

# A New Upper Bound for Cancellative Pairs

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## Abstract

A pair  $(\mathcal{A}, \mathcal{B})$  of families of subsets of an  $n$ -element set is called cancellative if whenever  $A, A' \in \mathcal{A}$  and  $B \in \mathcal{B}$  satisfy  $A \cup B = A' \cup B$ , then  $A = A'$ , and whenever  $A \in \mathcal{A}$  and  $B, B' \in \mathcal{B}$  satisfy  $A \cup B = A \cup B'$ , then  $B = B'$ . It is known that there exist cancellative pairs with  $|\mathcal{A}||\mathcal{B}|$  about  $2.25^n$ , whereas the best known upper bound on this quantity is  $2.3264^n$ . In this paper we improve this upper bound to  $2.2682^n$ . Our result also improves the best known upper bound for Simonyi's sandglass conjecture for set systems.

**Mathematics Subject Classifications:** 05D05

## 1 Introduction

The notion of a cancellative pair was introduced by Holzman and Körner [4]. We say that a pair  $(\mathcal{A}, \mathcal{B})$  of families of subsets of an  $n$ -element set  $S$  is *cancellative* if

$$\begin{aligned} &\text{whenever } A, A' \in \mathcal{A} \text{ and } B \in \mathcal{B} \text{ satisfy } A \cup B = A' \cup B \text{ then } A = A' \\ &\text{and whenever } A \in \mathcal{A} \text{ and } B, B' \in \mathcal{B} \text{ satisfy } A \cup B = A \cup B' \text{ then } B = B'; \end{aligned} \tag{1}$$

or, equivalently,

$$\begin{aligned} &\text{whenever } A, A' \in \mathcal{A} \text{ and } B \in \mathcal{B} \text{ satisfy } A \setminus B = A' \setminus B \text{ then } A = A' \\ &\text{and whenever } A \in \mathcal{A} \text{ and } B, B' \in \mathcal{B} \text{ satisfy } B \setminus A = B' \setminus A \text{ then } B = B'. \end{aligned} \tag{2}$$

We will usually take  $S = [n] = \{1, \dots, n\}$  and will call a cancellative pair with  $\mathcal{A} = \mathcal{B}$  a *symmetric cancellative pair*. Note that the assumption that  $(\mathcal{A}, \mathcal{A})$  is a symmetric cancellative pair is slightly stronger than the assumption that  $\mathcal{A}$  is a *cancellative family*, meaning no three distinct sets  $A, B, C \in \mathcal{A}$  satisfy  $A \cup B = A \cup C$  [3]. We mention that the concept of cancellative pairs corresponds to the information theoretic concept of

uniquely decodable code pairs for the binary multiplying channel without feedback (see e.g. Tolhuizen [8]).

In the case when  $n$  is a multiple of 3, we can obtain an example of a symmetric cancellative pair the following way. Partition  $S$  into  $n/3$  classes of size 3, and take  $\mathcal{A}$  (and  $\mathcal{B}$ ) to be the collection of subsets of  $S$  containing exactly one element from each class. It is not hard to verify that we get a cancellative pair. Here we have  $|\mathcal{A}||\mathcal{B}| = 3^{2n/3}$ , where  $3^{2/3} \approx 2.08$ . In the symmetric case, Erdős and Katona [5] conjectured this to be the maximal size for cancellative families. A counterexample was found by Shearer [6]. Tolhuizen [8] gave a beautiful construction to show that we can achieve  $(|\mathcal{A}||\mathcal{B}|)^{1/n} \rightarrow 9/4 = 2.25$ , even by symmetric pairs. This construction is (asymptotically) optimal in the symmetric case by a result of Frankl and Füredi [3].

In the general (non-symmetric) case, the exact value of  $\alpha = \sup(|\mathcal{A}||\mathcal{B}|)^{1/n}$  is not known. The best known upper bound is due to Holzman and Körner [4], who showed that  $|\mathcal{A}||\mathcal{B}| < \theta^n$  where  $\theta \approx 2.3264$ . No lower bound better than Tolhuizen's (symmetric) 2.25 is known. Our main aim in this paper is to improve the upper bound to  $2.2682^n$ . Our proof requires some numerical calculations by a computer.

