HIGHER-DIMENSIONAL DEDEKIND SUMS AND THEIR BOUNDS ARISING FROM THE DISCRETE DIAGONAL OF THE n-CUBE

MATTHIAS BECK, SINAI ROBINS, AND SHELEMYAHU ZACKS

Counting pairs is the oldest trick in combinatorics... Every time we count pairs, we learn something from it.
Gil Kalai

Abstract. We define a combinatorial game in $\mathbb{R}^d$ from which we derive numerous new inequalities between higher-dimensional Dedekind sums. Our approach is motivated by a recent article by Dilcher and Girstmair, who gave a nice probabilistic interpretation for the classical Dedekind sum. Here we introduce a game analogous to Dilcher and Girstmair's model in higher dimensions.

1. Introduction

Historically, Dedekind sums first appeared in Dedekind's transformation law of his η-function [3]. Dedekind sums have since become an integral part of combinatorial geometry (lattice point enumeration [9]), algebraic number theory (class number formulae [8]), topology (signature defects of manifolds [5]), and algorithmic complexity (pseudo random number generators [6]). We begin by defining the classical Dedekind sum, whose basic ingredient is the sawtooth function

$$((x)) = \begin{cases} \{x\} - \frac{1}{2} & \text{if } x \notin \mathbb{Z} \\ 0 & \text{if } x \in \mathbb{Z} \ . \end{cases}$$

Here $\{x\} = x - \lfloor x \rfloor$ denotes the fractional part of x.

Definition 1. *For any two positive integers a and b, we define the* classical Dedekind sum *as*

$$s(a,b) = \sum_{k \bmod b} \left(\left(\frac{ka}{b} \right) \right) \left(\left(\frac{k}{b} \right) \right) \ .$$

Here the sum is over a complete residue system modulo b.

The classic introduction to the arithmetic properties of the Dedekind sum is [10]. The Dedekind sums have recently been cast in a new light as essentially the second moments of an appealing probability model introduced by Dilcher and Girstmair [4]. They divide an interval of length a into b equal subintervals ("boxes") and count the number of integers in each subinterval.

Here we introduce a d-dimensional analog of this model. We begin gently with the two-dimensional extension: given three positive integers a, b, and c, divide one of the sides of the square $[0,a) \times [0,a)$ into b parts of length a/b, and the other side into c parts of length a/c. This division induces a grid (see Figure 1 for an example). We thus have bc boxes of equal size. We think of each box as half

Key words and phrases. Dedekind sums, probability models, moments.
Version of 11/6/2002. To appear in *Advances in Applied Mathematics*.

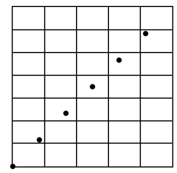

FIGURE 1. $a = 6,\ b = 5,\ c = 7$

open: we count the left (excluding the highest point) and bottom side (excluding the right-most point) as belonging to the box. Let's mark each box by a pair of integers (j,k) where $0 \le j \le b-1$ and $0 \le k \le c-1$. We will study the integer lattice points in the square; note that the box (j,k) contains the point $(m,n) \in \mathbb{Z}^2$ if and only if

$$\frac{ja}{b} \le m < \frac{(j+1)a}{b} \qquad \text{and} \qquad \frac{ka}{c} \le n < \frac{(k+1)a}{c} \ . \tag{1}$$

Equivalent to this condition is the following:

$$j \le \frac{mb}{a} < j+1 \qquad \text{and} \qquad k \le \frac{nc}{a} < k+1 \ ,$$

which can be rewritten in compact form using the greatest integer function $\lfloor x \rfloor$ (the greatest integer not exceeding x):

$$j = \left\lfloor \frac{mb}{a} \right\rfloor \qquad \text{and} \qquad k = \left\lfloor \frac{nc}{a} \right\rfloor \ . \tag{2}$$

We formalize the distribution of integer points within each of the bc boxes as follows.

Definition 2. *Let $f_{a;b,c}(j,k)$ denote the number of lattice points on the diagonal in the box (j,k).*

(So the vast majority of those numbers will be zero.) We can evaluate the following sum in two ways according to the equivalence of (1) and (2):

$$\sum_{j=0}^{b-1} \sum_{k=0}^{c-1} j\, k\, f_{a;b,c}(j,k) = \sum_{m=0}^{a-1} \left\lfloor \frac{mb}{a} \right\rfloor \left\lfloor \frac{mc}{a} \right\rfloor \ . \tag{3}$$

(A similar duality is central to Dilcher and Girstmair's work. There's was a one-dimensional problem, so they did not have to bother with diagonals.) A special case of this is $b = c$, for which we make the following definition.

Definition 3. *Here $f_{a;b}(j)$ denotes the number of integers in the j^{th} subinterval when we divide $[0,a)$ into b equal parts.*

We remark that $f_{a;b}(j) = f_{a;b,b}(j)$. Now the problem reduces to the one-dimensional case studied by Dilcher and Girstmair:

$$\sum_{j=0}^{b-1} \sum_{k=0}^{c-1} j\, k\, f_{a;b,b}(j,k) = \sum_{j=0}^{b-1} j^2 f_{a;b}(j) = \sum_{m=0}^{a-1} \left\lfloor \frac{mb}{a} \right\rfloor^2 \ . \tag{4}$$

The sum on the right hand is essentially a classical Dedekind sum: If a and b are relatively prime,

$$\begin{aligned}\sum_{m=0}^{a-1}\left\lfloor\frac{mb}{a}\right\rfloor^2 &= \sum_{m=1}^{a-1}\left(\frac{mb}{a}-\left\{\frac{mb}{a}\right\}\right)^2\\ &= \sum_{m=1}^{a-1}\left(\frac{mb}{a}\right)^2 - 2\sum_{m=1}^{a-1}\frac{mb}{a}\left\{\frac{mb}{a}\right\}+\sum_{m=1}^{a-1}\left\{\frac{mb}{a}\right\}^2\\ &= \frac{b^2}{a^2}\sum_{m=1}^{a-1}m^2 - 2b\sum_{m=1}^{a-1}\left(\frac{m}{a}-\frac{1}{2}\right)\left(\left\{\frac{mb}{a}\right\}-\frac{1}{2}\right) - 2b\sum_{m=1}^{a-1}\frac{m}{a}+\frac{2b(a-1)}{4}+\sum_{m=1}^{a-1}\left(\frac{m}{a}\right)^2\\ &= \frac{(b^2+1)(a-1)(2a-1)}{6a} - 2b\,s(b,a) - \frac{1}{2}b(a-1)\end{aligned}$$

This and similar sums coming from the one-dimensional case will appear repeatedly in the exposition that follows, which is a good reason to give them a name.

Definition 4. *For any two positive integers a and b, we define*

$$M_r(a;b) = \frac{1}{a}\sum_{m=0}^{a-1}\left\lfloor\frac{mb}{a}\right\rfloor^r .$$

M_r is the r^{th} moment of the Dilcher-Girstmair probability distribution. By (4), the definition of M_r is equivalent to

$$M_r(a;b) = \frac{1}{a}\sum_{j=0}^{b-1} j^r f_{a;b}(j) .$$

We just showed above that M_2 corresponds to a classical Dedekind sum:

$$M_2(a;b) = \frac{(b^2+1)(a-1)(2a-1)}{6a^2} - \frac{(a-1)b}{2a} - \frac{2b}{a}\,s(b,a) . \tag{5}$$

For larger r, we have similar correspondences, though the classical Dedekind sum does not suffice to describe M_r in these cases; one needs "higher-dimensional" Dedekind sums which have more than just two factors being summed. Naturally, there are many ways to define such extensions of the classical Dedekind sum; one could, for example, study sums of the form

$$\sum_{k \bmod a}\left(\left(\frac{ka_1}{a}\right)\right)\cdots\left(\left(\frac{ka_d}{a}\right)\right) , \tag{6}$$

and these sums arise in various contexts, for example, lattice-point problems in polyhedra [1]. $M_r(b,a)$ can be expressed as a linear combination of special cases of this sum, namely,

$$\sum_{k \bmod a}\left(\left(\frac{kb}{a}\right)\right)^m\left(\left(\frac{k}{a}\right)\right)^n$$

for some integers m and n.

