

Our main theorem is given below. The second part of the theorem requires that $D_{f_1}, \ldots, D_{f_m}$ are finite divergences. We say that a divergence $D_f$ is finite if $\sup_{P,Q} D_f(P||Q) < \infty$. The supremum here is taken over all probability measures over all possible measurable spaces. See Remark 3.2 for a detailed explanation of finite divergences.

**Theorem 2.1.** For every $D_1, \ldots, D_m \geq 0$, we have

\[
A(D_1, \ldots, D_m) = A_{m+2}(D_1, \ldots, D_m).
\]

Further if $D_{f_1}, \ldots, D_{f_m}$ are all finite, then

\[
B(D_1, \ldots, D_m) = B_{m+2}(D_1, \ldots, D_m).
\]
The conclusions of the above theorem may be better appreciated in the following optimization form. Theorem 2.1 states that the quantity $A(D_1, \ldots, D_m)$ equals the optimal value of the following finite-dimensional optimization problem:

$$\max_{p, q \in [0, 1]^{m+2}} \sum_{j: q_j > 0} q_j f\left(\frac{p_j}{q_j}\right) + f'(\infty) \sum_{j: q_j = 0} p_j$$

subject to

$$p_j \geq 0, \quad q_j \geq 0 \quad \text{for all} \quad j = 1, \ldots, m + 2 \quad (7)$$

$$\sum_{j: q_j > 0} q_j f_i\left(\frac{p_j}{q_j}\right) + f'_i(\infty) \sum_{j: q_j = 0} p_j \leq D_i$$

for $i = 1, \ldots, m$. Similarly, when $D_{f_1}, \ldots, D_{f_m}$ are all finite, $B(D_1, \ldots, D_m)$ equals the optimal value of

$$\min_{p, q \in [0, 1]^{m+2}} \sum_{j: q_j > 0} q_j f\left(\frac{p_j}{q_j}\right) + f'(\infty) \sum_{j: q_j = 0} p_j$$

subject to

$$p_j \geq 0, \quad q_j \geq 0 \quad \text{for all} \quad j = 1, \ldots, m + 2 \quad (8)$$

$$\sum_{j: q_j > 0} q_j f_i\left(\frac{p_j}{q_j}\right) + f'_i(\infty) \sum_{j: q_j = 0} p_j \geq D_i$$

for $i = 1, \ldots, m$. The proof of Theorem 2.1 is provided in the next section. In Section 4, we argue that Theorem 2.1 is tight in general and also comment on the assumption of finiteness of $D_{f_1}, \ldots, D_{f_m}$ for the validity of identity (6). We also describe an attempt to prove this theorem via joint ranges but this only yields a weaker result.

3 Proof of the Main Result

3.1 Testing Representation

For two probability measures $P$ and $Q$, let us define the function $\psi_{P, Q} : [0, \infty) \to [0, 1]$ by

$$\psi_{P, Q}(s) := \int \min(p, q s) d\lambda \quad \text{for} \quad s \in [0, \infty)$$

where $p$ and $q$ denote the densities of $P$ and $Q$ with respect to a common measure $\lambda$ (which can, for example, be taken to be $P + Q$). This function $\psi_{P, Q}$ is nonnegative, concave, non-decreasing and satisfies the inequality $0 \leq \psi_{P, Q}(s) \leq \min(1, s)$ for all $s \geq 0$. In other words, $\psi \in \mathcal{C}$ where $\mathcal{C}$ denotes the class of all functions $\psi$ on $[0, \infty)$ that are nonnegative, concave, non-decreasing and satisfy the inequality $\psi(s) \leq \min(1, s)$ for all $s \geq 0$. Moreover, it is true (see, for example, [28, Corollary 5]) that every function $\psi \in \mathcal{C}$ equals $\psi_{P, Q}$ for some pair of probability measures $P$ and $Q$.

For each divergence $D_f$, let us associate the measure $\nu_f$ on $(0, \infty)$ defined by

$$\nu_f(a, b) := \partial f(b) - \partial f(a) \quad \text{for} \quad 0 < a < b < \infty$$
where $\partial^r$ denotes the right derivative operator (note that by convexity $\partial^r f(x)$ exists for every $x \in (0, \infty)$).

We also associate the functional $I_f : C \to [0, \infty]$ by

$$I_f(\psi) := \int_0^\infty (\min(1, s) - \psi(s)) \, d\nu_f(s).$$

(9)

There is a precise connection between $D_f$ and $I_f$ that is given below:

**Lemma 3.1.** For every pair of probability measures $P$ and $Q$, we have

$$D_f(P||Q) = I_f(\psi_{P,Q}).$$

(10)

Lemma 3.1 is not new although the form in which it is stated above is non-standard. The more standard version simply involves writing the integral in (9) over the interval $(0, 1)$ by the change of variable $t = s/(1 + s)$. In this modified form, Lemma 3.1 has been proved in [24] in the case when $f$ is twice differentiable and in [20] in the general case. A short proof is available in [19, Theorem 2.3].

**Remark 3.1** (Primitive $f$-divergences). For each $s > 0$, let $u_s(t) := \min(1, s) - \min(t, s)$ for $t \in (0, \infty)$. Clearly, $u_s$ is a convex function on $(0, \infty)$ such that $u_s(1) = 0$. Moreover, it is a very simple convex function in the sense that it is piecewise linear with just two linear parts. It is straightforward to check that the divergence corresponding to $u_s$ is given by:

$$D_{u_s}(P||Q) = \min(1, s) - \psi_{P,Q}(s).$$

Lemma 3.1 therefore asserts that any arbitrary $f$-divergence can be written as an integral of the primitive divergences $D_{u_s}$ with respect to the measure $\nu_f$ on $(0, \infty)$. The most well-known of these primitive divergences is the total variation distance which corresponds to $s = 1$. Indeed,

$$D_{u_1}(P||Q) = 1 - \int \min(p, q) \, d\lambda = \frac{1}{2} \int |p - q| \, d\lambda =: V(P, Q)$$

Every primitive divergence $D_{u_s}(P||Q)$ is closely related to the smallest weighted average error (Bayes risk) in the problem of statistical testing between the hypotheses $P$ against $Q$ based on an observation $X$ (see, for example, [28, Lemma 3]).

**Remark 3.2** (Finiteness of a divergence). Lemma 3.1 implies that

$$\sup_{P,Q} D_f(P||Q) = \int_0^\infty \min(1, s) \, d\nu_f(s) = f(0) + f'(\infty).$$

(11)

The supremum above is taken over all probability measures $P$ and $Q$ defined on all possible measurable spaces. To see (11), just note that, by Lemma 3.1, we have

$$\sup_{P,Q} D_f(P||Q) = \sup_{P,Q} I_f(\psi_{P,Q}) = \sup_{\psi \in C} I_f(\psi) = I_f(0).$$

Intuitively, $\psi_{P,Q}(s) = 0$ for all $s$ implies that $P$ and $Q$ are maximally separated (mutually singular) and thus the maximum value of $I_f(\psi)$ is achieved when $\psi$ is the identically zero function. The definition of $I_f$ gives that

$$I_f(0) = \int_0^\infty \min(1, s) \, d\nu_f(s)$$
Moreover, for the probability measures \(P^* = (1,0)\) and \(Q^* = (0,1)\) in \(P_2\), the function \(\psi_{P,Q}\) equals 0. Therefore,
\[
I_f(0) = D_f(P^*||Q^*) = f(0) + f'(\infty),
\]
which proves (11).

Recall that an \(f\)-divergence is finite if \(\sup_{P,Q} D_f(P||Q) < \infty\). By (11), an \(f\)-divergence is finite if and only if
\[
\int_0^\infty \min(1,s)d\nu_f(s) = f(0) + f'(\infty) < \infty. \tag{12}
\]
Well known examples of finite divergences are the primitive divergences, the square of the Hellinger distance and the capacitory discrimination (which corresponds to the convex function (53)).

For each \(f\) and \(D \geq 0\), let us define
\[
C_1(f, D) := \{\psi \in C : I_f(\psi) \leq D\}
\]
and
\[
C_2(f, D) := \{\psi \in C : I_f(\psi) \geq D\}
\]
As a consequence of Lemma 3.1, we obtain that
\[
A(D_1, \ldots, D_m) = \sup \{I_f(\psi) : \psi \in \cap_{i=1}^m C_1(f_i, D_i)\} \tag{13}
\]
and
\[
B(D_1, \ldots, D_m) = \inf \{I_f(\psi) : \psi \in \cap_{i=1}^m C_2(f_i, D_i)\}. \tag{14}
\]
The following lemma on the derivatives of the function \(\psi_{P,Q}\) (the left and right derivative operators are denoted by \(\partial^l\) and \(\partial^r\) respectively) will be useful in the sequel.

**Lemma 3.2.** For every function \(\psi = \psi_{P,Q}\) in \(C\), we have
\[
\partial^l \psi(s) = Q\{p > sq\} \quad \text{for } s > 0 \tag{15}
\]
and
\[
\partial^r \psi(s) = Q\{p \geq sq\} \quad \text{for } s \geq 0. \tag{16}
\]

**Proof.** For every \(s > 0\),
\[
\partial^l \psi(s) = \lim_{\epsilon \downarrow 0} \frac{\psi(s) - \psi(s - \epsilon)}{\epsilon}
\]
and
\[
\frac{\psi(s) - \psi(s - \epsilon)}{\epsilon} = \int \frac{\min(p, qs) - \min(p, qs - \epsilon)}{\epsilon} d\lambda
\]
It is easy to check that the integrand above is bounded in absolute value by \(q\) and converges as \(\epsilon \downarrow 0\) to \(q\{p \geq q\} s\}. The identity (15) therefore follows by the dominated convergence theorem. The proof of (16) is similar. \(\Box\)
3.2 Reduction to Extreme Points

Let us first recall the definition of extreme points. Let $S$ be a subset of a vector space $V$. A point $a \in S$ is called an extreme point of $S$ if $a = (b + c)/2$ for $b, c \in S$ implies that $a = b = c$. In other words, $a$ cannot be the mid-point of a non-trivial line segment whose end points lie in $S$. We denote the set of all extreme points of $S$ by $\text{ext}(S)$.

An important result about extreme points in infinite dimensional topological vector spaces is Choquet’s theorem (see, for example, [25, Chapter 3]). We shall use the following version of Choquet’s theorem in this section:

\textbf{Theorem 3.3 (Choquet).} Let $K$ be a metrizable, compact convex subset of a locally convex space $V$ and let $x_0$ be an element of $K$. Then there exists a Borel probability measure $\mu_0$ on $K$ which is concentrated on the extreme points of $K$ and which satisfies $L(x_0) = \int_K L(x) d\mu_0(x)$ for every continuous linear functional $L$ on $V$.

The goal of this section is to prove the following:

\textbf{Lemma 3.4.} For every $D_1, \ldots, D_m \geq 0$, we have

$$A(D_1, \ldots, D_m) = \sup \{ I_f(\psi) : \psi \in \text{ext} (\bigcap_{i=1}^m C_1(f_i, D_i)) \}$$

and further, if $D_{f_1}, \ldots, D_{f_m}$ are all finite, we have

$$B(D_1, \ldots, D_m) = \inf \{ I_f(\psi) : \psi \in \text{ext} (\bigcap_{i=1}^m C_2(f_i, D_i)) \}$$

\textbf{Proof.} The proof is based on Theorem 3.3. Let $C[0, \infty)$ denote the space of all continuous functions on $[0, \infty)$ equipped with the topology given by the metric:

$$\rho(f, g) := \sum_{k \geq 1} 2^{-k} \min \left( \sup_{0 \leq x \leq k} |f(x) - g(x)|, 1 \right). \quad (17)$$

It is a fact (see, for example, [29, Chapter 1]) that $C[0, \infty)$ is a locally convex vector space under this topology. We shall apply Choquet’s theorem to $V = C[0, \infty)$ and $K = \bigcap_{i=1}^m C_1(f_i, D_i)$ for the first identity and $K = \bigcap_{i=1}^m C_2(f_i, D_i)$ for the second identity. It is obvious that $C$ is a subset of $C[0, \infty)$.