A related concept is that of a recovering pair. A pair  $(\mathcal{A}, \mathcal{B})$  of collections of subsets of an  $n$ -element set  $S$  is called *recovering* [1, 4] if for all  $A, A' \in \mathcal{A}$  and  $B, B' \in \mathcal{B}$  we have

$$A \setminus B = A' \setminus B' \implies A = A' \quad \text{and} \quad B \setminus A = B' \setminus A' \implies B = B'. \quad (3)$$

So any recovering pair is cancellative (cf. (2)). Simonyi's sandglass conjecture for set systems [1] states that  $|\mathcal{A}||\mathcal{B}| \leq 2^n$  for a recovering pair. (The value of  $2^n$  may be obtained by taking  $\mathcal{A} = \mathcal{P}(S_1)$ ,  $\mathcal{B} = \mathcal{P}(S \setminus S_1)$  for any  $S_1 \subseteq S$ . There is a more general sandglass conjecture for lattices, due to Ahlswede and Simonyi [1].) Our upper bound of  $2.2682^n$  is an improvement on the previously best known bounds of about  $2.28^n$  (Etkin and Ordentlich [2], using the terminology of information theory, and Soltész [7]).

## 2 Proof of the upper bound

Let  $h(x) = -x \log_2 x - (1-x) \log_2 (1-x)$  be the binary entropy function (with the convention  $0 \log_2 0 = 0$ ). Define  $\mathcal{A}_i = \{A \in \mathcal{A} \mid i \notin A\}$  and  $p_i = |\mathcal{A}_i|/|\mathcal{A}|$ ;  $q_i$  is defined similarly for  $\mathcal{B}$ . We quote the following result of Holzman and Körner [4]. (We will ignore the case when  $\mathcal{A}$  or  $\mathcal{B}$  is empty.)

**Proposition 1** (Holzman and Körner [4]). *For a cancellative pair  $(\mathcal{A}, \mathcal{B})$ , we have*

$$\log_2 [|\mathcal{A}||\mathcal{B}|] \leq \sum_{i=1}^n f(p_i, q_i) \quad (4)$$

where  $f(p, q) = ph(q) + qh(p)$ .

The result above can be established by considering the entropies of each of the random variables of the form  $\xi^B = A \setminus B$ , where  $B \in \mathcal{B}$  is fixed and  $A \in \mathcal{A}$  is chosen uniformly at random (and doing the same with  $\mathcal{A}, \mathcal{B}$  interchanged). Holzman and Körner [4] used (4) and induction to establish their upper bound of  $|\mathcal{A}||\mathcal{B}| < \theta^n$  ( $\theta \approx 2.3264$ ).

However, this argument can be improved. We call a cancellative pair *k-uniform* if  $|A| = |B| = k$  for all  $A \in \mathcal{A}, B \in \mathcal{B}$ . As we will see, bounding  $|\mathcal{A}||\mathcal{B}|$  for *k-uniform* families enables us to give bounds for general (non-uniform) pairs. For  $n/k$  small it is easy to give efficient bounds, and for  $n/k$  large we will use that the growth speed of the maximum of  $|\mathcal{A}||\mathcal{B}|$  (with  $k$  fixed,  $n$  increasing) can be bounded.

If  $(\mathcal{A}, \mathcal{B})$  and  $(\mathcal{A}', \mathcal{B}')$  are cancellative pairs over disjoint ground sets  $S$  and  $S'$ , define their product  $(\mathcal{A}'', \mathcal{B}'')$  by

$$\mathcal{A}'' = \{A \cup A' \mid A \in \mathcal{A}, A' \in \mathcal{A}'\}$$

$$\mathcal{B}'' = \{B \cup B' \mid B \in \mathcal{B}, B' \in \mathcal{B}'\}$$

giving a cancellative pair over  $S \cup S'$  with  $|\mathcal{A}''||\mathcal{B}''| = |\mathcal{A}||\mathcal{B}||\mathcal{A}'||\mathcal{B}'|$ .