The model that we described above extends naturally to higher dimensions. Instead of considering a square, let's divide the d-dimensional cube $[0,a)\times\cdots\times[0,a)$ into $b_1\cdots b_d$ equal boxes by a similar construction as above: now we divide the first side into b_1 equal intervals, the next one into b_2 equal intervals, and so on. Again we will count the number of integer lattice point on the diagonal of this cube, according to the box they are in. As above we will label each box, say by

$(k_1, \dots, k_d)$, $0 \le k_j \le b_j - 1$, and we will denote the function counting the lattice points in box $(k_1, \dots, k_d)$ by

$$f_{a;b_1,\dots,b_d}(k_1, \dots, k_d) \ .$$

As before, an elementary counting-two-ways argument yields

$$\sum_{k_1=0}^{b_1-1} \cdots \sum_{k_d=0}^{b_d-1} k_1 \cdots k_d \, f_{a;b_1,\dots,b_d}(k_1, \dots, k_d) = \sum_{m=0}^{a-1} \left\lfloor \frac{mb_1}{a} \right\rfloor \cdots \left\lfloor \frac{mb_d}{a} \right\rfloor \ .$$

This naturally leads to the following definition.

Definition 5. *For positive integers $a, b_1, b_2, \dots, b_d$, we define*

$$S_d(a; \mathbf{b}) = S_d(a; b_1, b_2, \dots, b_d) = \frac{1}{a} \sum_{m=0}^{a-1} \left\lfloor \frac{mb_1}{a} \right\rfloor \cdots \left\lfloor \frac{mb_d}{a} \right\rfloor \ ,$$

This is a generalized Dedekind sum. In fact, we can express this sum as a linear combination of sums of the form (6). Our goal is to find relations for the sums $S_d(a; \mathbf{b})$.

2. The two-dimensional frequency distribution $\{f_{a;b,c}(j,k)\}$ and its marginal distributions

In this section we focus on the study of the distribution numbers $f_{a;b,c}(j,k)$ using the duality interpretation given by (3). It appears impossible to derive a closed formula for the number of diagonal lattice points that belong to the (j,k)th rectangle, that is, $f_{a;b,c}(j,k)$, $j = 0, \dots, b-1$, $k = 0, \dots, c-1$. We develop an algorithm, given in the appendix, which computes the values of $f_{a;b,c}(j,k)$ and of the marginal frequencies

$$f_{a;b}(j) = \sum_{k=0}^{c-1} f_{a;b,c}(j,k) \qquad \text{and} \qquad f_{a;c}(k) = \sum_{j=0}^{b-1} f_{a;b,c}(j,k) \ .$$

Example. In Table 2 we present these distributions for the case $a = 50, b = 13, c = 7$. From this table we can immediately verify that

$$\sum_{j=0}^{12} \sum_{k=0}^{6} k \, j \, f_{50;13,7}(j,k) = \sum_{m=0}^{49} \left\lfloor \frac{13m}{50} \right\rfloor \left\lfloor \frac{7m}{50} \right\rfloor = 1236 \ .$$

By analyzing the structure of the marginal distributions we can arrive at closed formulae for $M_r(a; b)$. For example, one can immediately verify that if $a = bn$, $n \in \mathbb{N}$ then

$$f_{a;b}(j) = n = \left\lfloor \frac{a}{b} \right\rfloor, \ j = 0, \dots, b-1$$

and if $a = 1 + bn$ then

$$f_{a;b}(j) = \begin{cases} \left\lfloor \frac{a}{b} \right\rfloor + 1 & \text{if } j = 0, \\ \left\lfloor \frac{a}{b} \right\rfloor & \text{if } j > 0. \end{cases}$$

$j\backslash k$	0	1	2	3	4	5	6	$f_b^a(j)$
0	4	0	0	0	0	0	0	4
1	4	0	0	0	0	0	0	4
2	0	4	0	0	0	0	0	4
3	0	3	1	0	0	0	0	4
4	0	0	4	0	0	0	0	4
5	0	0	2	2	0	0	0	4
6	0	0	0	3	0	0	0	3
7	0	0	0	2	2	0	0	4
8	0	0	0	0	4	0	0	4
9	0	0	0	0	1	3	0	4
10	0	0	0	0	0	4	0	4
11	0	0	0	0	0	0	4	4
12	0	0	0	0	0	0	3	3
$f_c^a(k)$	8	7	7	7	7	7	7	50

FIGURE 2. The two-dimensional distribution and its marginals for $a = 50, b = 13, c = 7$

Thus for $a \equiv 0, 1 \mod b$ we immediately obtain

$$M_r(a;b) = \frac{1}{a} \left\lfloor \frac{a}{b} \right\rfloor \sum_{j=1}^{b-1} j^r \ .$$

In general, the one-dimensional frequencies can be bounded as

$$\left\lfloor \frac{a}{b} \right\rfloor \le f_{a;b}(j) < \left\lceil \frac{a}{b} \right\rceil \ . \tag{7}$$

A book-keeping device that will help us keep track of the difference between the frequency and $\left\lfloor \frac{a}{b} \right\rfloor$ is the following.

Definition 6. $I_{a;b}(j) = f_{a;b}(j) - \left\lfloor \frac{a}{b} \right\rfloor$.

Notice that by (7) we have $I_{a;b}(j) = 0, 1$ for all $a, b, j = 0, \dots, b-1$. Accordingly we rewrite the r^{th} moment of the Dilcher-Girstmair distribution as follows.

$$M_r(a;b) = \frac{1}{a} \left(\left\lfloor \frac{a}{b} \right\rfloor \sum_{j=1}^{b-1} j^r + \sum_{j=1}^{b-1} j^r I_{a;b}(j) \right) . \tag{8}$$

The second sum allows for a finer analysis of these moments. A trivial example follows from the fact that $I_{a;b}(j) \ge 0$:

$$M_r(a;b) \ge \frac{1}{a} \left\lfloor \frac{a}{b} \right\rfloor \sum_{j=1}^{b-1} j^r \ .$$

[Bernoulli functions!] This bound gets achieved, for example, when $a \equiv 0, 1 \mod b$. In the following section, we study $I_{a;b}(j)$ for the second moments.