Clearly both the sets $\bigcap_i C_1(f_i, D_i)$ and $\bigcap_i C_2(f_i, D_i)$ are convex. Also, by Fatou’s lemma, $\bigcap_i C_1(f_i, D_i)$ is closed under pointwise convergence i.e., if $\psi_n \in \bigcap_i C_1(f_i, D_i)$ and $\psi_n \to \psi$ pointwise, then $\psi \in \bigcap_i C_1(f_i, D_i)$. To see this, observe that by Fatou’s lemma, for each $i = 1, \ldots, m$,

$$I_{f_i}(\psi) = \int_0^\infty (\min(1, s) - \psi(s)) \ d\nu_{f_i}(s)$$

$$= \int_0^\infty \liminf_{n \to \infty} (\min(1, s) - \psi_n(s)) \ d\nu_{f_i}(s)$$

$$\leq \liminf_{n \to \infty} \int_0^\infty (\min(1, s) - \psi_n(s)) \ d\nu_{f_i}(s) \leq D_i.$$
On the other hand, if each \( D_{f_i} \) is a finite divergence, then by the dominated convergence theorem, \( \cap_i C_2(f_i, D_i) \) is also closed under pointwise convergence. Indeed, if \( \psi_n \to \psi \) pointwise and \( D_{f_i} \) is a finite divergence, then by the dominated convergence (since \( 0 \leq \min(1, s) - \psi_n(s) \leq \min(1, s) \)), we have \( I_{f_i}(\psi_n) \to I_{f_i}(\psi) \).

In Lemma 3.5 below, we show that \( C \) is a compact subset of \( C[0, \infty) \) under the topology given by the metric \( \rho \). Moreover, it is easy to see that convergence in the metric \( \rho \) implies pointwise convergence. It follows hence that \( \cap_i C_1(f_i, D_i) \) is a compact, convex subset of \( C[0, \infty) \) and if each \( D_{f_i} \) is a finite divergence, then \( \cap_i C_2(f_i, D_i) \) is also a compact, convex subset of \( C[0, \infty) \).

For each \( \epsilon > 0 \), let us define the functional \( \Lambda_\epsilon \) on \( C[0, \infty) \) by
\[
\Lambda_\epsilon(\psi) = \int (\min(1, s) - \psi(s)) \{ \epsilon \leq s \leq 1/\epsilon \} d\nu_f(s)
\]
When restricted to the interval \([\epsilon, 1/\epsilon]\), the measure \( \nu_f \) is a finite measure. Hence, \( \Lambda_\epsilon \) is a continuous, linear functional on \( C[0, \infty) \). Thus, by Theorem 3.3, we get that for every \( \psi_0 \in \cap_i C_1(f_i, D_i) \), there exists a Borel probability measure \( \tau_0 \) that is concentrated on the set of extreme points, \( ext(\cap_i C_1(f_i, D_i)) \), of \( \cap_i C_1(f_i, D_i) \) such that
\[
\Lambda_\epsilon(\psi_0) = \int \Lambda_\epsilon(\psi)d\tau_0(\psi),
\]
for every \( \epsilon > 0 \). Now, by the monotone convergence theorem,
\[
\Lambda_\epsilon(\psi) \uparrow I_f(\psi) \quad \text{as} \quad \epsilon \downarrow 0
\]
for every \( \psi \in C \). As a result, we can use the monotone convergence theorem again to assert that
\[
\int \Lambda_\epsilon(\psi)d\tau_0(\psi) \uparrow \int I_f(\psi)d\tau_0(\psi) \quad \text{as} \quad \epsilon \downarrow 0.
\]
We therefore obtain
\[
I_f(\psi_0) = \int I_f(\psi)d\tau_0(\psi).
\]
Since this is true for all functions \( \psi_0 \) in \( \cap_i C_1(f_i, D_i) \), we obtain
\[
\sup_{\psi \in \cap_i C_1(f_i, D_i)} I_f(\psi) = \sup_{\psi \in ext(\cap_i C_1(f_i, D_i))} I_f(\psi)
\]
The proof of the first assertion of Lemma 3.4 is now complete by (13). Similarly, when each divergence \( D_{f_i} \) is finite, we can prove that
\[
\inf_{\psi \in \cap_i C_2(f_i, D_i)} I_f(\psi) = \inf_{\psi \in ext(\cap_i C_2(f_i, D_i))} I_f(\psi)
\]
and this, together with (14), completes the proof of Lemma 3.4.

In the above proof, we used the fact that \( C \) is compact in \( C[0, \infty) \), the space of all continuous functions on \([0, \infty)\). We prove this fact below.

**Lemma 3.5.** The class \( C \) is compact in \( C[0, \infty) \) equipped with the topology given by the metric (17).
Proof. We show that $C$ is sequentially compact. Consider a sequence $\{\psi_n\}$ in $C$. For every fixed $s_0 \in [0, \infty)$, the sequence $\{\psi_n(s_0)\}$ is a sequence of real numbers in $[0, 1]$ and hence has a convergent subsequence. By a standard diagonalization argument, we assert the existence of a subsequence $\{\phi_k\}$ of $\{\psi_n\}$ that converges pointwise over the set of all nonnegative rational numbers (denoted by $\mathbb{Q}_+$).

Let us now fix $\epsilon > 0$ and a real number $s_0 \in [0, \infty)$. Choose $r_1, r_2 \in \mathbb{Q}_+$ such that $r_1 \leq s_0 \leq r_2$ and such that $r_2 - r_1 < \epsilon/4$. Also, let $N \geq 1$ be large enough so that

$$|\phi_k(r_i) - \phi_l(r_i)| < \epsilon/4 \quad \text{for } k, l \geq N$$

and for $i = 1, 2$. Using properties of functions in $C$, we get that

$$|\phi_k(s_0) - \phi_l(s_0)| < |\phi_k(r_1) - \phi_l(r_2)| + |\phi_k(r_2) - \phi_l(r_1)|$$

$$< 2|\phi_k(r_1) - \phi_l(r_1)| + 2|r_1 - r_2| < \epsilon.$$

In the last inequality above, we have used the fact that functions in $C$ are Lipschitz with constant 1 (this can be proved for instance using the derivatives given by Lemma 3.2). It therefore follows that the sequence $\{\phi_k\}$ converges pointwise on $[0, \infty)$. The proof is now complete by the observation that convergence in the metric $\rho$ is equivalent to pointwise convergence on $[0, \infty)$.

\[\square\]

### 3.3 Characterization of Extreme Points

Lemma 3.4 asserts that for the purposes of finding the supremum or infimum of $I_f$ subject to constraints on $I_f$, it is enough to focus on the extreme points of the constraint set. In the next theorem, we provide a necessary condition for a function in the constraint set to be an extreme point of the constraint set.

**Theorem 3.6.** Let $\psi$ be a function in $\cap_i C_i(f_i, D_{i})$ and let $k$ be the number of indices $i$ for which $I_{f_i}(\psi) = D_{f_i}$. Then a necessary condition for $\psi$ to be extreme in $\cap_i C_i(f_i, D_{i})$ is that $\psi$ equals $\psi_{P,Q}$ for two probability measures $P, Q \in \mathcal{P}_{k+2}$. The same conclusion also holds for extreme functions in $\cap_i C_2(f_i, D_{i})$ provided all the involved divergences $D_{f_1}, \ldots, D_{f_m}$ are finite.

**Remark 3.3.** When $m = k = 0$, the sets $\cap_i C_1(f_i, D_{i})$ and $\cap_i C_2(f_i, D_{i})$ can both be taken to be equal to $C$. As will be clear from the proof, the above theorem will also be true in this case where it states that a necessary condition for a function $\psi$ to be extreme in $C$ is that $\psi$ equals $\psi_{P,Q}$ for two probability measures $P, Q \in \mathcal{P}_{2}$.

The proof of Theorem 3.6 relies on the following lemma whose proof is provided after the proof of Theorem 3.6.

**Lemma 3.7.** Let $P$ and $Q$ be two probability measures on a space $\mathcal{X}$ having densities $p$ and $q$ with respect to $\lambda$. Let $l \geq 1$ be fixed. Suppose that for every decreasing sequence $s_1 > \cdots > s_l$ of positive real numbers, the following condition holds:

$$\min_{1 \leq j \leq l+1} (P(B_j) + Q(B_j)) = 0$$
where \( B_1 = \{ p \geq q s_1 \}, B_i = \{ q s_i \leq p < q s_{i-1} \} \) for \( i = 2, \ldots, l \) and \( B_{i+1} = \{ p < q s_i \} \). Then \( \psi_{P,Q} \) can be written as \( \psi_{P',Q'} \) for two probability measures \( P', Q' \in \mathcal{P}_l \).

Proof of Theorem 3.6. Let \( \psi \) be a function in \( \text{ext}(\cap_i \mathcal{C}_i(f_i, D_i)) \). Since \( \psi \in \mathcal{C} \), we can write \( \psi(s) = \psi_{P,Q}(s) = \int \min(p, sq) d\lambda \) for some probability measures \( P \) and \( Q \) on a measurable space \( \mathcal{X} \) having densities \( p \) and \( q \) with respect to a common sigma finite measure \( \lambda \). Without loss of generality, we assume that

\[
I_{f_i}(\psi) = D_{f_i}(P||Q) = D_i \quad \text{for } i = 1, \ldots, k
\]
and

\[
I_{f_i}(\psi) = D_{f_i}(P||Q) < D_i \quad \text{for } i = k + 1, \ldots, m.
\]

Let \( \alpha : \mathcal{X} \to (-1, 1) \) be a function satisfying

\[
\int \alpha p d\lambda = \int \alpha q d\lambda = 0.
\]
Note that \((1 + \alpha)p, (1 - \alpha)p, (1 + \alpha)q, (1 - \alpha)q\) are all probability densities with respect to \( \lambda \). Let \( P^+, P^-, Q^+, Q^- \) be probability measures having densities \( p_+ := (1 + \alpha)p, p_- := (1 - \alpha)p, q_+ := (1 + \alpha)q, q_- := (1 - \alpha)q \) respectively with respect to \( \lambda \). Also, let

\[
\psi_+(s) := \psi_{P^+, Q^+}(s) = \int (1 + \alpha) \min(p, sq) d\lambda
\]
and

\[
\psi_-(s) := \psi_{P^-, Q^-}(s) = \int (1 - \alpha) \min(p, sq) d\lambda
\]
so that \( \psi = (\psi_+ + \psi_-)/2 \). For every \( i = 1, \ldots, m \), we observe that

\[
I_{f_i}(\psi_+) = D_{f_i}(P_+||Q_+)
= \int q_+ f_i \left( \frac{p_+}{q_+} \right) d\lambda + f_i'(\infty) P_+ \{ q_+ = 0 \}.
\]
Writing \((1 + \alpha)p\) and \((1 + \alpha)q\) for \( p_+ \) and \( q_+ \) respectively and noting that \( 1 + \alpha > 0 \) because \( \alpha \) takes values in \((-1,1)\), we obtain

\[
I_{f_i}(\psi_+) = I_{f_i}(\psi) + \int \alpha r_id\lambda
\]
where

\[
r_i := q f_i \left( \frac{p}{q} \right) + f_i'(\infty) p \{ q = 0 \}.
\]
It follows similarly that

\[
I_{f_i}(\psi_-) = I_{f_i}(\psi) - \int \alpha r_id\lambda
\]
We observe that \( \int r_id\lambda \leq D_i \) for each \( i = 1, \ldots, m \) which implies that

\[
\int |\alpha r_i|d\lambda < \infty
\]
for every function \( \alpha \) that takes values in \((-1,1)\) and \( i = 1, \ldots, m \).
From (19), (22) and (23), it follows that the two inequalities:

\[ I_f(\psi_+) \leq D_i \quad \text{and} \quad I_f(\psi_-) \leq D_i \]

will be satisfied for \( i = 1, \ldots, k \) if and only if

\[ \int \alpha r_i d\lambda = 0 \quad \text{for} \quad i = 1, \ldots, k. \]

(26)

Moreover, from (20), (22) and (23), it follows that if \( \sup_{x \in X} |\alpha(x)| \) is sufficiently small, then (25) will be satisfied also for \( i = k + 1, \ldots, m \). Let us say that \( \alpha \) is a good function if it satisfies (21) and (26) and if \( \sup_{x} |\alpha(x)| \) is sufficiently small. We have thus proved that if \( \alpha \) is a good function, then both \( \psi_+ \) and \( \psi_- \) belong to \( \cap_i C_i(f_i, D_i) \). Because \( \psi \) is extreme and \( \psi = (\psi_+ + \psi_-)/2 \), we assert that \( \psi = \psi_+ = \psi_- \) for every good function \( \alpha \). As a result, \( \partial \psi(s) = \partial \psi_+(s) \) for every \( s > 0 \) and \( \partial \psi(s) = \partial \psi_+(s) \) for every \( s \geq 0 \). Because of Lemma 3.2 and the relations \( \psi \) for every \( s > 0 \) and \( s \geq 0 \), we have therefore shown that both \( \psi \) and \( \psi_+ \) hold for every decreasing sequence \( s_1 > \cdots > s_{k+2} \) of positive real numbers, the following condition must hold

\[ \min_{1 \leq j \leq k+3} (P(B_j) + Q(B_j)) = 0 \]

(29)

where \( B_1 = \{ p \geq q_{s_1} \} \), \( B_i = \{ q_{s_i} \leq p < q_{s_i-1} \} \) for \( i = 2, \ldots, k+2 \), and \( B_{k+3} = \{ p < q_{s_{k+2}} \} \). The proof would then be completed by Lemma 3.7.