(Note that the cancellative pair in the Introduction is just the product of cancellative pairs of the form  $n = 3$ ,  $\mathcal{A} = \mathcal{B} = \{\{1\}, \{2\}, \{3\}\}$ .) Let  $c(n)$  be the maximum of  $|\mathcal{A}||\mathcal{B}|$  for a cancellative pair over an  $n$ -element set, and let  $c_k(n)$  be the maximum considering only *k-uniform* pairs. Similarly to Soltész [7], we prove the following lemma.

**Lemma 2.** *Let  $M$  be a fixed positive integer, and suppose that  $\beta > 0$  is such that  $c_k(n) \leq \beta^n$  for all  $k$  divisible by  $M$  and for all  $n \geq k$ . Then  $c(n) \leq \beta^n$  for all  $n$ .*

*Proof.* Suppose the conditions above are satisfied but  $|\mathcal{A}||\mathcal{B}| = \omega^n$  for some  $\omega > \beta$ . Take the product of  $(\mathcal{A}, \mathcal{B})$  with (a copy of)  $(\mathcal{B}, \mathcal{A})$  to get a cancellative pair  $(\mathcal{A}_{(1)}, \mathcal{B}_{(1)})$  over some set  $S$  with  $|\mathcal{A}_{(1)}| = |\mathcal{B}_{(1)}| = \omega^{|S|/2}$  and  $\mathcal{A}_{(1)}$  and  $\mathcal{B}_{(1)}$  containing the same number of sets of size  $t$  for any  $t$ . Also, we can take the product of  $(\mathcal{A}_{(1)}, \mathcal{B}_{(1)})$  with (copies of) itself several times to get a pair with similar properties, so we may assume that  $|S|$  is large enough so that  $\omega^{|S|}/(|S| + 1)^2 > \beta^{|S|}$ . Take  $k_0 \in \{0, 1, \dots, |S|\}$  such that  $\mathcal{A}_{(1)}, \mathcal{B}_{(1)}$  each contain at least  $\omega^{|S|/2}/(|S| + 1)$  sets of size  $k_0$ , let  $(\mathcal{A}_{(2)}, \mathcal{B}_{(2)})$  contain only these  $k_0$ -sets. So  $|\mathcal{A}_{(2)}||\mathcal{B}_{(2)}| > \beta^{|S|}$  and  $(\mathcal{A}_{(2)}, \mathcal{B}_{(2)})$  is  $k_0$ -uniform cancellative. Take the product of  $(\mathcal{A}_{(2)}, \mathcal{B}_{(2)})$  with itself several times to obtain  $(\mathcal{A}_{(2)}^M, \mathcal{B}_{(2)}^M)$ , an  $(Mk_0)$ -uniform cancellative family contradicting our assumptions.  $\square$

We also need a simple observation.

**Lemma 3.** *If  $k$  and  $n \geq k$  are positive integers, then  $c_k(n) \leq 2^{2(n-k)}$ . In particular,  $c_k(n) \leq 2^n$  for  $n \leq 2k$ .*

*Proof.* Given  $A \in \mathcal{A}$ , all  $B \in \mathcal{B}$  have to differ on the complement of  $A$ , hence  $|\mathcal{B}| \leq 2^{n-k}$ . Similarly  $|\mathcal{A}| \leq 2^{n-k}$ .  $\square$

We note that we have equality for  $k \leq n \leq 2k$  (i.e.  $c_k(n) = 2^{2(n-k)}$ ), even in the symmetric case [3]. Also, we could deduce Lemma 3 from (4), observing that  $\sum p_i = \sum q_i = n - k$ .