3. Dilcher and Girstmair's two-variable case revisited

Of special interest is $M_2(a;b)$, due to its relationship to the Dedekind sum $s(b,a)$. According to (8)

$$a\, M_2(a;b) = \left\lfloor \frac{a}{b} \right\rfloor \frac{(b-1)b(2b-1)}{6} + \sum_{j=1}^{b-1} j^2 I_{a;b}(j) \ . \tag{9}$$

One may think about this identity in terms of the Dilcher-Girstmair distribution model: Among the a integers in $[0,a)$, we have $\lfloor a/b \rfloor$ of them for sure in each interval

$$\left[\frac{ka}{b}, \frac{(k+1)a}{b} \right), \qquad k = 0, \dots, b-1 \ .$$

These integers are represented in the first term on the right-hand side of (9). Suppose $a \equiv l \mod b$ where $0 < l < b$ (the case $b|a$ is special and very easy to handle: $I_{a;b}(j) = 0$ for all j); then there are $l-1$ integers "left" which haven't been accounted for (note that the first interval $[0, a/b)$ contains $\lfloor a/b \rfloor + 1$ integers). These $l-1$ integers are represented in the second term on the right-hand side of (9). In fact, one can say more about them. Because they are uniformly distributed among the b intervals, we obtain

$$D_2(a;b) = \sum_{j=1}^{b-1} j^2 I_{a;b}(j) = \sum_{m=1}^{l-1} \left\lfloor \frac{mb}{l} \right\rfloor^2 = l\, M_2(l;b). \tag{10}$$

[This is equivalent to two applications of Dedekind's reciprocity law!] Note that, in particular, $D_2(a;b)$ depends on a only via $l \equiv a \mod b$. In special cases of $a \equiv l \mod b$, we can obtain closed formulas for $D_2(a;b)$, given in the following table.

l	$D_2(a;b)$	
0,1	0	
2	$\left\lfloor \frac{b}{2} \right\rfloor^2$	
3	$5 \left\lfloor \frac{b}{3} \right\rfloor^2$	if $b \equiv 0,1 \mod 3$
	$5 \left\lfloor \frac{b}{3} \right\rfloor^2 + 4 \left\lfloor \frac{b}{3} \right\rfloor + 1$	if $b \equiv 2 \mod 3$
4	$14 \left\lfloor \frac{b}{4} \right\rfloor^2$	if $b \equiv 0,1 \mod 4$
	$14 \left\lfloor \frac{b}{4} \right\rfloor^2 + 10 \left\lfloor \frac{b}{4} \right\rfloor + 2$	if $b \equiv 2 \mod 4$
	$14 \left\lfloor \frac{b}{4} \right\rfloor^2 + 16 \left\lfloor \frac{b}{4} \right\rfloor + 5$	if $b \equiv 3 \mod 4$
5	$30 \left\lfloor \frac{b}{5} \right\rfloor^2$	if $b \equiv 0,1 \mod 5$
	$30 \left\lfloor \frac{b}{5} \right\rfloor^2 + 14 \left\lfloor \frac{b}{5} \right\rfloor + 2$	if $b \equiv 2 \mod 5$
	$30 \left\lfloor \frac{b}{5} \right\rfloor^2 + 26 \left\lfloor \frac{b}{5} \right\rfloor + 6$	if $b \equiv 3 \mod 5$
	$30 \left\lfloor \frac{b}{5} \right\rfloor^2 + 40 \left\lfloor \frac{b}{5} \right\rfloor + 14$	if $b \equiv 4 \mod 5$

Figure 3. $D_2(a;b)$ for $a \equiv l \mod b$

In general, one can use (10) to obtain inequalities for $D_2(a;b)$ and hence for $M_2(a;b)$. To this extend, we use the fact that

$$\left(m \left\lfloor \frac{b}{l} \right\rfloor \right)^2 \le \left\lfloor \frac{mb}{l} \right\rfloor^2 \le \left\lfloor \left(\frac{mb}{l} \right)^2 \right\rfloor \ ,$$

which implies the following bounds:

$$\left\lfloor \frac{b}{l} \right\rfloor^2 \sum_{m=1}^{l-1} m^2 = \left\lfloor \frac{b}{l} \right\rfloor^2 \frac{(l-1)l(2l-1)}{6} \le D_2(a;b) \le \left\lfloor \left(\frac{b}{l}\right)^2 \frac{(l-1)l(2l-1)}{6} \right\rfloor = \left\lfloor \sum_{m=1}^{l-1} \left(\frac{mb}{l}\right)^2 \right\rfloor .$$

Accordingly, we have the following:

Proposition 1.

$$M_2(a;b) \ge \left\lfloor \frac{a}{b} \right\rfloor \frac{(b-1)b(2b-1)}{6} + \left\lfloor \frac{b}{l} \right\rfloor^2 \frac{(l-1)l(2l-1)}{6} . \tag{11}$$

and

$$M_2(a;b) \le \left\lfloor \frac{a}{b} \right\rfloor \frac{(b-1)b(2b-1)}{6} + \left\lfloor \frac{b^2(l-1)(2l-1)}{6l} \right\rfloor . \tag{12}$$

Recall that these bounds are for the cases $a \equiv l \mod b$ where $0 < l < b$; for $l = 0$ or 1 we obtained

$$M_2(a;b) = \left\lfloor \frac{a}{b} \right\rfloor \frac{(b-1)b(2b-1)}{6} .$$

Naturally, (10) can be refined further to give even better bounds. We illustrate one further step here. Suppose as before that $a \equiv l \mod b$ where $1 < l < b$, and moreover that $b = \lfloor b/l \rfloor l + k$, so that $0 \le k \le l-1$. According to (10) this gives

$$\begin{aligned} D_2(a;b) &= \sum_{m=1}^{l-1} \left\lfloor \frac{mb}{l} \right\rfloor^2 = \sum_{m=1}^{l-1} \left\lfloor \frac{m(\lfloor b/l \rfloor l + k)}{l} \right\rfloor^2 = \sum_{m=1}^{l-1} \left(m \left\lfloor \frac{b}{l} \right\rfloor + \left\lfloor \frac{mk}{l} \right\rfloor \right)^2 \\ &= \left\lfloor \frac{b}{l} \right\rfloor^2 \frac{(l-1)l(2l-1)}{6} + 2 \left\lfloor \frac{b}{l} \right\rfloor \sum_{m=1}^{l-1} m \left\lfloor \frac{mk}{l} \right\rfloor + \sum_{m=1}^{l-1} \left\lfloor \frac{mk}{l} \right\rfloor^2 . \end{aligned}$$

Thus, if $k = 0, 1,\ l \ge 2$ then

$$D_2(a;b) = \left\lfloor \frac{b}{l} \right\rfloor^2 \frac{(l-1)l(2l-1)}{6} .$$

If $k = 2,\ l \ge 2$ then

$$D_2(a;b) = \left\lfloor \frac{b}{l} \right\rfloor^2 \frac{(l-1)l(2l-1)}{6} + \begin{cases} \left\lfloor \frac{b}{l} \right\rfloor \left((l-1)l - \frac{1}{4}l(l-2)\right) + \frac{l}{2} & \text{if } l \text{ is even,} \\ \left\lfloor \frac{b}{l} \right\rfloor (l-1)l - \left\lfloor \frac{l}{2} \right\rfloor \left(1 + \left\lfloor \frac{l}{2} \right\rfloor\right) + \left\lfloor \frac{l}{2} \right\rfloor & \text{if } l \text{ is odd.} \end{cases} \tag{13}$$

For example, if $l = 4, k = 2$

$$D_2(4,b) = \left\lfloor \frac{b}{4} \right\rfloor^2 \frac{3 \cdot 4 \cdot 7}{6} + 10 \left\lfloor \frac{b}{4} \right\rfloor + 2 ,$$

and if $l = 5, k = 2$

$$D_2(5,b) = \left\lfloor \frac{b}{5} \right\rfloor^2 \frac{4 \cdot 5 \cdot 9}{6} + 14 \left\lfloor \frac{b}{5} \right\rfloor + 2 ,$$

as stated in Figure 3. Finally, since $\left\lfloor \frac{mk}{l} \right\rfloor \ge \left\lfloor \frac{m2}{l} \right\rfloor$ for all $k \ge 2$, the above formula of $D_2(a;b)$ for $k = 2$ is a lower bound.