We prove (29) via contradiction. Suppose that the condition (29) does not hold for some \( s_1 > \cdots > s_{k+2} \). Let \( \alpha = \sum_{j=1}^{k+3} \alpha_j I_{B_j} \) where \( \alpha_1, \ldots, \alpha_{k+3} \) are real numbers in \((-1,1)\) and \( I_{B_j} \) denotes the indicator function of \( B_j \). We claim that for this \( \alpha \), the conditions (27) and (28) cannot hold unless \( \alpha_1 = \cdots = \alpha_{k+3} = 0 \). To see this, note that (27) and (28) for \( s = s_1 \) give \( \alpha_1 (P(B_1) + Q(B_1)) = 0 \). But since \( P(B_1) + Q(B_1) \) is strictly positive (we are assuming that (29) does not hold), it follows that \( \alpha_1 = 0 \). We now use (27) and (28) for \( s = s_2 \) to obtain \( \alpha_2 = 0 \). Continuing this argument, we get that (27) and (28) cannot hold unless \( \alpha_1 = \cdots = \alpha_{k+3} = 0 \). As a result, it follows that \( \alpha = \sum_{j=1}^{k+3} \alpha_j I_{B_j} \) is not a good function for every non-zero vector \( (\alpha_1, \ldots, \alpha_{k+3}) \) in \( \mathbb{R}^{k+3} \).

On the other hand, as can be easily seen by writing down the conditions (21) and (26), for \( \alpha = \sum_{j=1}^{k+3} \alpha_j I_{B_j} \) to be a good function, \( \max_j |\alpha_j| \) needs to be sufficiently small and the following equalities need to be satisfied:

\[ \sum_{j=1}^{k+3} \alpha_j P(B_j) = 0 = \sum_{j=1}^{k+3} \alpha_j Q(B_j) \]
and

\[ \sum_{j=1}^{k+3} \alpha_j \int_{B_j} r_j d\lambda = 0 \quad \text{for } i = 1, \ldots, k. \]

If (29) is not satisfied, then the above represent \(k+2\) linear equalities for the \(k+3\) variables \(\alpha_1, \ldots, \alpha_{k+3}\). Therefore, a solution exists where \(\alpha_1, \ldots, \alpha_{k+3}\) are non-zero (and where \(\max_j |\alpha_j|\) is small) for which \(\alpha = \sum_{j=1}^{k+3} \alpha_j I_{B_j}\) becomes a good function. Since this is a contradiction, we have established (29).

By Lemma 3.7, it follows that \(\psi\) can be written as \(\psi_{P',Q'}\) for two probability measures \(P'\) and \(Q'\) on \(\{1, \ldots, k+2\}\). This proves the first part of the theorem. The case of \(\cap_i C_2(f_i, D_i)\) is very similar. In the above argument, the only place where we used the fact that the constraints in \(\cap_i C_1(f_i, D_i)\) are of the \(\leq\) form is in asserting (24). In the case of \(\cap_i C_2(f_i, D_i)\), the statement (24) still holds under the assumption that each divergence \(D_{f_i}\) is finite. The rest of the proof proceeds exactly as before.

Below, we provide the proof of Lemma 3.7 which was used in the above proof.

**Proof of Lemma 3.7.** Let \(\eta\) denote the probability measure \((P + Q)/2\). Suppose

\[ N := \{x \in (0, 1) : x = \eta\{p \geq qs\} \text{ for some } s \in (0, \infty)\}. \]

We claim that \(N\) is a finite set having cardinality at most \(l - 1\). To see this, suppose, if possible, that there exist points \(0 < x_1 < \cdots < x_l < 1\) in \(N\). Then, we can write \(x_i = \eta\{p \geq qs\}\) for some \(s_1 > \cdots > s_l > 0\). But then \(\eta(B_1) = x_1, \eta(B_i) = x_i - x_{i-1} > 0\) for \(i = 2, \ldots, l\) and \(\eta(B_{l+1}) = 1 - x_l > 0\) which contradicts the condition given in the lemma. Let us therefore assume that the cardinality of \(N\) equals \(k \leq l - 1\) and let \(N = \{x_1, \ldots, x_k\}\) where \(0 < x_1 < \cdots < x_k < 1\). Let

\[ s_i^* := \sup \{s > 0 : \eta\{p \geq qs\} = x_i\} \]

for \(i = 1, \ldots, k\). Also let

\[ s_{k+1}^* := \sup \{s > 0 : \eta\{p \geq qs\} = 1\} \]

if there exists \(s > 0\) with \(\eta\{p \geq qs\} = 1\). If there exists no such \(s > 0\), we define \(s_{k+1}^* = 0\). It is easy to see that \(s_1^* \in (0, \infty]\) and \(s_{k+1}^* \in [0, \infty)\) while \(s_2^*, \ldots, s_k^* \in (0, \infty)\). Let us first consider the case when \(s_1^* < \infty\) and \(s_{k+1}^* > 0\). In this case, for each \(i = 1, \ldots, k+1\), there exists a sequence \(\{t_n(i)\}\) with \(0 < t_n(i) \uparrow s_i^*\) such that \(\eta\{p \geq qt_n(i)\} = x_i\) (we take \(x_{k+1} = 1\)). Because the sets \(\{p \geq qt_n(i)\}\) decrease to \(\{p \geq qs_i^*\}\) as \(n \to \infty\), it follows that \(\eta\{p \geq qs_i^*\} = x_i\) for each \(i = 1, \ldots, k+1\). Also it is easy to see that

\[ \eta\{p > qs_i^*\} = \lim_{s_i^* \downarrow s_i^*} \eta\{p \geq qs\} = x_{i-1} \]

for each \(i = 1, \ldots, k + 1\) where we take \(x_0 = 0\). It follows therefore that \(\eta\{p = qs_i^*\} = x_i - x_{i-1}\) for \(1 \leq i \leq k + 1\). Because \(\sum_{i=1}^{k+1} (x_i - x_{i-1}) = x_{k+1} - x_0 = 1\), it follows that

\[ \sum_{i=1}^{k+1} \eta\{p = qs_i^*\} = 1. \quad (30) \]
It can be checked that the above statement is also true in the case when $s^*_1 = \infty$ and/or $s^*_{k+1} = 0$ provided we interpret

$\{p = q \cdot \infty\} = \{q = 0\}$ and $\{p = q \cdot 0\} = \{p = 0\}$.

The equality (30) is the same as

$$\sum_{i=1}^{k+1} P\{p = qs^*_i\} = 1 \quad \text{and} \quad \sum_{i=1}^{k+1} Q\{p = qs^*_i\} = 1.$$  \hfill (31)

Let $p_i = P\{p = qs^*_i\}$ and $q_i = Q\{p = qs^*_i\}$ for $i = 1, \ldots, k+1$ so that $P' = (p_1, \ldots, p_{k+1})$ and $Q' = (q_1, \ldots, q_{k+1})$ are probability measures on $\{1, \ldots, k+1\}$. For each $i = 1, \ldots, k+1$, we have

$$p_i = P\{p = qs^*_i\} = \int_{p = qs^*_i} p d\lambda = s^*_i \int_{p = qs^*_i} q d\lambda = s^*_i q_i$$

where the above statement is to be interpreted as $q_1 = 0$ if $s^*_1 = \infty$ and as $p_{k+1} = 0$ if $s^*_{k+1} = 0$. Also

$$\int_{p = qs^*_i} \min(p, qs) d\lambda = \min(s^*_i, s) Q\{p = qs^*_i\} = \min(p_i, q_i s)$$

for every $s \geq 0$ and $i = 1, 2, \ldots, k+1$. Therefore,

$$\psi_{P, Q}(s) = \int \min(p, qs) d\lambda = \sum_{i=1}^{k+1} \int_{p = qs^*_i} \min(p, qs) d\lambda = \psi_{P', Q'}(s).$$

The proof is complete because $k + 1 \leq l$. \hfill $\square$

### 3.4 Completion of the Proof

We shall prove (5). The proof of (6) is entirely analogous. Theorem 3.6 states that every function in $\cap_i C_1(f_i, D_i)$ that is extreme equals $\psi_{P, Q}$ for some $P, Q \in P_{m+2}$. Therefore, by Lemma 3.4, we get that $A(D_1, \ldots, D_m)$ equals

$$\sup \{I_f(\psi_{P, Q}) : \psi_{P, Q} \in \cap_i C_1(f_i, D_i) \text{ and } P, Q \in P_{m+2}\}.$$

Because $I_f(\psi_{P, Q})$ equals $D_f(P \| Q)$, the constraint $\psi \in \cap_i C_1(f_i, D_i)$ is equivalent to $D_f(P \| Q) \leq D_i$ for all $i = 1, \ldots, m$. The proof is therefore complete.

### 4 Remarks and Extensions

#### 4.1 Stronger Version

The proof of Theorem 2.1 actually yields a smaller expression for $A(D_1, \ldots, D_m)$ than $A_{m+2}(D_1, \ldots, D_m)$ and a larger expression for $B(D_1, \ldots, D_m)$ than $B_{m+2}(D_1, \ldots, D_m)$. For each subset $J$ of $\{1, \ldots, m\}$, let
$A^J(D_1, \ldots, D_m)$ denote the supremum of $D_f(P||Q)$ over all probability measures $P, Q \in \mathcal{P}_{k+2}$ (where $k$ is the cardinality of $J$) for which $D_{f_i}(P||Q) = D_i$ for $i \in J$ and $D_{f_i}(P||Q) < D_i$ for $i \notin J$. It is clear that

$$A^J(D_1, \ldots, D_m) \leq A^{m+2}(D_1, \ldots, D_m)$$

for each $J \subseteq \{1, \ldots, m\}$. The following is therefore a stronger version of Theorem 2.1:

$$A(D_1, \ldots, D_m) = \max_{J \subseteq \{1, \ldots, m\}} A^J(D_1, \ldots, D_m)$$ (32)

An analogous statement also holds for $B(D_1, \ldots, D_m)$. Let us now show that our proof of Theorem 2.1 given in Section 3.4 results in (32). By Theorem 3.6, every function $\psi$ in $\cap_i C_1(f_i, D_i)$ that is extreme equals $\psi_{P,Q}$ for some $P, Q \in \mathcal{P}_{k+2}$ where $k$ is the number of indices $i$ for which $I_{f_i}(\psi) = D_{f_i}(P||Q) = D_i$. Therefore, if $J$ denotes these indices, then

$$I_f(\psi) = D_f(P||Q) \leq A^J(D_1, \ldots, D_m)$$

$$\leq \max_{J \subseteq \{1, \ldots, m\}} A^J(D_1, \ldots, D_m)$$

for every $\psi \in \text{ext}(\cap_i C_1(f_i, D_i))$. The equality (32) therefore follows from Lemma 3.4.