In order to state our key proposition, we need a definition. For  $\gamma, x \geq 2$ , consider the following optimisation problem:

$$\begin{aligned} & \text{maximize} && \frac{1}{n} \sum_{i=1}^n f(p_i, q_i) \\ & \text{subject to} && p_i q_i \leq 1/\gamma \quad \text{for } i = 1, \dots, n \\ & && \sum_{i=1}^n p_i = \sum_{i=1}^n q_i \geq n(1 - 1/x) \\ & && 0 \leq p_i, q_i \leq 1 \quad \text{for } i = 1, \dots, n \\ & && n \in \mathbb{N} \end{aligned} \tag{5}$$

(Note that the positive integer  $n$  is not fixed.) We write  $\varphi(\gamma, x)$  for the solution (i.e. the supremum) of (5).

**Proposition 4.** *Suppose  $k$  is a positive integer,  $2 \leq \lambda$  such that  $\lambda k$  is an integer, and  $2 \leq r_1 \leq \gamma$ . Suppose that  $c_k(\lambda k) \leq r_1^{\lambda k}$  and*

$$r_1 \geq 2^{\varphi(\gamma, \lambda)}. \tag{6}$$

*Then, for  $\lambda k \leq n$ ,*

$$c_k(n) \leq r_1^{\lambda k} \gamma^{n-\lambda k}.$$

*In particular, if  $\mu > \lambda$ ,  $\mu k$  is an integer and  $r_2 = r_1^{\lambda/\mu} \gamma^{1-\lambda/\mu}$ , then  $c_k(n) \leq r_2^n$  for  $\lambda k \leq n \leq \mu k$ .*

*Proof.* Notice that  $\gamma \geq r_2 \geq r_1$ . We know the given inequality holds for  $n = \lambda k$ . Suppose it is false for some  $n$ ,  $\lambda k + 1 \leq n$ ,  $n$  minimal.

Then  $c_k(n)/c_k(n-1) > \gamma$ . So we must have  $p_i q_i < 1/\gamma$  (or else  $|\mathcal{A}_i| |\mathcal{B}_i| > c_k(n-1)$  and  $(\mathcal{A}_i, \mathcal{B}_i)$  is cancellative over  $S \setminus \{i\}$ ).

We also have  $\sum p_i = \sum q_i = n - k = n(1 - k/n) \geq n(1 - 1/\lambda)$ . Hence  $\sum f(p_i, q_i) \leq n\varphi(\gamma, \lambda)$  (by the definition of  $\varphi$ ). So then, by (4), we get

$$|\mathcal{A}| |\mathcal{B}| \leq 2^{n\varphi(\gamma, \lambda)} \leq r_1^n \leq r_1^{\lambda k} \gamma^{n-\lambda k},$$

contradiction.

For  $\lambda k \leq n \leq \mu k$ , we have  $c_k(n)^{1/n} \leq (r_1/\gamma)^{\lambda k/n} \gamma \leq (r_1/\gamma)^{\lambda/\mu} \gamma = r_2$ . □

Proposition 4 enables us to implement the following method. Let  $2 = \lambda_0 < \lambda_1 < \dots < \lambda_N$ , and let  $\rho_0 = 2$ . Using a computer program, we find some  $\rho_1 \geq \rho_0$ , then  $\rho_2 \geq \rho_1$ , and so on, finally  $\rho_N$ , such that the conditions of Proposition 4 hold for  $\lambda = \lambda_i$ ,  $\mu = \lambda_{i+1}$ ,  $r_1 = \rho_i$ ,  $r_2 = \rho_{i+1}$  and the corresponding value of  $\gamma$  ( $i = 0, 1, \dots, N-1$ ). So then  $c_k(n) \leq \rho_N^n$  for  $n/k \leq \lambda_N$ . (Note that the values  $\rho_i, \lambda_i$  do not depend on  $k$ .)

To be able to apply this method, we make the following observations.