Similar bounds can be derived "classically" by applying Dedekind's famous reciprocity law:

Theorem 2 (Dedekind)**.** *If a and b are relatively prime then*

$$s(a,b)+s(b,a)=-\frac{1}{4}+\frac{1}{12}\left(\frac{a}{b}+\frac{1}{ab}+\frac{b}{a}\right) .$$

Denote the rational function appearing in Theorem 2 by

$$R(a,b)=-\frac{1}{4}+\frac{1}{12}\left(\frac{a}{b}+\frac{1}{ab}+\frac{b}{a}\right) .$$

Then we obtain for $a \equiv l \mod b$, where a and b are relatively prime and $1<l<b$,

$$s(b,a)=R(a,b)-s(a,b)=R(a,b)-s(l,b)=R(a,b)-R(b,l)+s(b,l) .$$

It is well known (and a straightforward exercise) that

$$|s(b,l)| \le s(1,l)=\frac{l}{12}-\frac{1}{4}+\frac{1}{6l} ,$$

which gives the following bounds:

$$R(a,b)-R(b,l)-s(1,l) \le s(b,a) \le R(a,b)-R(b,l)+s(1,l) .$$

These inequalities, in turn, can be transformed into inequalities for M_2 via (5):

$$M_2(a;b) \ge \frac{(b^2+1)(a-1)(2a-1)}{6a^2}-\frac{(a-1)b}{2a}-\frac{2b}{a}\left(R(a,b)-R(b,l)+s(1,l)\right) . \tag{14}$$

$$M_2(a;b) \le \frac{(b^2+1)(a-1)(2a-1)}{6a^2}-\frac{(a-1)b}{2a}-\frac{2b}{a}\left(R(a,b)-R(b,l)-s(1,l)\right) . \tag{15}$$

In the following table we give the exact values of $aM_2(a;b)$ and their lower bounds. We denote by

flb1 the lower bound according to (11),
flb2 the lower bound according to (13),
rlb the lower bound according to (14),
fub the upper bound according to (12),
rub the upper bound according to (15).

Note that we can compute rlb and rub only when a and b are relatively prime.

a	b	exact	flb1	flb2	rlb	fub	rub
5	2	2	2	2	2	2	2
5	3	6	6	6	6	6	6
5	4	14	14	14	14	14	14
6	2	3	3	3		3	
6	3	10	10	10		10	
6	4	18	18	18		18	
6	5	30	30	30	30	30	30
7	2	3	3	3	3	3	3
7	3	10	10	10	10	10	10
7	4	19	19	19	19	19	19.9
7	5	34	34	34	34	34	34
7	6	55	55	55	55	55	55
35	7	455	455	455		455	
39	7	490	469	481	486.5	497	490
40	7	501	485	501	498.2	513	503.8
41	7	510	510	510	510	529	517.8
10	3	15	15	15	15	15	15
11	3	16	16	16	16	16	16
21	6	185	185	185		185	
20	6	174	174	174		174	
11	7	126	105	117	122.5	133	126
10	9	204	204	204	204	204	204
11	9	220	220	220	220	220	220
12	9	249	249	249		249	
13	9	260	260	260	260	274	264.5
14	9	288	234	250	280.8	301	288
15	9	315	259	286		327	
16	9	328	295	328	322.9	354	335.7
17	9	344	344	344	344	381	359.75
24	10	648	626	648		657	

4. The Cauchy-Schwartz inequality and bounds to generalized Dedekind sums: the case $d = 2$

4.1. **Applications of the Cauchy-Schwartz inequality.** In the present section we discuss some relationships between the S and the M-functions. By definition, if $b_1 = \cdots = b_d$

$$S_d(a; b\ \mathbf{1}_d) = M_d(a; b)\ ,\ \ d = 1, 2, \ldots$$

Here $\mathbf{1}_d$ denotes the d-dimensional vector each of whose components is 1. The Cauchy-Schwartz inequality yields immediately, for $d = 2$, the inequality

$$S_2(a; b_1, b_2) \leq (M_2(a; b_1) M_2(a; b_2))^{1/2}\ \ ,$$

with equality if and only if $b_1 = b_2$.

Let

$$R_2(a;b_1,b_2) = \frac{S_2(a;b_1,b_2)}{\sqrt{M_2(a;b_1)M_2(a;b_2)}} \ .$$

In the following table we give a few values of $R_2(a;b_1,b_2)$.

a	b_2	$R_2(a;2,b_2)$	$R_2(a;3,b_2)$
11	7	0.9163	0.9799
21	5	0.9237	0.9721
18	11	0.9297	0.9729
73	39	0.9189	0.9695
99	33	0.9192	0.9707

It is interesting to observe in this table that all these $R_2(a;b,c)$-values are close to 1, and that among these values $R_2(a;2,b_2) < R_2(a;3,b_2)$. The question is whether this inequality is always true. A partial answer is given in Lemma 6 of Section 4.2. Empirical evaluations lead us to the following conjecture:

Conjecture 1. *For all $a,b,c \ge 3$,*

$$R_2(a;b,c) \ge R_2(5;2,3) = \frac{\sqrt{3}}{2} \ .$$

Notice that according to the previous definitions, $R_2(a;b,c)$ is the cosine of the angle between the two vectors

$$\mathbf{v}_b = \left(\left\lfloor \frac{bm}{a} \right\rfloor : m = 1, \dots, a-1 \right) \qquad \text{and} \qquad \mathbf{v}_c = \left(\left\lfloor \frac{cm}{a} \right\rfloor : m = 1, \dots, a-1 \right) \ .$$

In section 4.2 we present the geometrical correspondence, which is utilized to obtain further results.

Exact formulae can be derived for $R_2(a;2,a)$, $a \ge 3$. Indeed

$$S_2(a;2,a) = \begin{cases} \frac{a-1}{2} - \frac{\lfloor a/2 \rfloor (1 + \lfloor a/2 \rfloor)}{2a} & \text{if } \left\lfloor \frac{a}{2} \right\rfloor < \frac{a}{2}, \text{ i.e., } a \text{ is odd,} \\ \frac{a-1}{2} - \frac{1}{4}\left(\frac{a}{2} - 1\right) & \text{if } \left\lfloor \frac{a}{2} \right\rfloor = \frac{a}{2}, \text{ i.e., } a \text{ is even.} \end{cases}$$

Moreover

$$M_2(a;2) = \frac{1}{a} \left\lfloor \frac{a}{2} \right\rfloor \ ,$$

and

$$M_2(a;a) = \frac{2a^2 - 3a + 1}{6} \ .$$

Accordingly

$$R_2(a;2,a) = \begin{cases} R_2^*(a) \left(a - 1 - 1/a \lfloor a/2 \rfloor (1 + \lfloor a/2 \rfloor)\right) & \text{if } \left\lfloor \frac{a}{2} \right\rfloor < \frac{a}{2}, \text{ i.e., } a \text{ is odd,} \\ R_2^*(a) \left(a - 1 - 1/2(a/2 - 1)\right) & \text{if } \left\lfloor \frac{a}{2} \right\rfloor = \frac{a}{2}, \text{ i.e., } a \text{ is even,} \end{cases}$$

where

$$R_2^*(a) = \frac{\sqrt{6a}}{2\sqrt{\lfloor a/2 \rfloor (2a^2 - 3a + 1)}} \ .$$

A graph of $R_2(a;2,a)$ for $a = 3, \dots, 50$ is given in Figure 4. Notice that $\lim_{a \to \infty} R_2(a;2,a) = \frac{3\sqrt{6}}{8}$.