### 4.2 Joint Ranges

Recall that the joint range of divergences $D_{f_1}, \ldots, D_{f_m}$ is denoted by $\mathcal{R}(f_1, \ldots, f_m)$ and is defined as the set of all vectors in $\mathbb{R}^m$ that equal $(D_{f_1}(P||Q), \ldots, D_{f_m}(P||Q))$ for some $P$ and $Q$. The quantities $A(D_1, \ldots, D_m)$ and $B(D_1, \ldots, D_m)$ can easily be calculated from knowledge of $\mathcal{R}(f_1, \ldots, f_m)$. It therefore makes sense to try to prove Theorem 2.1 by trying to determine the joint range $\mathcal{R}(f_1, \ldots, f_m)$. We argue here that this approach is not good enough to prove Theorem 2.1; it results in the weaker identities (36) and (37).

In the following theorem, we characterize the joint range $\mathcal{R}(f_1, \ldots, f_m)$ for every arbitrary set of $m$ divergences. We show that it suffices to restrict attention to pairs of probability measures in $\mathcal{P}_{m+2}$. For each $k \geq 1$, let

$$\mathcal{R}_k(f_1, \ldots, f_m) := \{(D_{f_1}(P||Q), \ldots, D_{f_m}(P||Q)) : P, Q \in \mathcal{P}_k\}.$$ 

**Theorem 4.1.** For every $m \geq 1$ and divergences $D_{f_1}, \ldots, D_{f_m}$, we have

$$\mathcal{R}(f_1, \ldots, f_m) = \mathcal{R}_{m+2}(f_1, \ldots, f_m).$$

For the special case $m = 2$, this theorem has already been proved by [15]. The short proof given below uses the Caratheodory theorem and was communicated to us by an anonymous referee. In contrast, the proof given in [15] for $m = 2$ is much more elaborate. The counterexamples in [15] show the tightness of this theorem. After the proof, we describe an attempt to prove Theorem 2.1 via Theorem 4.1.
Proof. We just need to prove that $R(f_1, \ldots, f_m) \subseteq R_{m+2}(f_1, \ldots, f_m)$. Let $u \in R(f_1, \ldots, f_m)$. Then $u = (D_{f_1}(P||Q), \ldots, D_{f_m}(P||Q))$ for some pair of probability measures $P$ and $Q$. If $p$ and $q$ denote the densities of $P$ and $Q$ with respect to a common measure $\lambda$, then

$$u = \int_{\{q > 0\}} \left( f_1 \left( \frac{p}{q} \right), \ldots, f_m \left( \frac{p}{q} \right) \right) dQ + P\{q = 0\} \left( f_1^1(\infty), \ldots, f_m^1(\infty) \right).$$

(33)

Let $S \subseteq \mathbb{R}^{m+1}$ be defined by $S := \{(s, f_1(s), \ldots, f_m(s)) : s \geq 0\}$. Then clearly the vector

$$\int_{\{q > 0\}} \left( \frac{p}{q}, f_1 \left( \frac{p}{q} \right), \ldots, f_m \left( \frac{p}{q} \right) \right) dQ$$

lies in the convex hull of $S$. Because $S$ is a connected subset of $\mathbb{R}^{m+1}$, we can use Caratheodory’s theorem (see, for example, [2]) to assert that any point in its convex hull can be written as a convex combination of at most $m + 1$ points in $S$. As a result, we can write

$$\int_{\{q > 0\}} \left( \frac{p}{q}, f_1 \left( \frac{p}{q} \right), \ldots, f_m \left( \frac{p}{q} \right) \right) dQ = \sum_{i=1}^{m+1} \alpha_i \left( s_i, f_1(s_i), \ldots, f_m(s_i) \right)$$

(34)

for some $\alpha_1, \ldots, \alpha_{m+1} \geq 0$ with $\sum_i \alpha_i = 1$ and $s_1, \ldots, s_{m+1} \geq 0$. One consequence of this representation is that

$$\sum_{i=1}^{m+1} \alpha_i s_i = \int_{q > 0} \left( \frac{p}{q} \right) dQ = P\{q > 0\}.$$  

(35)

We now define two probability measures $P'$ and $Q'$ in $\mathcal{P}_{m+2}$ as follows: $P'\{i + 1\} = \alpha_i s_i$ for $1 \leq i \leq m + 1$ and $P'\{1\} = P\{q = 0\}$; and $Q'\{i + 1\} = \alpha_i$ for $1 \leq i \leq m + 1$ and $Q'\{1\} = 0$. The fact that $\sum_{i=1}^{m+2} P'\{i\} = 1$ follows from (35). The equalities (33) and (34) together clearly imply that $u = (D_{f_1}(P'||Q'), \ldots, D_{f_m}(P'||Q'))$. Thus $u \in R_{m+2}(f_1, \ldots, f_m)$ and this completes the proof. □

Clearly $A(D_1, \ldots, D_m)$ and $B(D_1, \ldots, D_m)$ can be written as functions of the joint range $R(f, f_1, \ldots, f_m)$. Therefore, Theorem 4.1 immediately therefore implies

$$A(D_1, \ldots, D_m) = A_{m+3}(D_1, \ldots, D_m)$$

(36)

and

$$B(D_1, \ldots, D_m) = B_{m+3}(D_1, \ldots, D_m).$$

(37)

These results are clearly weaker than those given by Theorem 2.1. Strictly speaking, one can deduce a slightly stronger conclusion than (36) and (37) from Theorem 4.1. A probability measure on $\{1, \ldots, m+3\}$ is determined by $m + 2$ real numbers. Therefore, a pair of probability measures in $\mathcal{P}_{m+2}$ are determined by $2m + 4$ real numbers. The inequalities (36) and (37) therefore reduce the optimization problems for $A(D_1, \ldots, D_m)$ and $B(D_1, \ldots, D_m)$ into optimization problems over $2m + 4$ variables. A closer inspection at the proof of Theorem 4.1 shows that one actually gets a reduction to $2m + 3$ variables. This is because the probability measure $Q'$ in the proof satisfies $Q'\{1\} = 0$. Therefore, by an argument based solely on the joint range of $D_f, D_{f_1}, \ldots, D_{f_m}$, one can reduce the optimization problems for $A(D_1, \ldots, D_m)$ and $B(D_1, \ldots, D_m)$ into optimization problems over $2m + 3$ variables. Because of the tightness of Theorem 4.1, this is the best reduction that one can hope for the quantities $A(D_1, \ldots, D_m)$ and $B(D_1, \ldots, D_m)$ via an argument based on the joint range alone. On the other hand, Theorem 2.1 achieves a reduction to $2m + 2$ variables.
4.3 Tightness

The conclusion of Theorem 2.1 is tight in the sense that, in general, one cannot reduce the optimization problems to pairs of probability measures on spaces of cardinality strictly smaller than \( m + 2 \). We shall demonstrate this fact in this section by means of an example. We also explain this fact numerically in Example 6.6.

Consider the problem of maximizing an \( f \)-divergence subject to a upper bound on the total variation distance. In other words, let

\[
A(V) := \sup\{D_f(P||Q) : V(P, Q) \leq V\}
\]

where \( D_f \) is an arbitrary \( f \)-divergence. In this case, Theorem 2.1 asserts that \( A(V) \) equals \( A_3(V) \) where, as before,

\[
A_k(V) := \sup\{D_f(P||Q) : P, Q \in \mathcal{P}_k, V(P, Q) \leq V\}.
\]

We shall show below that when \( D_f \) is a finite divergence and when \( f \) is strictly convex on \((0, \infty)\), the quantity \( A_3(V) \) is strictly larger than \( A_2(V) \) for all \( V \in (0, 1) \).

The quantity \( A_3(V) = A(V) \) can be determined precisely. The easiest way is to use Lemma 3.1. Because

\[
V(P, Q) = D_{a_1}(P||Q) = 1 - \psi_{P, Q}(1),
\]

the constraint \( V(P, Q) \leq V \) is equivalent to \( \psi_{P, Q}(1) \geq 1 - V \). Therefore, by Lemma 3.1, we get

\[
A(V) = \sup\{I_f(\psi) : \psi \in \mathcal{C} \text{ and } \psi(1) \geq 1 - V\}.
\]

It is obvious that the supremum above is achieved for \( \psi(s) = (1 - V) \min(1, s) \) which equals \( \psi_{P', Q'} \) for \( P' = (1 - V, V, 0) \) and \( Q' = (1 - V, 0, V) \). Thus

\[
A(V) = D_f(P'||Q') = V f(0) + f'(\infty).
\]

In other words, by Remark 3.2, the quantity \( A(V) \) equals \( V \) times the maximum possible value of the divergence \( D_f \).

Let us now consider the quantity \( A_2(V) \). By compactness and the form of the constraint, it follows that there exist two probability measures \( P^* \) and \( Q^* \) in \( \mathcal{P}_2 \) with \( V(P^*, Q^*) = V \) and \( D_f(P^*||Q^*) = A_2(V) \). We can then, without loss of generality, parametrize \( P^* \) and \( Q^* \) by \( P^* = (\rho, 1 - \rho) \) and \( Q^* = (\rho + V, 1 - \rho - V) \) for some \( 0 \leq \rho \leq 1 - V \). Consider now the probability measures

\[
\hat{P} = \left(\frac{\rho}{2}, \frac{\rho}{2}, 1 - \rho\right) \quad \text{and} \quad \hat{Q} = \left(\frac{\rho}{2} + \frac{V}{4}, \frac{\rho}{2} + \frac{3V}{4}, 1 - \rho - V\right)
\]

in \( \mathcal{P}_3 \). If \( V \in (0, 1) \), by strict convexity of the function \( f \), it is easy to see that

\[
D_f(\hat{P}||\hat{Q}) > D_f(P^*||Q^*) = A_2(V).
\]
On the other hand, it is easy to see that $V(\hat{P}, \hat{Q})$ equals $V$ and hence $A_3(V) > D_f(\hat{P}||\hat{Q})$. Therefore, $A_3(V) > A_2(V)$. Thus, Theorem 2.1 is tight in general. However, in some special cases, one can obtain stronger conclusions, see Sections 5.1 and 5.2.

4.4 Finiteness assumption for $B(D_1, \ldots, D_m)$

In order to prove (6), we required that all the divergences $D_{f_1}, \ldots, D_{f_m}$ are finite. The reason is mainly technical and the finiteness assumption was crucially used in the proof of Lemma 3.4. The set $\cap_i C_2(f_i, D_i)$ will not be closed (in $C[0, \infty)$ equipped with the metric $\rho$) if some of the divergences $D_{f_i}$ were non-finite (closedness of $\cap_i C_2(f_i, D_i)$ was critical in the application of Choquet’s theorem in Lemma 3.4). To illustrate this non-closedness, let us consider $m = 1$ and the set $C_2(f_1, D_1)$ for some non-finite divergence $D_{f_1}$ and $D_1 > 0$. By (12), because $D_{f_1}$ is non-finite, we have

$$\int_0^{\infty} \min(1, s) d\nu_{f_1}(s) = \infty.$$  

The function $\psi_0(s) = \min(1, s)$ clearly does not belong to $C_2(f_1, D_1)$ because $I_{f_1}(\psi_0) = 0$. But we shall show that $\psi_0$ belongs to the closure of $C_2(f_1, D_1)$. Indeed, if

$$\psi_n(s) := \left(1 - \frac{1}{n}\right) \min(1, s) \quad \text{for } s \geq 0,$$

then clearly $\psi_n$ converges to $\psi$ in the metric $\rho$. Moreover, for each $n$, $\psi_n \in C$ and

$$I_{f_1}(\psi_n) = \frac{1}{n} \int_0^{\infty} \min(1, s) d\nu_{f_1}(s) = \infty.$$  

Thus $\psi_n \in C_2(f_1, D_1)$ for each $n \geq 1$ which implies that $\psi_0$ belongs to the closure of $C_2(f_1, D_1)$. Therefore, $C_2(f_1, D_1)$ is not closed.

The quantity $B(D_1, \ldots, D_m)$ behaves strangely when some of the divergences $D_{f_i}$ are non-finite and when $D_f$ is finite. Indeed, in this case, one can simply drop the constraints corresponding to the non-finite divergences and reduce the problem to the case when all divergences are finite. This is the content of the next lemma.