1. If  $\lambda_i$  is rational for all  $i$ , then we are allowed to assume that  $\lambda_i k$  is an integer (since we may assume  $M$  divides  $k$  for any fixed  $M$  positive integer).
2. We do not need to consider  $n/k > 3.6$ . Indeed, for  $n/k > 3.6$  we have  $p_i + q_i > 2(1 - 1/3.6) = 13/9$  for some  $i$ , so then  $p_i q_i > 1.4/9 = 1/2.25$ . Hence  $c_k(n) < 2.25c_k(n-1)$ , as  $(\mathcal{A}_i, \mathcal{B}_i)$  is cancellative.
3. We need to find an upper bound on  $\varphi(\gamma, x)$ . Details on how this is done are given in the Appendix, however, we note the following simple result.  
 Let  $\gamma \geq 2.25$ ,  $x \geq 2$  and let  $(p_0, q_0)$  satisfy  $p_0 + q_0 = 2(1 - 1/x)$  and  $p_0 q_0 = 1/\gamma$ .  
 If  $0 \leq p_0, q_0 \leq 1$ ,  $p_0 \neq q_0$ , then  $\varphi(\gamma, x) = f(p_0, q_0)$ .

Now we are ready to prove our result using the method described above. Choose, for example,  $N = 100000$  and  $\lambda_i = 2 + i(3.6 - 2)/N$ . Then find appropriate values of  $\rho_1, \dots, \rho_N$  using a computer program. Details about our implementation are given in the Appendix. Our program gives  $\rho_N = 2.268166\dots$ , whence  $c_k(n) \leq 2.2682^n$  for all  $n$  (and  $k$  a multiple of an appropriate  $M$ ). By Lemma 2, we get our main result.

**Theorem 5.** *For a cancellative pair  $(\mathcal{A}, \mathcal{B})$  over an  $n$ -element set, we have  $|\mathcal{A}||\mathcal{B}| \leq 2.2682^n$ .*  $\square$

### 3 Remarks

**Recovering pairs** Since any recovering pair is also cancellative, the result above immediately gives the following corollary.

**Corollary 6.** *For a recovering pair  $(\mathcal{A}, \mathcal{B})$  over an  $n$ -element set, we have  $|\mathcal{A}||\mathcal{B}| \leq 2.2682^n$ .*  $\square$

We remark that a bound stronger than  $2^{2k}$  for  $k$ -uniform recovering pairs over a  $2k$ -element set would give a stronger bound on the maximal value of  $|\mathcal{A}||\mathcal{B}|$  using the argument above (we could choose  $\rho_0$  to be smaller). Note that the product of recovering families is recovering [7], so our arguments would still be valid.

**Uniform constructions** We now discuss how our upper bound on  $c_k(n)$  is related to the best known  $k$ -uniform constructions as  $n/k$  varies. Tolhuizen [8] gave a family of symmetric  $k$ -uniform pairs for all values of  $k$  and  $n$  having  $|\mathcal{A}| \geq \nu \binom{n}{k} 2^{-k}$ , where  $\nu$  is a constant. It follows that for  $n/k = x > 2$ , we have

$$c_k(n)^{1/n} \geq 2^{2(h(1/x) - 1/x) + o(1)}.$$

This construction is known to be asymptotically optimal in the symmetric  $k$ -uniform case [3, 8]. (As pointed out after Lemma 3, the exact value of  $c_k(n)$  is known for  $n/k \leq 2$ .)

Figure 1 shows the upper bound we obtain by the argument above for  $c_k(n)^{1/n}$ , together with the lower bound from Tolhuizen's construction ( $n/k$  fixed,  $n$  large). We note that, with a slight modification of Proposition 4, our upper bound could be decreased for  $n/k$  large (instead of becoming constant at the maximum value). However, this would not improve our constant of 2.2682, and it requires more care to find bounds for the optimization problem (5) when  $\gamma$  is small.