FIGURE 4. $R_2(a; 2, a)$ for $a = 3, \ldots, 50$

We provide here a few auxiliary results. First, if $c = l + ia$ (i.e., $a \equiv l \mod c$) then

$$S_2(a; b, c) = \sum_{m=0}^{a-1} \left\lfloor \frac{bm}{a} \right\rfloor \left\lfloor \frac{(l+ia)m}{a} \right\rfloor = i \sum_{m=1}^{a-1} m \left\lfloor \frac{bm}{a} \right\rfloor + S_2(a; b, l) \ .$$

Similarly,

$$aM_2(a; l+ia) = \sum_{m=0}^{a-1} \left\lfloor \frac{(l+ia)m}{a} \right\rfloor^2 = i^2 \frac{(a-1)a(2a-1)}{6} + 2i \sum_{m=1}^{a-1} m \left\lfloor \frac{lm}{a} \right\rfloor + aM_2(a, l) \ .$$

Accordingly,

$$R_2(a; b, l+ia) = \frac{i \sum_{m=1}^{a-1} m \left\lfloor \frac{bm}{a} \right\rfloor + aS_2(a; b, l)}{D_i}$$

where

$$D_i = i \left(aM_2(a; b) \frac{(a-1)a(2a-1)}{6} + \frac{2}{i} \sum_{m=1}^{a-1} m \left\lfloor \frac{lm}{a} \right\rfloor + \frac{a}{i^2} M_2(a, l) \right)^{1/2} .$$

Thus,

$$\lim_{c \to \infty} R_2(a; b, c) = \lim_{i \to \infty} R_2(a; b, l+ia) = R_2(a; b, a) \ .$$

Now,

$$aS_2(a; ja, a) = \sum_{m=0}^{a-1} \left\lfloor \frac{mja}{a} \right\rfloor \left\lfloor \frac{ma}{a} \right\rfloor = j \sum_{m=0}^{a-1} m^2 = j \frac{(a-1)a(2a-1)}{6}$$

and

$$aM_2(a;ja) = j^2 \sum_{m=0}^{a-1} m^2 = j^2 \frac{(a-1)a(2a-1)}{6} ,$$

whence

$$R_2(a;ja,a) = 1 \qquad \text{for all } j \geq 1 .$$

We consider now $R_2(a;b,a)$ with $a \to \infty$. Let $a = jb$. For $j \geq 2$

$$R_2(jb;b,jb) = \frac{\sum_{m=j}^{jb-1} m \left\lfloor \frac{m}{j} \right\rfloor}{\left(\sum_{m=j}^{jb-1} \left\lfloor \frac{m}{j} \right\rfloor^2 \frac{(a-1)a(2a-1)}{6} \right)^{1/2}}$$

$$\sum_{m=j}^{jb-1} m \left\lfloor \frac{m}{j} \right\rfloor = \sum_{l=1}^{b-1} l \sum_{m=lj}^{(l+1)j-1} m = \frac{bj(b-1)(4bj+j-3)}{12}$$

$$\sum_{m=j}^{jb-1} \left\lfloor \frac{m}{j} \right\rfloor^2 = j \sum_{l=1}^{b-1} l^2 = j \frac{(b-1)b(2b-1)}{6} .$$

Thus

$$R_2^*(b) = \lim_{j\to\infty} R_2(jb;b,jb) = \lim_{j\to\infty} \frac{(b-1)\left((4b+1)j-3\right)}{2\left((b-1)(2b-1)(jb-1)(2jb-1)\right)^{1/2}} = \frac{\sqrt{2}(b-1)(4b+1)}{4b\sqrt{(b-1)(2b-1)}} .$$

Some values of the limit are given in the table below.

b	$R_2^*(b)$
2	0.918558
3	0.96896
4	0.9836

FIGURE 5. Some values of $R_2^*(b) = \lim_{j\to\infty} R_2(jb;b,jb)$

4.2. **Geometrical correspondence.** Since the Dedekind-like sums $S_2(a;b,c)$ and $M_2(a;b)$ could be considered as inner products, for a given integer $a \geq 3$, we construct within the vector space $\mathbb{R}^{a-1}$ the subspace of all vectors

$$\mathbf{v}_b = \left(\left\lfloor \frac{b}{a} \right\rfloor, \left\lfloor \frac{2b}{a} \right\rfloor, \dots, \left\lfloor \frac{(a-1)b}{a} \right\rfloor \right).$$

As stated earlier, the significance of these vectors to this paper is that $R_2(a;b,c)$ is the cosine of the angle between the two vectors $\mathbf{v}_b$ and $\mathbf{v}_c$. Notice that $\mathbf{v}_1 = \mathbf{0} = (0,\dots,0)$ and $\mathbf{v}_a = (1,2,\dots,a-1)$. For $b = 2,3,\dots,a-1$, the vectors $\mathbf{v}_b$ are

$$\mathbf{v}_2 = (0,\dots,0,1,\dots,1), \mathbf{v}_3 = (0,\dots,0,1,\dots,1,2,\dots,2), \dots, \mathbf{v}_{a-1} = (0,1,\dots,a-2) .$$

Also note that if $b = ka + l$, $k \geq 0$, $0 \leq l < a$, then $\mathbf{v}_b = k\mathbf{v}_a + \mathbf{v}_l$. Since $\mathbf{v}_1 = 0$, we have $\mathbf{v}_{ka} = \mathbf{v}_{ka+1}$. Moreover, if P_l $(2 \leq l \leq a-1)$ denotes the 2-dimensional plane containing the vectors $\mathbf{v}_l$ and $\mathbf{v}_a$, then all the vectors $\mathbf{v}_{ka+l}$, $k = 0,1,\dots$ belong to P_l. Notice that for different values of l, say l and $l' \neq l$, P_l and $P_{l'}$ are two different planes which have the ray

$$R_a = \{c\,\mathbf{v}_a : \ c \geq 0\}$$

in common (see Lemma 3). In Figure 6 we plot the three-dimensional vector space corresponding to $a = 4$. Notice that $\mathbf{v}_2$ and $\mathbf{v}_3$ lie in the same plane but are linearly independent. Also, $\mathbf{v}_4$ is linearly independent of both $\mathbf{v}_2$ and $\mathbf{v}_3$.

FIGURE 6. The vector space for $a = 4$. $\mathbf{v}_2 = (0, 1, 1), \mathbf{v}_3 = (0, 1, 2), \mathbf{v}_4 = (1, 2, 3)$

The vectors $\mathbf{v}_2, \ldots, \mathbf{v}_a$ are not always linearly independent. One can easily check that if $a = 3, 4, 6$ then these vectors are linearly independent, and when $a = 5, 7, 8, 9, \ldots$ they are not. However, one can prove the following:

Lemma 3. *For each $a \geq 4$, the vectors $\mathbf{v}_a, \mathbf{v}_l, \mathbf{v}_{l'}$, where $1 < l, l' < a$ and $l \neq l'$, are linearly independent.*

Proof. For each $a \geq 4$, $\mathbf{v}_a = (1, 2, \ldots, a-1)$, while the first component of both $\mathbf{v}_l$ and $\mathbf{v}_{l'}$ is zero; thus $\mathbf{v}_a$ is linearly independent of $\{\mathbf{v}_l, \mathbf{v}_{l'}\}$. Moreover, $\mathbf{v}_l$ and $\mathbf{v}_{l'}$ do not lie on the same ray. □

Lemma 4. *For each $a \geq 3$, if $b_1 = k_1 a + l$ and $b_2 = k_2 a + l$, where $1 \leq k_1 < k_2$, then*

$$R_2(a; l, a) < R_2(a; l, b_2) < R_2(a; l, b_1)$$

for all $1 < l < a$.