**Lemma 4.2.** Let $D_f, D_{f_1}, \ldots, D_{f_m}$ be finite divergences and let $D_{f_{m+1}}, \ldots, D_{f_{m+l}}$ be non-finite divergences. Then

$$B(D_1, \ldots, D_{m+l}) = B(D_1, \ldots, D_m).$$

**Proof.** We shall work with (14). Because $\cap_{i=1}^{m+l} C_2(f_i, D_i)$ is contained in $\cap_{i=1}^{m} C_2(f_i, D_i)$, it follows that $B(D_1, \ldots, D_{m+l})$ is larger than or equal to $B(D_1, \ldots, D_m)$. To prove the other inequality, let $\psi \in \cap_{i=1}^{m} C_2(f_i, D_i)$. For each $n \geq 1$, define

$$\psi_n(s) = \min\left[\left(1 - \frac{1}{n}\right) \min(1, s), \psi(s)\right]$$
It is easy to check that $\psi_n \in \mathcal{C}$. Note that for $1 \leq i \leq m$,

$$I_f(\psi_n) = \int_0^\infty (\min(1, s) - \psi_n(s)) \, d\nu_f(s)$$

$$\geq \int_0^\infty (\min(1, s) - \psi(s)) \, d\nu_f(s) = I_f(\psi) \geq D_i.$$ 

Moreover, for $m < i \leq m + l$, we have

$$I_f(\psi_n) = \int_0^\infty (\min(1, s) - \psi_n(s)) \, d\nu_f(s)$$

$$\geq \frac{1}{n} \int_0^\infty \min(1, s) \, d\nu_f(s) = \infty \geq D_i.$$ 

It therefore follows that $\psi_n \in \bigcap_{i=1}^{m+l} \mathcal{C}_2(f_i, D_i)$ for every $n \geq 1$. Consequently,

$$I_f(\psi_n) \geq B(D_1, \ldots, D_{m+l}) \quad \text{for every } n \geq 1.$$ 

Observe that $\psi_n(s)$ converges to $\psi(s)$ for every $s \geq 0$. Thus, because $D_f$ is a finite divergence, it follows by the dominated convergence theorem that $I_f(\psi_n)$ converges to $I_f(\psi)$ which results in

$$I_f(\psi) \geq B(D_1, \ldots, D_{m+l}).$$ 

Finally, because $\psi \in \bigcap_{i=1}^m \mathcal{C}_2(f_i, D_i)$ is arbitrary, we have proved that $B(D_1, \ldots, D_m)$ is larger than or equal to $B(D_1, \ldots, D_{m+l})$ which completes the proof of the lemma.

**Remark 4.1.** If $D_f$ is finite and if all the divergences $D_{f_1}, \ldots, D_{f_m}$ are non-finite, then Lemma 4.2 gives that

$$B(D_1, \ldots, D_m) = 0$$ 

(38)

for all values of $D_1, \ldots, D_m$. Here is a special instance of this result. Suppose that $D_f$ denotes the total variation distance, $m = 1$ and that $D_{f_1}$ is the Kullback-Leibler divergence. Then (38) shows that the smallest value of the total variation distance over all probability measures with Kullback-Leibler divergence at least 5 (say) equals 0. The same conclusion holds for multiple non-finite divergence constraints as well.

Theorem 2.1 gives a formula for $B(D_1, \ldots, D_m)$ for arbitrary $D_f$ and for finite $D_{f_1}, \ldots, D_{f_m}$. In Lemma 4.2, we showed that when $D_f$ is finite, then the case when one of more of $D_{f_1}, \ldots, D_{f_m}$ are non-finite can be reduced to the case where all the constraint divergences are finite which is handled by Theorem 2.1. The case that we are unable to resolve is $B(D_1, \ldots, D_m)$ when $D_f$ is non-finite and when one or more of $D_{f_1}, \ldots, D_{f_m}$ are non-finite. This case is neither covered by Theorem 2.1 nor by Lemma 4.2.

### 4.5 Sufficiency of the extreme point characterization

In Theorem 3.6, we gave a necessary condition for functions in the classes $\cap_i \mathcal{C}_1(f_i, D_i)$ and $\cap_i \mathcal{C}_2(f_i, D_i)$ to be extreme. As we have seen, this necessary condition was enough to prove Theorem 2.1. For the sake
of completeness, in this section, we investigate whether the condition in Theorem 3.6 is sufficient as well for extremity.

Let \( j \in \{1, 2\} \) and let \( \psi \) be a function in \( \cap_i \mathcal{C}_j(f_i, D_i) \). Suppose \( \psi \) satisfies the condition given in Theorem 3.6 i.e., let \( \psi = \psi_{P,Q} \) for two probability measures \( P, Q \in \mathcal{P}_{k+2} \) where \( k \) is the number of indices where \( I_{f_i}(\psi) = D_i \). Here, we explore the question of extremity of \( \psi \) in \( \cap_i \mathcal{C}_j(f_i, D_i) \).

Let \( l \leq k + 2 \) be the size of the (finite) support set of the measure \( P + Q \) and let \( P = \{ p_1, \ldots, p_l \} \) and \( Q = \{ q_1, \ldots, q_l \} \), then \( \psi(s) = \sum_{i=1}^{l} \min(p_i, q_i s) \). Because the size of the support set of \( P + Q \) is \( l \), it follows that \( \max(p_i, q_i) > 0 \) for every \( i \). It is easy to check that \( \psi \) is piecewise linear with knots at \( p_i/q_i \) (this ratio can equal 0 or \( \infty \) as well).

Suppose that \( \psi = (\psi_1 + \psi_2)/2 \) for two functions \( \psi_1 \) and \( \psi_2 \) in \( \cap_i \mathcal{C}_j(f_i, D_i) \). Because \( \psi_1 \) and \( \psi_2 \) are both concave, it follows that they both have to be linear in the regions where \( \psi \) is linear. As a result, one can write

\[
\psi_1(s) = \sum_{i=1}^{l} (1 + \alpha_i) \min(p_i, q_i s)
\]

and

\[
\psi_2(s) = \sum_{i=1}^{l} (1 - \alpha_i) \min(p_i, q_i s)
\]

for some \( \alpha_1, \ldots, \alpha_n \in [-1, 1] \) satisfying

\[
\sum_{i=1}^{l} \alpha_i p_i = \sum_{i=1}^{l} \alpha_i q_i = 0. \tag{39}
\]

Now, whenever \( I_{f_i}(\psi) = D_i \), because of the above, we must have \( I_{f_i}(\psi_1) = D_i \). This latter equality can be written as a linear equality in \( \alpha_1, \ldots, \alpha_l \). Because \( I_{f_i}(\psi) = D_i \) for \( k \) indices \( i \), we obtain \( k \) linear equations for \( \alpha_1, \ldots, \alpha_l \). These, together with (39), give rise to \( k + 2 \) linear equations for the \( l \leq k + 2 \) variables \( \alpha_1, \ldots, \alpha_l \). Under appropriate linear independence conditions on the measures \( \nu_{f_i} \), these would imply that \( \alpha_i = 0 \) for every \( 1 \leq i \leq l \) which would further imply that \( \psi_1 = \psi = \psi_2 \) and that \( \psi \) is extreme.

In the case when \( m \leq 1 \) however, no such explicit linear independence conditions are necessary and, moreover, one can also give a geometric proof of the sufficiency characterization of the extreme points. We do this below in two parts: Lemma 4.3 deals with \( m = 0 \) (i.e., extreme points of \( \mathcal{C} \)) and Lemma 4.4 deals with the \( m = 1 \) case.

**Lemma 4.3.** For every \( P, Q \in \mathcal{P}_2 \), the function \( \psi_{P,Q} \) is extreme in \( \mathcal{C} \).

**Proof.** Fix two probability measures \( P \) and \( Q \) on \( \{1, 2\} \) and let \( J \) denote the smallest open interval (possibly infinite) such that \( \psi_{P,Q}(s) = \min(1, s) \) for \( s \notin J \). By explicitly writing down the expression for \( \psi \) in terms of \( P\{1\} \) and \( Q\{1\} \), it is easy to see that if \( J \) is non-empty, then \( \psi_{P,Q} \) is linear on \( J \).
Suppose now that $\psi_{P,Q}$ equals the convex combination $(\psi_1 + \psi_2)/2$ for two functions $\psi_1$ and $\psi_2$ in $\mathcal{C}$. If $J$ is empty, then $\psi_{P,Q}$ equals the function $\min(1, s)$ for all $s$ and since all functions in $\mathcal{C}$ and bounded from above by $\min(1, s)$, it follows that

$$
\psi_{P,Q}(s) = \psi_1(s) = \psi_2(s) = \min(1, s)
$$

(40)

for all $s \geq 0$.

Let us therefore assume that $J$ is non-empty. In this case, again it is obvious that (40) holds for $s \notin J$. Concavity of functions in $\mathcal{C}$ and linearity of $\psi$ in $J$ would then imply that $\psi_1 \geq \psi_{P,Q}$ and $\psi_2 \geq \psi_{P,Q}$. Since $\psi_{P,Q}$ is the average of $\psi_1$ and $\psi_2$, this can happen only when $\psi_{P,Q} = \psi_1 = \psi_2$. The proof is complete.

**Lemma 4.4.** Let $j \in \{1, 2\}$ and consider the class $\mathcal{C}_j(f_1, D_1)$ for $D_1 > 0$. For every $P, Q \in \mathcal{P}_3$ with $D_{f_1}(P||Q) = D_1$, the function $\psi_{P,Q}$ is extreme in $\mathcal{C}_j(f_1, D_1)$.

**Proof.** Fix two probability measures $P$ and $Q$ in $\mathcal{P}_3$ with $D_{f_1}(P||Q) = D_1$ so that $I_{f_1}(\psi_{P,Q}) = D_1$. For notational convenience, let us denote $\psi_{P,Q}$ by $\psi$. As in the proof of Lemma 4.3, let $J$ denote the smallest interval outside which $\psi(s)$ equals $\min(1, s)$. If $J$ is empty, then $\psi$ equals the function $\min(1, s)$ which is obviously extreme. So let us assume that $J$ is non-empty. In that case, because $P, Q \in \mathcal{P}_3$, it can be checked that $\psi$ is piecewise linear with at most two segments in $J$.

Suppose that $\psi = (\psi_1 + \psi_2)/2$ for two functions $\psi_1, \psi_2 \in \mathcal{C}_j(f_1, D_1)$. Because, $I_{f_1}(\psi) = D_{f_1}(P||Q) = D_1$, it follows that

$$
I_{f_1}(\psi_1) = I_{f_1}(\psi_2) = I_{f_1}(\psi) = D_{f_1}(P||Q) = D_1.
$$

(41)

If $\psi$ has exactly one segment in $J$, then, by concavity, the inequalities $\psi_1(s) \geq \psi(s)$ and $\psi_2(s) \geq \psi(s)$ hold for all $s$. Because $\psi_1$ and $\psi_2$ average out to $\psi$, we must then have $\psi = \psi_1 = \psi_2$.

Now suppose that $\psi$ has exactly two segments in $J$. Let $a$ be the point in $J$ such that $\psi$ is linear on both $J \cap [0, a]$ and $J \cap [a, \infty)$. We shall show that $\psi(a) = \psi_1(a) = \psi_2(a)$. Concavity of $\psi_1$ and $\psi_2$ and linearity of $\psi$ on $J \cap [0, a]$ and $J \cap [a, \infty)$ can then be used to show that $\psi = \psi_1 = \psi_2$. Suppose, if possible, that $\psi_1(a) > \psi(a)$. Using the concavity of $\psi_1$, it then follows that $\psi_1(s) > \psi(s)$ for all $s \in J$. Because of (41), it follows that

$$
\int_J (\psi_1(s) - \psi(s)) d\nu_{f_1}(s) = \int_0^\infty (\psi_1(s) - \psi(s)) d\nu_{f_1}(s) = 0
$$

This implies that $\nu_{f_1}(J) = 0$. But then

$$
D_1 = I_{f_1}(\psi) = \int_J (\min(1, s) - \psi(s)) d\nu_{f_1}(s) = 0
$$

which contradicts the fact that $D_1 > 0$. We have thus obtained $\psi_1(a) \leq \psi(a)$. Similarly, $\psi_2(a) \leq \psi(a)$ and since $\psi(a)$ is an average of $\psi_1(a)$ and $\psi_2(a)$, it follows that $\psi(a) = \psi_1(a) = \psi_2(a)$. The proof is complete.
5 Applications and Special Cases

5.1 Primitive Divergences

In this section, we consider the case of the quantity $B(D_1, \ldots, D_m)$ where all the divergences $D_{f_1}, \ldots, D_{f_m}$ are primitive divergences (see Remark 3.1). In Theorem 5.1 below, we show that, in this case, $B(D_1, \ldots, D_m)$ actually equals $B_{m+1}(D_1, \ldots, D_m)$ as opposed to $B_{m+2}(D_1, \ldots, D_m)$.