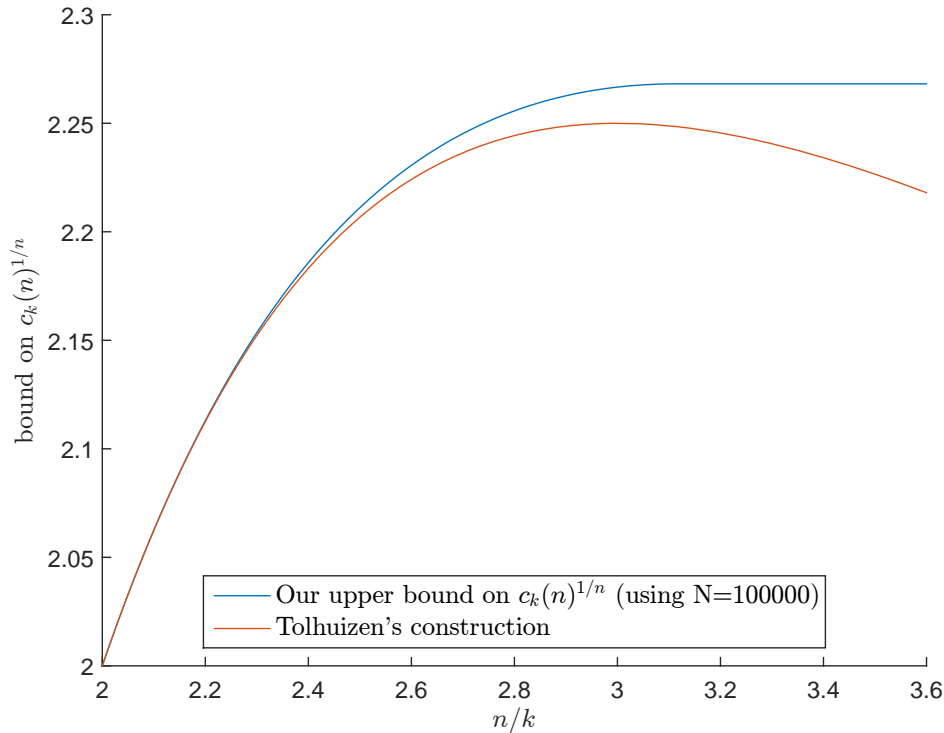


Figure 1: Graphical representation of the lower and upper bounds for uniform pairs.

**The symmetric case** In the case  $\mathcal{A} = \mathcal{B}$ , an argument similar to the one considered above gives the best possible bound of  $2.25^n$ . In fact, our argument is equivalent to that of Frankl and Füredi [3]. For convenience, we consider  $G_k(n)$ , the largest possible size of  $\mathcal{A}$  if  $(\mathcal{A}, \mathcal{A})$  is  $k$ -uniform cancellative. (So then  $c_k(n) \geq G_k(n)^2$ .) In this case, we have  $p_i = q_i$  for each  $i$ . If  $G_k(n)/G_k(n-1) = \gamma$ , then  $p_i \leq 1/\gamma$  for all  $i$ . But  $\sum p_i = n - k$ , hence  $\gamma \leq \frac{n}{n-k}$ . As  $G_k(2k) \leq 2^k$ , induction gives (for  $n \geq 2k$ )

$$G_k(n) \leq 2^k \binom{n}{k} / \binom{2k}{k}$$

This is exactly the formula obtained by Frankl and Füredi [3]. This is not surprising: their argument is essentially the same, but instead of removing elements one-by-one (i.e. inducting from  $n-1$  to  $n$ ), they consider a random set of size  $2k$ . (It is not hard to deduce the bound  $(3/2)^{2n}$  for symmetric pairs from here, noticing that subexponential factors can be ignored by a product argument. The asymptotic optimality of Tolhuizen's construction for  $k$ -uniform symmetric cancellative pairs ( $n \rightarrow \infty$ ,  $n/k \rightarrow x > 2$ ) also follows [8].)