Proof. The vectors $\mathbf{v}_{b_1}$ and $\mathbf{v}_{b_2}$ lie in P_l. Moreover, $\mathbf{v}_{b_1} = k_1 \mathbf{v}_a + \mathbf{v}_l$ and $\mathbf{v}_{b_2} = k_2 \mathbf{v}_a + \mathbf{v}_l$. Hence

$$\angle(\mathbf{v}_l, \mathbf{v}_a) > \angle(\mathbf{v}_{b_1}, \mathbf{v}_a) > \angle(\mathbf{v}_{b_1}, \mathbf{v}_a) \ .$$

But $\angle(\mathbf{v}_b, \mathbf{v}_l) = \angle(\mathbf{v}_a, \mathbf{v}_l) - \angle(\mathbf{v}_a, \mathbf{v}_b)$, and the inequalites in the statement follow by taking cosines. □

Notice that due to the monotonicity stated in the last lemma,

$$\lim_{k \to \infty} R_2(a; l, ka + l) = R_2(a; l, a) \ .$$

It is interesting to notice that in the case of $a = 3$, all vectors $\mathbf{v}_b$ are between $\mathbf{v}_2 = (0, 1)$ and $\mathbf{v}_3 = (1, 2)$. The cosine of the angle between these two vectors is $2/\sqrt{5}$.

Lemma 5. (i) *If $a = 3, 5$ then $R_2(a; 2, b) < R_2(a; 3, b)$ for all $b \geq 3$.*
(ii) *If $a = 4$ then $R_2(4; 2, b) < R_2(4; 3, b)$ for all $b \neq 6$. If $b = 6$ then $R_2(4; 2, 6) = 0.9708$ and $R_2(4; 3, 6) = 0.9647$.*

Proof. (i) The case $a = 3$ follows immediately from Lemma 4. For $a = 5$ we have

$$\begin{aligned}
\mathbf{v}_2 &= (0, 0, 1, 1), \qquad |\mathbf{v}_2| = \sqrt{2} \\
\mathbf{v}_3 &= (0, 1, 1, 2), \qquad |\mathbf{v}_3| = \sqrt{6} \\
\mathbf{v}_4 &= (0, 1, 2, 3), \qquad |\mathbf{v}_4| = \sqrt{14} \\
\mathbf{v}_5 &= (1, 2, 3, 4), \qquad |\mathbf{v}_5| = \sqrt{30} \ .
\end{aligned}$$

Let $(\cdot,\cdot)$ denote the inner product of two vectors. For any $b = 5k + l,\ k = 1, 2, \dots,\ l = 2, 3, 4,$

$$R_2(5; 2, 5k + l) < R_2(5; 3, 5k + l)$$

if and only if

$$\frac{1}{\sqrt{2}} (\mathbf{v}_2, \mathbf{v}_{5k+l}) < \frac{1}{\sqrt{6}} (\mathbf{v}_3, \mathbf{v}_{5k+l}) \ .$$

This is equivalent to

$$\sqrt{6}k\,(\mathbf{v}_2, \mathbf{v}_5) + \sqrt{6}\,(\mathbf{v}_2, \mathbf{v}_l) < \sqrt{2}k\,(\mathbf{v}_3, \mathbf{v}_5) + \sqrt{2}\,(\mathbf{v}_3, \mathbf{v}_l) \ ,$$

or

$$k\left(13\sqrt{2} - 7\sqrt{6}\right) > \sqrt{6}\,(\mathbf{v}_2, \mathbf{v}_l) - \sqrt{2}\,(\mathbf{v}_3, \mathbf{v}_l) \ .$$

Thus, for $l = 2$ the inequality is true for all $k > 0.53$; for $l = 3$ or 4 it is true for all $k \geq 0$. Notice that for $l = 2$, if $k = 0$ then $b = 2$.

(ii) For $a = 4$, if $b = 4k + 2$ then the inequality is true for all $k > 1.72$. For this reason, the inequality between $R_2(4; 2, 6)$ and $R_2(4; 3, 6)$ is reversed. If $b = 4k + 3$ the inequality is true for all $k \geq 0$. □

Empirical evidence suggests that $R_2(a; 2, b) < R_2(a; 3, b)$ for $a \geq 6$ and $b \geq 3$. We do not give a formal proof.

[Possibly inclde the lemma $R_2(a; 2, a) < R_2(a; 3, a)$ here.]

Lemma 6. *For each $a \geq 3$ and each $b, c \geq 2$*

$$R_2(a; b, c) \geq \min\left(R_2(a; l', a), R_2(a; l, a), R_2(a; l', l)\right)$$

where $b \equiv l \mod a,\ c \equiv l' \mod a$.

Proof. If $l, l' \equiv 0, 1 \mod a$, both $\mathbf{v}_b$ and $\mathbf{v}_c$ are on the ray R_a, and $R_2(a; b, c) = 1$.

If $l = l' = 2, \dots, a - 1$ then $\mathbf{v}_b$ and $\mathbf{v}_c$ belong to P_l and $R_2(a; b, c) \geq R_2(a; l, a)$.

Finally, if $l \neq l'$ one establishes the inequality by comparing the arcs on the unit sphere corresponding to the angles. These are the arcs between the points on the sphere on the rays generated by $\mathbf{v}_a$, $\mathbf{v}_l$, $\mathbf{v}_{l'}$, $\mathbf{v}_b$, and $\mathbf{v}_c$. □

To prove Conjecture 1 one has to show that

$$\min_{a\geq 3,\ b,c\geq 2} R_2(a; b, c) \geq R_2(5; 2, 3) \ .$$

Let $R_2^*(a) = \min_{b,c\geq 2} R_2(a; b, c)$. According to Lemma 6, for each $a \geq 3$

$$R_2^*(a) = \min_{1<l,l'<a} \min\left(R_2(a; l', a), R_2(a; l, a), R_2(a; l', l)\right) \ ,$$

whence

$$\min_{a\geq 3,\ b,c\geq 2} R_2(a; b, c) = \min_{a\geq 3} R_2^*(a) \ .$$

In Figure 7 we present a plot of $R_2^*(a)$ for $a = 3, \dots, 53$. We see that in this range, $R_2(5; 2, 3)$ is the minium.

FIGURE 7. $R_2^*(a)$ for $a = 3, \ldots, 53$

5. Upper bounds for generalized Dedekind sums: higher dimensions

5.1. **Probability models.** We introduce now a probability space and random variables, whose (mixed) moments yield the S- and M-functions. Let $\mathcal{D}_d^{(a)}$ be a d-dimensional discrete sample space, consisting of a^d poins, that is,

$$\mathcal{D}_d^{(a)} = \{(m_1, \ldots, m_d) : \ m_j = 0, \ldots, a-1, \ j = 1, \ldots, d\}.$$

A point in $\mathcal{D}_d^{(a)}$ is a d-dimensional vector $\mathbf{m} = (m_1, \ldots, m_d)$. Consider the probability function on $\mathcal{D}_d^{(a)}$,

$$P(\mathbf{m}) = \begin{cases} 1/a & \text{if } \mathbf{m} = j\mathbf{1}_d, \ j = 0, \ldots, a-1, \\ 0 & \text{otherwise.} \end{cases} \tag{16}$$

This probability function is concentrated on the main diagonal points of $\mathcal{D}_d^{(a)}$. Define the random variables

$$X_i^{(a)}(\mathbf{m}; \mathbf{b}) = \begin{cases} \left\lfloor \frac{mb_i}{a} \right\rfloor & \text{if } \mathbf{m} = m\mathbf{1}_d, \ m = 0, \ldots, a-1, \\ 0 & \text{otherwise,} \end{cases} \tag{17}$$

where $\mathbf{b} = (b_1, \ldots, b_d)$. It follows immediately that

$$S_d(a; \mathbf{b}) = E_P \left\{ \prod_{i=1}^d X_i^{(a)}(\mathbf{m}; \mathbf{b}) \right\}, \tag{18}$$

where $E_P\{\ \}$ denotes the expected value of the term in braces with respect to the probability function P. Moreover,

$$M_k(a; b_i) = E_P \left\{ \left(X_i^{(a)}(\mathbf{m}; \mathbf{b}) \right)^k \right\}. \tag{19}$$