The problem of minimizing an $f$-divergence subject to constraints on primitive divergences and the related problem of obtaining inequalities between $f$-divergences and primitive divergences has received much attention in the literature and has a long history. Let us briefly mention some important works in this area. The most well-known such inequality is Pinsker’s inequality which states that $D_{KL}(P||Q) \geq 2V^2(P, Q)$ where $D_{KL}$ is the Kullback-Leibler divergence which corresponds to $f(x) = x \log x$ and $V$ is the total variation distance. Pinsker [26] proved this inequality with the constant 2 replaced by 1. The inequality with the constant 2 (which cannot be improved further) has been proved independently almost at the same time by Csiszar [5], Kemperman [16] and Kullback [17].

Although Pinsker’s inequality is very useful, it is not sharp in the sense that

$$\inf \{D_{KL}(P||Q) : V(P, Q) \geq V \} > 2V^2$$

for every $V \neq 0$. The problem of finding sharp inequalities between $D_{KL}(P||Q)$ and $V(P, Q)$ was solved in [9] where an implicit expression for the infimum in the left hand side above was provided.

The more general problem of finding the best lower bound for an arbitrary $f$-divergence given a lower bound on total variation distance was solved by Gilardoni in [11]. The problem of finding lower bounds for $f$-divergences given constraints on a finite number of primitive divergences was studied by [28]. In Remark 5.1, we explain how our theorem below gives an equivalent but simpler solution compared to the solution of [28].

**Theorem 5.1.** Suppose that $D_f$ is an arbitrary divergence and that all divergences $D_{f_1}, \ldots, D_{f_m}$ are primitive divergences. Then

$$B(D_1, \ldots, D_m) = B_{m+1}(D_1, \ldots, D_m).$$

**Proof.** Theorem 2.1 states that $B(D_1, \ldots, D_m)$ equals $B_{m+2}(D_1, \ldots, D_m)$. We shall show therefore that $B_{m+2}(D_1, \ldots, D_m)$ equals $B_{m+1}(D_1, \ldots, D_m)$.

It is obvious that

$$B_{m+2}(D_1, \ldots, D_m) \leq B_{m+1}(D_1, \ldots, D_m)$$

because we have a minimization problem and the constraint set is larger in the case of $B_{m+2}(D_1, \ldots, D_m)$.
It is therefore enough to prove that

\[ B_{m+2}(D_1, \ldots, D_m) \geq B_{m+1}(D_1, \ldots, D_m). \]

Fix two probability measures \( P = (p_1, \ldots, p_{m+2}) \) and \( Q = (q_1, \ldots, q_{m+2}) \) in \( \mathcal{P}_{m+2} \) with \( D_{f_i}(P||Q) \geq D_i \)
for every \( i = 1, \ldots, m \). We show below that

\[ D_{f_i}(P||Q) \geq B_{m+1}(D_1, \ldots, D_m) \]

which will complete the proof.

Without loss of generality, we assume that \( p_i + q_i > 0 \) for each \( i \) and that the likelihood ratios \( r_i := p_i / q_i \in [0, \infty] \) satisfy \( r_1 \leq \cdots \leq r_{m+2} \). Because each divergence \( D_{f_i} \) is assumed to be primitive, the convex function \( f_i \) is piecewise linear with exactly two linear parts. As a result, there exists some index \( j \in \{1, \ldots, m+1\} \) such that all the functions \( f_1, \ldots, f_m \) are linear in the interval \([r_j, r_{j+1}]\).

Now consider the two probability measures \( P^* \) and \( Q^* \) in \( \mathcal{P}_{m+1} \) defined by

\[ P^* := (p_1, \ldots, p_{j-1}, p_j + p_{j+1}, p_{j+2}, \ldots, p_{m+2}) \]

and

\[ Q^* := (q_1, \ldots, q_{j-1}, q_j + q_{j+1}, q_{j+2}, \ldots, q_{m+2}) \]

Because of the linearity of \( f_1, \ldots, f_m \) on \([r_j, r_{j+1}]\), it is easy to check that

\[ D_{f_i}(P^*||Q^*) = D_{f_i}(P||Q) \geq D_i \quad \text{for all} \quad 1 \leq i \leq m. \]

As a result, we have

\[ D_{f_i}(P^*||Q^*) \geq B_{m+1}(D_1, \ldots, D_m). \]

On the other hand, by convexity or as a consequence of the data processing inequality for \( f \)-divergences (see, for example, [8, Lemma 4.1]), it follows that

\[ D_{f_i}(P||Q) \geq D_{f_i}(P^*||Q^*) \geq B_{m+1}(D_1, \ldots, D_m). \]

The proof is complete. \( \square \)

**Remark 5.1.** Let \( 0 < s_1 < \cdots < s_m < \infty \) and let \( D_{f_i} \) be the primitive divergence corresponding to \( f_i = u_{s_i} \) (the functions \( u_{s_i} \) are defined in Remark 3.1). Then the optimization problem corresponding to

\[ B_{m+1}(D_1, \ldots, D_m) \]

can be written as:

\[
\begin{align*}
\text{minimize} & \quad \sum_{p,q \in [0,1]^{m+1}} q_j f \left( \frac{p_j}{q_j} \right) + f'(\infty) \sum_{j : q_j = 0} p_j \\
\text{subject to} & \quad p_j \geq 0, \quad q_j \geq 0 \quad \text{for all} \quad j = 1, \ldots, m+1 \\
& \quad \sum_j p_j = \sum_j q_j = 1 \\
& \quad \sum_j \min(p_j, q_j, s_i) \leq \min(1, s_i) - D_i 
\end{align*}
\]
for $i = 1, \ldots, m$. According to Theorem 5.1, the optimal value of this problem equals $B(D_1, \ldots, D_m)$. As we mentioned before, the problem of determining $B(D_1, \ldots, D_m)$ when the divergences $D_f$, are all primitive divergences has been studied by [28]. Their main result [28, Theorem 6] gives a characterization of $B(D_1, \ldots, D_m)$ that is much more complicated than (42). However, the two forms are essentially equivalent. To understand the equivalence, observe that, by Lemma 3.1, $D_f(P||Q)$ can be written as an integral functional of $\psi_{P,Q}$. It is possible to precisely characterize the form of the function $\psi_{P,Q}$ when $P, Q \in \mathcal{P}_{m+1}$. As a result, the optimization problem (42) can be reformulated in terms of such concave functions $\psi$. This, after some tedious algebra, leads to the formula for $B(D_1, \ldots, D_m)$ given in [28, Theorem 6]. Our formula (42) is much simpler and, moreover, is conceptually easier to understand.

The special case of $m = 1$ in Theorem 5.1 asserts that in order to determine $B(D)$ when $D_f$ is a primitive divergence, one only needs to consider probabilities on $\{1, 2\}$. This fact is well-known at least in the case when $D_f$ is the total variation distance (see, for example, [11, Proposition 2.1]). It is then possible to give a more direct expression for $B(D)$ which is the content of the following lemma, whose special case for $s = 1$ appears in [11, Proposition 2.1].

**Lemma 5.2.** Let $m = 1$ and consider the quantity $B(D)$ where $D_f$ is an arbitrary $f$-divergence and $D_f$, is the primitive divergence corresponding to $f_1 = u_s$ for a fixed $s > 0$. Then, for every $0 \leq D \leq \min(1, s)$, the quantity $B(D)$ equals

$$
\inf_{0 \leq q \leq H/s} \left[ (1 - q)f \left( \frac{H - qs}{1 - q} \right) + qf \left( \frac{1 + qs - H}{q} \right) \right] \tag{43}
$$

where $H := \min(1, s) - D$.

**Proof.** We shall now show that $B_2(D)$ equals (43). Note that $B_2(0) = 0$ and (43) also equals 0 when $D = 0$. To see this, note that it is trivially zero (because $f(1) = 0$) when $s = 1$ and when $s \neq 1$, then it is zero because the value at $q = (1 - \min(1, s))/(1 - s)$ equals 0. So we shall assume below that $D > 0$. The optimization problem corresponding to $B_2(D)$ is:

$$
\begin{align*}
\text{minimize} & \quad \sum_{j: q_j > 0} p_j f \left( \frac{p_j}{q_j} \right) + f'(\infty) \sum_{j: q_j = 0} p_j \\
\text{subject to} & \quad p_j \geq 0, q_j \geq 0 \text{ for } j = 1, 2 \\
& \quad p_1 + p_2 = q_1 + q_2 = 1 \\
& \quad \min(p_1, q_1s) + \min(p_2, q_2s) = H. \tag{44}
\end{align*}
$$

Note that we have equality as opposed to $\leq$ in the last constraint above. This is because of the fact that for every $(p_1, p_2)$ and $(q_1, q_2)$ lying in the constraint set for which the last constraint is not tight, we can get $(\bar{p}_1, \bar{p}_2)$ and $(\bar{q}_1, \bar{q}_2)$ still lying in the constraint set with the last constraint satisfied with an equality sign and for which the objective function is reduced.

We will now finish the proof by showing that the optimal value of the optimization problem (44) is (43). Let $(p_1, p_2)$ and $(q_1, q_2)$ satisfy the constraint set with $p_1/q_1 \leq 1 \leq p_2/q_2$. If $s \notin [p_1/q_1, p_2/q_2]$, we
then clearly \( \min(p_1, q_1 s) + \min(p_2, q_2 s) = \min(1, s) \) and such \( (p_1, p_2) \) and \( (q_1, q_2) \) do not satisfy the
constraint set because \( D > 0 \). So we assume that \( s \in [p_1/q_1, p_2/q_2] \). In this case, the final constraint
gives \( p_1 = H - q_2 s \). We can therefore write each of \( p_1, p_2 \) and \( q_1 \) in terms of \( q_2 \). Plugging these values in
the objective function leads to the function in (43) (with \( q \) replaced by \( q_2 \)). The fact that each of \( p_1, p_2, q_1 \)
and \( q_2 \) need to lie between 0 and 1 gives the constraint \( 0 \leq q_2 \leq H/s \). The proof is complete.

For completeness, let us note the special case of the above lemma in the case of the total variation
distance, which corresponds to \( s = 1 \). This result is due to Gilardoni [11, Proposition 2.1].

**Corollary 5.3** (Gilardoni). Let \( m = 1 \) and consider the quantity \( B(V) \) where \( D_f \) is an arbitrary \( f \)-
divergence and \( D_{f_1}(P||Q) \) equals \( V(P, Q) \), the total variation distance between \( P \) and \( Q \). Then, for every
\( 0 \leq V \leq 1 \),
\[
B(V) := \inf \{ T(q, V) : 0 \leq q \leq 1 - V \}
\]
where
\[
T(q, V) := (1 - q)f\left(\frac{1 - V - q}{1 - q}\right) + qf\left(\frac{q + V}{q}\right).
\]
Consequently, for every pair of probability measures \( P \) and \( Q \), we have the inequality
\[
D_f(P||Q) \geq \inf \{ T(q, V(P, Q)) : 0 \leq q \leq 1 - V(P, Q) \}.
\]
Moreover, this represents the sharpest possible inequality between \( D_f \) and total variation distance.

Although the expression (45) cannot be simplified further in general, one can get much simpler
expressions for \( B(V) \) in certain special cases. One such special case of interest corresponds to symmetric
\( f \)-divergences. An \( f \)-divergence is said to be symmetric if the underlying convex function \( f \) satisfies the identity:
\( f(x) = xf(1/x) \) for all \( x \in (0, \infty) \). It is easy to check that under this condition, one has
\( D_f(P||Q) = D_f(Q||P) \) for all \( P \) and \( Q \). Examples of symmetric divergences include the total variation
distance, squared Hellinger distance, triangular discrimination and the Jensen-Shannon divergence. The
following result is due to Gilardoni [11]. We include it here for completeness and also because our proof
is more direct than that in [11].