**The choice of  $N$**  Increasing  $N$  over 100000 does not seem to change the first 5 digits after the decimal point in our upper bound  $2.268166\dots$ , e.g.  $N = 5 \cdot 10^6$  gives about 2.268164. We mention that using  $N = 5$  already improves the previously best known upper bound for cancellative pairs (it gives about  $2.3235^n$ ).

## Appendix

The appendix contains two main parts. In the first part, we give bounds for  $\varphi(\gamma, x)$ . In the second part, we briefly describe how we implement our argument using a computer program.

### Bounding the optimisation problem

**Lemma 7.** *Suppose  $\gamma \geq 2.25$  and  $\kappa \geq 0$ . Then the maximizer  $(p, q)$  of  $L_\kappa(p, q) = f(p, q) + \kappa(p + q)$  in the range  $0 \leq p, q \leq 1$ ,  $pq \leq 1/\gamma$  satisfies  $pq = 1/\gamma$ .*

*Proof.* Consider the maximizer. We may assume  $p \leq q$ . We show that if  $pq < 1/\gamma$  then  $\partial L_\kappa / \partial p > 0$ . We have

$$\partial L_\kappa / \partial p = h(q) + qh'(p) + \kappa \geq h(q) + qh'(p).$$

If  $p < 1/2$  then this is positive. If  $p \geq 1/2$ , then

$$\partial L_\kappa / \partial p \geq h\left(\frac{1}{2.25p}\right) + \frac{h'(p)}{2.25p}$$

which is positive on  $[1/2, 2/3]$ . □

**Lemma 8.** *Suppose  $\kappa \geq 0$ ,  $\gamma \geq 2.25$ ,  $x \geq 2$  and assume that for  $0 \leq p, q \leq 1$ ,  $pq = 1/\gamma$  the maximum of  $L_\kappa(p, q) = f(p, q) + \kappa(p + q)$  is  $\psi(\gamma, \kappa)$ . Then  $\varphi(\gamma, x) \leq \psi(\gamma, \kappa) - 2\kappa(1 - 1/x)$ .*

*Proof.* If  $(p_i)_{i=1}^n, (q_i)_{i=1}^n$  satisfy the constraints of (5), then

$$\frac{1}{n} \sum_{i=1}^n f(p_i, q_i) \leq \frac{1}{n} \sum_{i=1}^n (f(p_i, q_i) + \kappa(p_i + q_i)) - \frac{1}{n} \kappa \cdot 2n(1 - 1/x).$$

Using Lemma 7 and our assumptions above, the result follows. □

**Lemma 9.** *Suppose  $\kappa \geq 0$ ,  $q = q(p) = 1/(\gamma p)$ , and  $(p_0, q_0)$  satisfy  $p_0 q_0 = 1/\gamma$ ,  $0 \leq p_0, q_0 \leq 1$  and*

$$\kappa = \frac{p_0 q_0}{\log 2} \frac{g(p_0) - g(q_0)}{q_0 - p_0}$$

*where  $g(x) = \frac{\log(1-x)}{x}$ . Then  $L_\kappa(p, q(p))$  is maximal at  $(p_0, q_0)$ .*

*Proof.* We may assume  $q > p$ . As  $dq/dp = -q/p$ , we have (see [4] for more details)

$$\frac{d}{dp} \left[ f(p, q(p)) + \kappa(p + q(p)) \right] = q \left[ \frac{1}{p} \log_2(1-p) - \frac{1}{q} \log_2(1-q) \right] + \kappa(1 - q/p).$$

This has the same sign as

$$\frac{pq}{\log 2} \frac{g(p) - g(q)}{q - p} - \kappa$$

where  $g(x) = \frac{\log(1-x)}{x}$ . As  $pq$  is constant, it suffices to show that in the range  $\frac{1}{\gamma} \leq p < \frac{1}{\sqrt{\gamma}}$ , the function

$$\sigma(p) = \frac{g(p) - g(q(p))}{q(p) - p}$$

is strictly decreasing. We have

$$\sigma'(p) = \frac{(g'(p) - g'(q)(-q/p))(q-p) - (g(p) - g(q))(-q/p - 1)}{(q-p)^2}.$$