Notice that $M_k(a; b_i)$ is the k-th order moment of $X_i^{(a)}(\mathbf{m}; \mathbf{b})$. The Dilcher-Girstmair presentation of the S- and M-functions can be described as moments of the random variables

$$J_i^{(a)}(\mathbf{m}; \mathbf{b}) = \sum_{j=0}^{b_i - 1} j \, I \left\{ \mathbf{m} : \ \frac{ja}{b_i} \le m_i < \frac{(j+1)a}{b_i} \right\}, \ i = 1, \ldots, d, \tag{20}$$

where $I\{\mathbf{m} : \ldots\}$ is the indicator function. According to this definition,

$$S_d(a; \mathbf{b}) = E_P \left\{ \prod_{i=1}^d J_i^{(a)}(\mathbf{m}; \mathbf{b}) \right\} \tag{21}$$

and

$$M_k(a; b_i) = E_P \left\{ \left(J_i^{(a)}(\mathbf{m}; \mathbf{b}) \right)^k \right\}. \tag{22}$$

5.2. **Upper bounds for $S_d(a;\mathbf{b})$.** In the present section we use the random variables $X_i^{(a)}(\mathbf{m};\mathbf{b})$. Since a and $\mathbf{b}$ are fixed, we will simplify the notation to calling the random variables $X_1,\ldots,X_d$. Repeated application of the Cauchy-Schwartz inequality yields bounds in terms of the one-dimensional moments M. For example, for $d=2$ we obtain

$$E\left\{X_1X_2\right\} \le \left(E\left\{X_1^2\right\}E\left\{X_2^2\right\}\right)^{1/2},$$

and thus

$$S_2(a;b_1,b_2) \le \left(M_2(a,b_1)M_2(a,b_2)\right)^{1/2}.$$

For $d=3$ we get

$$E\left\{X_1X_2X_3\right\} \le \left(E\left\{X_1^2\right\}E\left\{X_2^2X_3^2\right\}\right)^{1/2} \le \left(E\left\{X_1^2\right\}\left(E\left\{X_2^4\right\}E\left\{X_3^4\right\}\right)^{1/2}\right)^{1/2}$$

or

$$S_3(a;b_1,b_2,b_3) \le M_2^{1/2}(a,b_1)M_4^{1/4}(a,b_2)M_4^{1/4}(a,b_3)\ . \tag{23}$$

By taking the geometric mean of the cyclical permutations, we get the symmetric upper bound

$$S_3(a;b_1,b_2,b_3) \le \left(\prod_{j=1}^{3} M_2(a,b_j)M_4(a,b_j)\right)^{1/6}.$$

Similarly, we obtain

$$S_4(a;b_1,b_2,b_3,b_4) \le \left(\prod_{j=1}^{4} M_4(a,b_j)\right)^{1/4}. \tag{24}$$

For $d=5$ we start with

$$\begin{aligned} S_5(a;\mathbf{b}) &= E_P\left\{X_1\cdots X_5\right\} \\ &\le \left(E_P\left\{X_1^2X_2^2\right\}\right)^{1/2}\left(E_P\left\{X_3^2X_4^2X_5^2\right\}\right)^{1/2} \\ &\le \left(M_4(a;b_1)M_4(a;b_2)\right)^{1/4}\left(\prod_{j=3}^{5} M_4(a;b_j)M_8(a;b_j)\right)^{1/12} \end{aligned}$$

Symmetrizing this upper bound by taking the geometric mean of the $\binom{5}{2}$ different bounds obtained by different selections of pairs and triplets gives

$$S_5(a;\mathbf{b}) \le \left(\prod_{j=1}^{5} M_4^3(a;b_j)M_8(a;b_j)\right)^{1/20}. \tag{25}$$

From the upper bound for S_3 we immediately obtain

$$S_6(a;\mathbf{b}) \le \left(\prod_{j=1}^{6} M_4(a;b_j)M_8(a;b_j)\right)^{1/12}. \tag{26}$$

Generally, if $d=2k,\ k=1,2,\ldots,$ we have

$$S_{2k}(a;\mathbf{b}) \le \left(E_P\left\{X_1^2\cdots X_k^2\right\}\right)^{1/2}\left(E_P\left\{X_{k+1}^2\cdots X_{2k}^2\right\}\right)^{1/2}, \tag{27}$$

from which we get, by utilizing previous results, symmetric upper bounds. For example,

$$S_8(a;\mathbf{b}) \le \left(M_8(a;b_1)\cdots M_8(a;b_4)\right)^{1/8}\left(M_8(a;b_5)\cdots M_8(a;b_8)\right)^{1/8} = \left(M_8(a;b_1)\cdots M_8(a;b_8)\right)^{1/8}, \tag{28}$$

and

$$S_{10}(a;\mathbf{b}) \le \left(\prod_{j=1}^{10} M_8^3(a;b_j)M_{16}(a;b_j)\right)^{1/40}. \tag{29}$$

We can immediately prove by induction that

$$S_{2^k}(a;\mathbf{b}) \le \left(\prod_{j=1}^{2^k} M_{2^k}(a;b_j)\right)^{1/2^k}, \quad k=1,2,\dots \tag{30}$$

Similarly we get for $k=0,1,\dots$

$$S_{3\cdot 2^k}(a;\mathbf{b}) \le \left(\prod_{j=1}^{3\cdot 2^k} M_{2^{k+1}}(a;b_j)M_{2^{k+2}}(a;b_j)\right)^{1/6\cdot 2^k} \tag{31}$$

and

$$S_{5\cdot 2^k}(a;\mathbf{b}) \le \left(\prod_{j=1}^{5\cdot 2^k} M^3_{2^{k+2}}(a;b_j)M_{2^{k+3}}(a;b_j)\right)^{1/20\cdot 2^k}. \tag{32}$$

If $d=2k+1$ one needs a two-stage process of first partitioning to

$$\left(E_P\left\{\prod_{j=1}^{k} X_j^2\right\}\right)^{1/2}\left(E_P\left\{\prod_{j=1}^{k+1} X_{k+j}^2\right\}\right)^{1/2}$$

and then symmetrizing.

Before concluding this section, we remark that the above upper bounds for the S-functions are generally not unique. By different partitions one can obtain different bounds. For example, in the case of S_5, one could start with

$$E_P\{X_1\cdots X_5\} \le \left(E_P\left\{X_1^2\right\}\right)^{1/2}\left(E_P\left\{X_2^2\cdots X_5^2\right\}\right)^{1/2} = \left(M_2(a;b_1)\right)^{1/2}\left(\prod_{j=2}^{5} M_8(a;b_j)\right)^{1/8}.$$

After symmetrization we get

$$S_5(a;\mathbf{b}) \le \left(\prod_{j=1}^{5} M_2(a;b_j)M_8(a;b_j)\right)^{1/10}. \tag{33}$$

The question is which upper bound should be used, (25) or (33)? For example, if $a=31$ and $\mathbf{b}=(3,5,7,11,13)$ then $S_5(a;\mathbf{b})=1213.806$. The upper bound given by (25) is 1321.321, whereas that given by (33) is 1456.985. In the following table we present some exact values of $S_5(a;\mathbf{b})$ and the two bounds (25) and (33). We also show $R_5(a;\mathbf{b})$, the ratio of $S_5(a;\mathbf{b})$ to the upper bound (25).

a	$\mathbf{b}$	S_5	bound (25)	bound (33)	R_5
31	(3, 5, 7, 11, 13)	1213.806	1321.321	1456.985	0.9186
21	(5, 7, 9, 11, 13)	4411.333	4668.719	5190.201	0.9449
23	(5, 9, 11, 13, 17)	11429.74	12050.58	13385.72	0.9485
27	(5, 11, 13, 17, 21)	28101.93	29617.94	33011.8	0.9488
33	(7, 11, 13, 19, 23)	51943.76	54384.26	60525.59	0.9551

FIGURE 8. Some values and bounds of S_5

It seems from Figure 8 that the upper bound given by (25) is closer to the exact value of $S_5(a;\mathbf{b})$ than (33). It is the preferred upper bound. It is also interesting that, like in the case of $R_2(a;\mathbf{b})$, all values of $R_5(a;\mathbf{b})$ in Figure 8 are greater than 0.9186.