**Corollary 5.4** (Gilardoni). Let \( m = 1 \) and consider the quantity \( B(V) \) where \( D_f \) is a symmetric \( f \)-
divergence and \( D_{f_1}(P||Q) \) equals \( V(P, Q) \), the total variation distance between \( P \) and \( Q \). Then, for every
\( 0 \leq V \leq 1 \),
\[
B(V) = (1 - V)f\left(\frac{1 + V}{1 - V}\right).
\]
Consequently, for every pair of probability measures \( P \) and \( Q \), we have
\[
D_f(P||Q) \geq (1 - V(P, Q))f\left(\frac{1 + V(P, Q)}{1 - V(P, Q)}\right).
\]
Moreover, this represents the sharpest possible inequality between the symmetric divergence \( D_f \) and total
variation distance.
Proof. We shall show that the right hand side of (45) equals the right hand side of (47) when $D_f$ is a symmetric divergence. Consider the quantity $T(q,V)$ defined in Corollary 5.3. Because $f(x) = xf(1/x)$, it can be easily checked that

$$T(q,V) = T(1 - q - V, V) \quad \text{for all } q \in [0, 1 - V].$$

In other words, the function $q \mapsto T(q,V)$ is symmetric in the interval $[0, 1 - V]$ about the mid-point $(1 - V)/2$. Moreover, as can be checked by taking derivatives (one-sided derivatives if $f$ is not differentiable), $q \mapsto T(q,V)$ is convex on $[0, 1 - V]$ (this fact does not require $f$ to be symmetric). These two facts clearly imply that

$$\inf_{0 \leq q \leq 1 - V} T(q,V) = T\left(\frac{1 - V}{2}, V\right) = (1 - V)f\left(\frac{1 + V}{1 - V}\right)$$

which completes the proof.

5.2 Chi-squared divergence

In this section, we describe another situation where the conclusion of Theorem 2.1 can be further simplified.

Theorem 5.5. Let $m = 1$ and consider the quantity $A(D)$ where $D_f$ is the chi-squared divergence, $\chi^2(P||Q)$ which corresponds to $f(x) := x^2 - 1$. Also let the function $f_1$ be such that the function $h : (0, \infty) \to (0, \infty)$ defined by $h(x) := (1 + f_1(x))/x$ is a strictly increasing, strictly convex, twice differentiable bijective mapping. Then $A(D) = h^{-1}(D + 1) - 1$, where $h^{-1}$ denotes the inverse function of $h$ on $(0, \infty)$.

Proof. By Theorem 2.1, $A(D)$ equals the optimal value of the problem:

$$\begin{align*}
\max_{p,q \in [0,1]^3} & \quad \sum_{j:q_j>0} \frac{p_j^2}{q_j} - 1 + \infty \cdot \sum_{j:q_j=0} p_j \\
\text{subject to} & \quad p_j \geq 0, q_j \geq 0 \text{ for all } j = 1, 2, 3 \\
& \quad \sum p_j = \sum q_j = 1 \\
& \quad \sum_{j:q_j>0} q_j f_1\left(\frac{p_j}{q_j}\right) + f_1'(\infty) \sum_{j:q_j=0} p_j \leq D
\end{align*}$$

By convexity of $h$, we have

$$h(x) \geq h(a) + h'(a)(x - a) \quad \text{(49)}$$

for every $x > 0$ and $a > 0$. One consequence of this and the fact that $h$ is strictly increasing is that

$$h(1) + h'(1)(x - 1) \leq h(x) \leq h(1)$$

for all $x \in (0,1)$. This implies that $\lim_{x \downarrow 0} xh(x) = 0$ and as a result

$$f_1(0) = \lim_{x \downarrow 0} f_1(x) = \lim_{x \downarrow 0} (xh(x) - 1) = -1$$
Further, because \( h \) is strictly increasing, we have \( h'(a) > 0 \) and thus

\[
f'_1(\infty) = \lim_{x \to \infty} h(x) = \infty
\]

which implies that we only need to consider \( P \) and \( Q \) for which \( \sum_j q_j = 0 \). Writing (49) in terms of \( f_1(x) \), we obtain

\[
1 + f_1(x) \geq x (h(a) - ah'(a)) + x^2 h'(a).
\]

for every \( x > 0 \) and also at \( x = 0 \) (because \( f_1(0) := \lim_{x \to 0} f_1(x) \)). Applying this inequality to \( x = p_j/q_j \) for \( q_j > 0 \) and then multiplying by \( q_j \), we obtain

\[
q_j + q_j f_1(p_j/q_j) \geq p_j (h(a) - ah'(a)) + \frac{p_j^2}{q_j} h'(a)
\]

for each \( j = 1, 2, 3 \). As a result, we get

\[
h'(a) \sum_{j : q_j > 0} \frac{p_j^2}{q_j} \leq \sum_{j : q_j > 0} q_j f_1 \left( \frac{p_j}{q_j} \right) + 1 - h(a) + ah'(a)
\]

Because \( P \) and \( Q \) satisfy the constraint, we have

\[
\sum_{j : q_j > 0} q_j f_1 \left( \frac{p_j}{q_j} \right) \leq D
\]

and hence

\[
\sum_{j : q_j > 0} \frac{p_j^2}{q_j} - 1 \leq \left[ \frac{D + 1 - h(a) + ah'(a)}{h'(a)} \right] - 1.
\]

Because \( a > 0 \) is arbitrary, we get

\[
A(D) \leq \inf_{a > 0} \left[ \frac{D + 1 - h(a) + ah'(a)}{h'(a)} \right] - 1.
\]

By elementary algebra, the above infimum is achieved at \( a^* = h^{-1}(D + 1) \) and we then obtain \( A(D) \leq h^{-1}(D + 1) - 1 \). To see that \( A(D) \) is exactly equal to \( h^{-1}(D + 1) - 1 \), observe that the probabilities \( P = (1, 0, 0) \) and \( Q = (1/a^*, 1 - 1/a^*, 0) \) satisfy \( D_{f_1}(P||Q) = D \) and \( \chi^2(P||Q) = h^{-1}(D + 1) - 1 \).

The function \( f_1(x) = x^l - 1 \) for \( l > 2 \) clearly satisfies the conditions of the above theorem. We therefore obtain the following result as a simple corollary.

**Corollary 5.6.** Let \( m = 1 \) and consider the quantity \( A(D) \) where \( D_{f_1}(P||Q) = \chi^2(P||Q) \) and \( D_{f_1} \) is the power divergence, \( D^{(l)}(P||Q) \), corresponding to \( f_1(x) = x^l - 1 \) for \( l > 2 \). Then \( A(D) = (1 + D)^{1/(l-1)} - 1 \). This yields the sharp inequality

\[
\chi^2(P||Q) + 1 \leq \left( 1 + D^{(l)}(P||Q) \right)^{1/(l-1)}
\]

between the chi-squared divergence and power divergence for \( l > 2 \).
6 Numerical Computation

In this section we explore numerical methods for solving the optimization problems (7) and (8) in order to compute \( A(D_1, \ldots, D_m) \) and \( B(D_1, \ldots, D_m) \) respectively. In Section 6.1, we consider the special case when \( D_f \) is a primitive divergence. This special case is motivated by the statistical problem of obtaining lower bounds for the minimax risk and we show that the quantity \( A(D_1, \ldots, D_m) \) can be computed exactly via convex optimization for every \( m \geq 1 \) and every arbitrary choice of \( D_{f_1}, \ldots, D_{f_m} \). In Section 6.2, we consider the special case \( m = 1 \) and demonstrate that (7) and (8) can be solved for practically any pair of \( f \)-divergences by a gridded search over the low-dimensional parameter space. We verify several known inequalities and also improve on some existing inequalities that are not sharp.

6.1 Maximizing Primitive Divergences

In this subsection we consider maximizing a primitive divergence subject to upper bounds on arbitrary \( f \)-divergences. While this optimization problem is not a-priori convex, we reduce it to a collection of convex problems.

The optimization problem (7) where \( D_f \) is a primitive divergence is, of course, closely related to the problem of bounding from above a primitive divergence subject to upper bounds on other \( f \)-divergences. This latter problem arises in obtaining lower bounds for the minimax risk in nonparametric statistical estimation (see, for example, [12, 13, 32, 34]). For example, Le Cam’s inequality, which is a popular technique for obtaining minimax lower bounds, says that the minimax risk is bounded from below by a multiple of the \( L_1 \) affinity between two probability measures \( P \) and \( Q \), where the \( L_1 \) affinity is defined as \( 1 - V(P, Q) \). The \( L_1 \) affinity also appears in Assouad’s Lemma, another technique for obtaining minimax lower bounds. Evaluating \( V(P, Q) \) is hard because \( P \) and \( Q \) are typically product distributions of the form \( P = \otimes_{i=1}^n P_i \) (or mixtures of such distributions), so it is difficult to express \( V(P, Q) \) in terms of \( V(P_i, Q_i) \) (which can be easier to compute).

Application of Le Cam’s inequality in practice, therefore, requires one to obtain a good upper bound on the total variation, \( V(P, Q) \). One typically first bounds \( D_f(P||Q) \) for an \( f \)-divergence that decouples for product distributions such as squared Hellinger, chi-squared, or Kullback-Leibler divergence and then translates this into a bound on \( V(P, Q) \). It is common to use crude bounds like Pinsker’s inequality for this purpose and we believe there is room for improvement by using tight bounds. Also, one typically uses only one \( f \)-divergence to bound \( V(P, Q) \); but we shall argue here that one gets better bounds (Figure 3) when using multiple divergences simultaneously. This is one of our motivations for studying the case \( m \geq 2 \) as opposed to just \( m = 1 \). The constants underlying minimax lower bounds might be improved by the use of these better bounds addressing a common criticism of minimax lower bound techniques.

Theorem 6.1 below solves the problem of maximizing a primitive divergence \( D_{u*} \) given constraints on
$m$ other divergences $D_f$, exactly via convex optimization. This leads to a fast algorithm with well-studied convergence properties.

For each $m \geq 1$, let

$$S_m = \{ \sigma \in \{-1, 1\}^{m+2} : \sigma_i \leq \sigma_j \text{ for } i \leq j \}$$

For each $\sigma \in S_m$, let us consider the following convex optimization problem and denote its optimal value by $V_{\sigma}(D_1, \ldots, D_m)$.

$$\begin{align*}
\max_{p,q \in [0,1]^{m+2}} & \quad \sum_{j=1}^{m+2} \sigma_j (p_j - sq_j) \\
\text{subject to} & \quad p_j \geq 0, q_j \geq 0 \text{ for all } j = 1, \ldots, m+2 \\
 & \quad \sum_j p_j = \sum_j q_j = 1 \\
 & \quad \sum_{j:q_j>0} q_j f_i \left( \frac{p_j}{q_j} \right) + f'_i(\infty) \sum_{j:q_j=0} p_j \leq D_i
\end{align*}$$

(50)

for $i = 1, \ldots, m$. Note that this problem is convex because the objective function is linear and the constraint set is convex in $p_1, \ldots, p_{m+2}, q_1, \ldots, q_{m+2}$. The fact that the constraint set is convex is a consequence of the convexity of $D_f(P||Q)$ in $(P, Q)$ (see, for example, [8, Lemma 4.1]). It is also clear that this is a $2m + 2$-dimensional optimization problem because there are $2m + 4$ variables in all which satisfy two linear equality constraints.

**Theorem 6.1.** Let $D_f$ denote the primitive $f$-divergence corresponding to $f = u_s$ for some $s > 0$. Then

$$A(D_1, \ldots, D_m) = -\frac{|s-1|}{2} + \max_{\sigma \in S_m} V_{\sigma}(D_1, \ldots, D_m)$$

(51)

Consequently, $A(D_1, \ldots, D_m)$ can be computed by solving the $|S_m| = m + 3$ convex optimization problems (50).