Since  $g'(x) = -\frac{1}{x(1-x)} - g(x)/x$ , we obtain

$$\begin{aligned} p(q-p)^2\sigma'(p) &= (q-p)(pg'(p) + qg'(q)) + (p+q)(g(p) - g(q)) \\ &= (q-p) \left( -\frac{1}{1-p} - g(p) - \frac{1}{1-q} - g(q) \right) + (p+q)(g(p) - g(q)) = \\ &= -(q-p) \left( \frac{1}{1-p} + \frac{1}{1-q} \right) + 2pg(p) - 2qg(q). \end{aligned}$$

Using the substitutions  $1-p=x$ ,  $1-q=y$ ,  $a=x/y > 1$ , we get

$$\begin{aligned} p(q-p)^2\sigma'(p) &= -(x-y) \left( \frac{1}{x} + \frac{1}{y} \right) + 2(\log x - \log y) \\ &= -a + \frac{1}{a} + 2 \log a. \end{aligned}$$

But this is negative for  $a > 1$ , since it is 0 at  $a = 1$  and its derivative is

$$-1 - \frac{1}{a^2} + \frac{2}{a} = -\frac{(1-a)^2}{a^2}.$$

So  $\sigma$  is strictly decreasing. □

**Lemma 10.** *Let  $\gamma \geq 2.25$ ,  $x \geq 2$  and let  $(p_0, q_0)$  satisfy  $p_0 + q_0 = 2(1 - 1/x)$  and  $p_0q_0 = 1/\gamma$ .*

*If  $0 \leq p_0, q_0 \leq 1$ ,  $p_0 \neq q_0$ , then  $\varphi(\gamma, x) = f(p_0, q_0)$ .*

*Proof.* Choose

$$\kappa = \frac{p_0q_0}{\log 2} \frac{g(p_0) - g(q_0)}{q_0 - p_0}$$

(this is positive, since  $g'(x) < 0$ , see [4].) By Lemma 9,  $\psi(\gamma, \kappa) = L_\kappa(p_0, q_0)$ . By Lemma 8,  $\varphi(\gamma, x) \leq f(p_0, q_0)$ . Equality can be achieved by choosing  $n = 2$ ,  $p_1 = q_2 = p_0$ ,  $p_2 = q_1 = q_0$ . □



## Implementation using a computer

The essence of our algorithm is the following. We choose  $\lambda_i$  ( $i = 0, \dots, N$ ) to be equally spaced between 2 and 3.6 and set  $\rho_0 = 2$ . In the  $i^{\text{th}}$  step, we find  $p_0, q_0$  such that  $0 \leq p_0, q_0 \leq 1$ ,  $p_0 + q_0 = 2(1 - 1/\lambda_i)$  and  $2^{f(p_0, q_0)} = \rho_i$ . Then we calculate  $\gamma_i = 1/(p_0 q_0)$  (so that  $\varphi(\gamma, \lambda_i) = f(p_0, q_0)$  by Lemma 10), and set  $\rho_{i+1} = \rho_i^{\lambda_i/\lambda_{i+1}} \gamma_i^{1-\lambda_i/\lambda_{i+1}}$ . Initially we have  $\lambda_0 = 2$ ,  $\rho_0 = 2$ ,  $\gamma_0 = 4$ . As  $\lambda_i$  increases, we have that  $\rho_i$  increases and  $\gamma_i$  decreases. The process stops when  $\gamma_i$  and  $\rho_i$  become equal. This happens at  $\lambda_i \approx 3.12$  with  $\rho_i \approx \gamma_i \approx 2.2682$ .

While doing the calculations, we check that Lemma 10 applies (e.g.  $\gamma \geq 2.25$ ). Also, we make some changes to the method described above to avoid rounding errors (e.g. we require  $2^{f(p_0, q_0)} + \delta \leq \rho_i$  for  $\delta = 10^{-8}$ ).

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