**Proof.** Theorem 2.1 asserts that $A(D_1, \ldots, D_m)$ equals the optimal value of the optimization problem (7). Note that the constraint sets of the problems (7) and (50) are the same. Let us denote this constraint set by $C_m$ so that

$$A(D_1, \ldots, D_m) = \max_{P,Q \in C_m} D_{u_s}(P||Q).$$

The objective of (7) can be written as

$$D_{u_s}(P||Q) = \min(1, s) - \sum_{j=1}^{m+2} \min(p_j, sq_j)$$

$$= \min(1, s) - \frac{1}{2} \sum_{j=1}^{m+2} p_j + sq_j - |p_j - sq_j|$$

$$= -\frac{|s-1|}{2} + \max_{\sigma \in \{-1, 1\}^{m+2}} \sum_{j=1}^{m+2} \sigma_j (p_j - sq_j).$$

Because two maxima can always be interchanged, we have

$$\max_{P,Q \in C_m} \left[ \max_{\sigma \in \{-1, 1\}^{m+2}} \sum_{j=1}^{m+2} \sigma_j (p_j - sq_j) \right] = \max_{\sigma \in \{-1, 1\}^{m+2}} \left[ \max_{P,Q \in C_m} \sum_{j=1}^{m+2} \sigma_j (p_j - sq_j) \right].$$
Note that the inner maximization in the right hand side above is precisely the convex problem (50).

Because the optimal value of (50) is invariant to permuting the indices of $\sigma$, we have the reduction

$$\max_{\sigma \in \{-1,1\}^{m+2}} \max_{P,Q \in \mathbb{C}_m} \sigma^T (P - sQ) = \max_{\sigma \in S_m} \max_{P,Q \in \mathbb{C}_m} \sigma^T (P - sQ).$$

This shows that we can restrict attention only to those problems (50) for $\sigma \in S_m$. It is obvious that $|S_m| = m + 3$. The proof is complete.

**Example 6.2.** Consider the special case of Theorem 6.1 when $m = 1$, $s = 1$ and when $D_{f_1}$ is the squared Hellinger distance which corresponds to $f_1(x) = (\sqrt{x} - 1)^2/2$. In other words, we consider the problem of maximizing the total variation distance subject to an upper bound on the Hellinger distance. The solution to this problem given by Theorem 6.1 is plotted in Figure 1(a). Each red dot shows $A(H) =: A_{TV}^1(H)$ computed by solving the four 4-dimensional convex optimization problems (50) (each corresponding to a $\sigma \in S_1$).

Note that the quantity $A_{TV}^1(H)$ can be obtained analytically in a closed form. Indeed, since $f_1$ is a symmetric divergence, the sharp inequality bounding the total variation distance by the squared Hellinger distance is given by (48) with $f(x) = (\sqrt{x} - 1)^2$ (this inequality is usually attributed to [18]) which implies that

$$A_{TV}^1(H) = \sqrt{2H} \sqrt{1 - \frac{H}{2}}.$$

We have plotted this function analytically by the solid cyan line in Figure 1(a). It is clear that our numerical optimization method given by Theorem 6.1 agrees with the known analytical bound.

**Example 6.3.** For another simple application of Theorem 6.1, consider maximizing the total variation subject to an upper bound on the Kullback-Leibler divergence. In other words, we take $m = 1$, $s = 1$ and $f_1(x) = x \log x$ and plot the solution given by Theorem 6.1 in Figure 1(b). Each black dot shows $A(K) =: A_{TV}^{KL}(K)$ for a different value of $K$, computed by solving the four 4-dimensional convex optimization problems (50). The solid green line shows Pinsker’s analytic upper bound $\sqrt{2K}$ which is not sharp for any $K > 0$.

**Example 6.4.** We now consider maximizing the total variation subject to constraints on both the Hellinger distance and Kullback-Leibler divergence. In other words, we take $m = 2$, $s = 1$, $f_1(x) = (\sqrt{x} - 1)^2/2$ and $f_2(x) = x \log x$. To the best of our knowledge, there does not exist a closed form analytical solution to this problem. However, numerical solution is straightforward by Theorem 6.1 as shown below.

According to Theorem 6.1, for fixed $H, K \geq 0$ we can compute $A(H, K) =: A_{TV}^{HKL}(H, K)$ by solving five 6-dimensional convex programs (50). Figure 2 shows the function $A_{TV}^{HKL}(H, K)$ interpolated from 14884 $(H, K)$ pairs. We used CVX in MATLAB to solve the convex programs. The height of each point in the surface shows how large the total variation can be when the squared Hellinger distance and Kullback-Leibler divergence are bounded by $H$ and $K$ respectively. As expected, the total variation is zero.
Figure 1: Two simple applications of Theorem 6.1 discussed in examples 6.2 and 6.3. Here and in all subsequent plots we set the axis limits to the maximum value of the relevant $f$-divergence and to 5 in the case of the Kullback-Leibler divergence (which has no maximum value).
when either $H = 0$ or $K = 0$, and it approaches 1 for large values of $H$ and $K$. Next, observe that the surface $A_{HKL}^{TV}(H,K)$ is flat as $K$ varies for small $H$, and vice-versa flat as $H$ varies for small $K$. This is because only one constraint is tight in these regions. In other words, the surface $A_{HKL}^{TV}(H,K)$ is approximately the point-wise minimum of the two surfaces $A_{H}^{TV}(H)$ and $A_{KL}^{TV}(K)$, with a diagonal ridge at the intersection of these two surfaces. But, as can be seen in Figure 3, our bound that simultaneously leverages both single-coordinate bounds is strictly better than the simple minimum of those two individual bounds for some $(H,K)$. In other words, there exist $(H,K)$ such that

$$\min (A_{H}^{TV}(H), A_{KL}^{TV}(K)) - A_{HKL}^{TV}(H,K) > 0$$

(52)

The left hand side above is positive when both single-coordinate bounds are informative, i.e. when both constraints in the optimization problem (7) are active. We will explain later (see Example 6.5 and Figure 4) that the location of this ridge is predicted by an inequality between $D_H(P||Q)$ and $D_{KL}(P||Q)$.

Figure 2: The height of each point in the surface above shows $A_{HKL}^{TV}(H,K)$ for a different $(H,K)$ pair—the the least upper bound on total variation when squared Hellinger distance and Kullback-Leibler divergence are bounded by $H$ and $K$ respectively (see example 6.4).

### 6.2 The General Case

Theorem 6.1 requires $D_f$ to be a primitive divergence. We do not know if, in general, the optimization problems (7) and (8) can be solved by convex optimization algorithms. However, if $m$ is not too large, heuristic optimization techniques can be used. We demonstrate this in this subsection for $m = 1$.

**Example 6.5.** Consider the optimization problem (7) for $m = 1$, $f(x) = (\sqrt{x} - 1)^2/2$ and $f_1(x) = x \log x$. In other words, we consider the problem of maximizing the squared Hellinger distance subject to an upper
bound on the Kullback-Leibler divergence. The optimization problem (7) is clearly 4-dimensional (there are six variables in all $p_1, p_2, p_3$ and $q_1, q_2, q_3$ but they satisfy two linear constraints as they sum to one). Because the variable space is only 4-dimensional, there was no trouble solving this by gridding the parameter space. We plot the solution in Figure 4(a) where each blue dot shows $A(K) =: A_{H,KL}^H(K)$ for a different value of $K$.

The quantity $A_{H,KL}^H(K)$ can be used to better understand the inequality (52). Indeed, when we overlay the curve $(K, A_{H,KL}^H(K))$ on Figure 3 (see Figure 4(b)), we see that the curve $(K, A_{K,L}^H(K))$ (plotted by the blue line) lies above the region where the inequality (52) holds. Only the constraint on $D_{KL}(P||Q)$ is active in the optimization problem considered in Example 6.4 when $H > A_{H,KL}^H(K)$. For such $(H, K)$, therefore, the inequality (52) does not hold.

Example 6.6. Consider maximizing the squared Hellinger distance between $P$ and $Q$ with the total variation between $P$ and $Q$, $V(P, Q)$, bounded by $V$. In other words, we consider the special case of the problem (7) for $m = 1$, $f(x) = (\sqrt{x} - 1)^2/2$ and $f_1(x) = |x - 1|/2$. This is a special case of the problem we considered in section 4.3 where we proved that $A_2(V) < A_3(V)$ for all $V \in (0, 1)$. Here we confirm this fact numerically.

We compute both the quantities $A_2(V)$ and $A_3(V)$ by a gridded search over pairs of probabilities satisfying the constraint in $P_2$ and $P_3$ respectively. These functions are plotted in Figure 5. Each red
Figure 4: A sharp inequality between squared Hellinger distance and Kullback-Leibler divergence bounds the support of the ridge. The upper panel displays a sharp inequality between squared Hellinger and Kullback-Leibler divergence. The height of each blue dot represents the optimal value $A^H_{KL}(K)$ with a different constraint, $K$, on the Kullback-Leibler divergence. The lower panel shows the same blue curve overlaid on Figure 3. Observe that the region with positive improvement is bounded by the blue curve from the upper panel.
triangle in Figure 5 shows $A_3(V)$ for a different $V$. Each point in the dotted blue line shows $A_2(V)$ for a different $V$. It is evident that the inequality $A_2(V) < A_3(V)$ holds for all $V \in (0, 1)$. In other words, when we restrict the constraint set to probability measures in $\mathcal{P}_2$, the maximum Hellinger distance is strictly smaller for all $V \in (0, 1)$. Therefore, Theorem 2.1 is in general tight and cannot be improved.

Note also that the plot $A_3(V)$ agrees with the form $A_3(V) = A(V) = V(f(0) + f'(\infty)) = V$ derived in Section 4.3. This gives rise to the sharp inequality $H^2(P, Q) \leq V(P, Q)$ which is again attributed to [18].

![Figure 5: Three point measures strictly improve on two point measures. Each red triangle shows $A_3(V)$ computed by a gridded search over pairs of probability measures in $\mathcal{P}_3$. Each blue dot shows $A_2(V)$ computed by a gridded search over pairs of probability measures in $\mathcal{P}_2$. The simulation over three point measures is exactly a straight line with slope one—agreeing with Le Cam’s bound $H^2 \leq V$. And $A_2(V) < A_3(V)$ for all $V \in (0, 1)$.](image_url)

**Example 6.7.** The capacitory discrimination between two probability measures $P$ and $Q$ is defined by

$$C(P, Q) = D_{KL}(P\|\frac{P + Q}{2}) + D_{KL}(Q\|\frac{P + Q}{2}).$$

It is easy to check that $C(P, Q)$ is an $f$-divergence that corresponds to the convex function:

$$x \log x - (x + 1) \log(x + 1) + 2 \log 2.$$  \hspace{1cm} (53)

The triangular discrimination $\Delta(P, Q)$ is another $f$-divergence that corresponds to the convex function

$$\frac{(x - 1)^2}{x + 1}.$$ \hspace{1cm} (54)
Topsøe proved the following inequality between these two \( f \)-divergences [31]:

\[
\frac{1}{2} \Delta(P, Q) \leq C(P, Q) \leq (\log 2) \Delta(P, Q).
\]  

(55)

Let us investigate here the sharpness of these inequalities. Let

\[ A(D_1) := \sup \{C(P, Q) : \Delta(P, Q) \leq D_1\} \]

and

\[ B(D_1) := \inf \{C(P, Q) : \Delta(P, Q) \geq D_1\} . \]

We solved the optimization problems (7) and (8) for \( m = 1 \), \( f(x) \) given by (53) and \( f_1(x) \) given by (54) by a gridded search. The resulting solutions for \( A(D_1) \) and \( B(D_1) \) are plotted in Figure 6, with red triangles corresponding to \( A(D_1) \) and blue dots corresponding to \( B(D_1) \). We have also plotted the bounds given by (55) in Figure 6 with the green line corresponding to \( \log 2 D_1 \) and the blue line to \( D_1/2 \). It is clear from the figure that the upper bound in (55) is sharp while the lower bound is not sharp. The sharp lower bound is given by \( B(D_1) \). We are unaware of an analytic formula for \( B(D_1) \), but we conjecture that \( B_2(D_1) = B_3(D_1) \) because this equality holds numerically. It may be possible to use this fact to find an analytic formula for \( B(D_1) \).

![Figure 6: The green line with slope \( \log 2 \) and the blue line with slope \( \frac{1}{2} \) trace the bounds in (55), while the red triangles and the black dots display \( A(D_1) \) and \( B(D_1) \) respectively.](image)
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