5.3. **Relationships to upper bounds revisited.** We study now upper bounds to S_d of the type given by (23)–(32). In particular, define

$$R_3(a;\mathbf{b}) = \frac{S_3(a;\mathbf{b})}{\left(\prod_{j=1}^{3} M_2(a,b_j)M_4(a,b_j)\right)^{1/6}} , \tag{34}$$

$$R_4(a;\mathbf{b}) = \frac{S_4(a;\mathbf{b})}{\left(\prod_{j=1}^{4} M_4(a,b_j)\right)^{1/4}} , \text{ and} \tag{35}$$

$$R_5(a;\mathbf{b}) = \frac{S_5(a;\mathbf{b})}{\left(\prod_{j=1}^{5} M_4^3(a;b_j)M_8(a;b_j)\right)^{1/20}} . \tag{36}$$

A few values of $R_5(a;\mathbf{b})$ are given in in Figure 8. It seems that the minimal $R_5(a;\mathbf{b})$ value is $R_5(7;2,3,4,5,6) = 0.8567$. It is also interesting to observe that R_5, as shown in Figure 8, is generally above 0.9, as in the case of R_2, despite the increase in dimension from 2 to 5. We try to explain this phenomenon in probability terms.

As shown in (18) and (21),

$$S_d(a;\mathbf{b}) = E_P\left\{X_1\cdots X_d\right\} = E_P\left\{J_1\cdots J_d\right\} .$$

Consider the case $d=2$. According to the law of iterated expectation [2],

$$S_2(a;b_1,b_2) = E_P\left\{J^{(a)}(\mathbf{m};b_1)E_P\left\{J^{(a)}(\mathbf{m};b_2) \mid J^{(a)}(\mathbf{m};b_1)\right\}\right\} , \tag{37}$$

where the second term on the right-hand side is the *conditional expectation* of $J^{(a)}(\mathbf{m};b_2)$, given $J^{(a)}(\mathbf{m};b_1)$. Notice that in the notation of Section 2,

$$S_2(a;b,c) = \frac{1}{a}\sum_{j=0}^{b-1}\sum_{l=0}^{c-1} jl f_{a;b,c}(j,l) = \frac{1}{a}\sum_{j=0}^{b-1} j f_{a;b}(j)\sum_{l=0}^{c-1} l\frac{f_{a;b,c}(j,l)}{f_{a;b}(j)} . \tag{38}$$

The key to understanding the phenomenon is that the joint frequencies $f_{a;b,c}(j,l)$ are distributed along the main diagonal, as illustrated in Figure 2. In the special case that $b=c$,

$$f_{a;b,c}(j,l) = \begin{cases} f_{a;b}(j) = f_{a;c}(j) & \text{if } j \neq l, \\ 0 & \text{otherwise.} \end{cases}$$

In this case,

$$\sum_{l=0}^{b-1} l \frac{f_{a;b,c}(j,l)}{f_{a;b}(j)} = j$$

and

$$S_2(a;b,b) = \frac{1}{a}\sum_{j=0}^{b-1} j^2 f_{a;b}(j) = M_2(a;b) \ ,$$

as expected. When $b \neq c$ then R_2 is always smaller than 1, but might be quite close to it, even when b and c are different. For example, $R_2(50;7,13) = 0.9955$.

5.4. **One-dimensional moments relationships.** We present here some inequalities between $M_r(a;b)$ for fixed values of a and b. First, by Liapounov's inequality of moments [7, p. 627] we have

$$M_1 < M_2^{1/2} < M_3^{1/3} < \dots$$

By factoring $\lfloor \dots \rfloor^{2k+1} = \lfloor \dots \rfloor^{k} \lfloor \dots \rfloor^{k+1}$ we obtain the inequality

$$M_{2k+1}^2(a;b) < M_{2k}(a;b)M_{2k+2}(a;b)$$

for all $k \geq 1$. In particular one obtains

$$\frac{M_{2k+1}(a;b)}{M_{2k+2}(a;b)} < \frac{M_{2k}(a;b)}{M_{2k+1}(a;b)}$$

for all $k \geq 1$. Accordingly,

$$2\log M_{2k+1}(a;b) + \log M_{2k}(a;b) + \log M_{2k+2}(a;b) > 0 \ ,$$

that is, $M_k(a;b)$ is log-convex in k.

Appendix

Algorithm for Determining $f_b^a(i),\ i = 0, \dots, b-1$

```
STEP 0:
Set:
(i) r = a/b;
(ii) l = a-b*[r];
(iii) f = 0(1,b);          # b-dimensional vector of zeros

STEP 1:

Compute:
f [0] <- 1+[r];
f [ i ] <- [(i+1)*r]- [i*r], i=1,..,(b-2);
f [ b-1] <- a-1- [(b-1)*r];

STEP 2:

IF((l=0) or (b=2)) { GOTO STEP 3 };
ELSE {
```

```
FOR ( i=1,...,b-2) {
IF( [(i+1)*r] = r*(i+1) ) {
f[i] <- f[i]-1;
f[i+1] <- f[i+1]+1;
}
}

STEP 3:

PRINT f

END.
```

Algorithm for Determining $f^a_{bc}(i,j)$

```
STEP 0:

Set:
r1 <- a/b;
r2 <- a/c;
l1 <- a -b*[r1];
l2 <- a - c*[r2];
  CT <- O((b+1),(c+1));    # matrix of zeros, of dimensions (b+1)*(c+1)
t1 <- O(b,1);
t2 <- O(1,c);

STEP 1:

Compute:
CT[i,(c+1)] <- f_b[i-1], i=1,...,b;
CT[(b+1), j] <- f_c[j-1], j=1,...,c;
CT[(b+1),(c+1)] <- a;
CT[1,1] <- min( CT[1,c+1], CT[b+1,1]);
t2[1] <- t2[1] + CT[1,1];

STEP 2:

Compute:
FOR (i=2,...,b) {
CT[i,1] <- max(0, min(f_c[1]-t2[1], f_b[i-1])));
t2[1] <- t2[1] + CT[i,1];
}
t1 <- CT[1:b,1];

STEP 3:

Compute:
FOR (j=2,...,c) {
CT[1,j] <- max(0,min(f_b[0]-t1[1], f_c[j-1]));
t1[1] <- t1[1] + CT[1,j];
t2[j] <- t2[j] + CT[1,j];
```

```
}

STEP 4:

Compute:
FOR (i=2,...,b) {
FOR(j=2,...,c) {
cty<- max(0, min(f_b[i-1]- t1[i], f_c[j-1]));
ctx <- max(0, min(f_c[j-1]-t2[j], f_b[i-1]));
CT[i,j] <- min(ctx,cty)
t1[ i ] <- t1 [ i ]+  CT [ i, j];
t2[ j ] <- t2 [ j ] + CT [i , j];
}
}

STEP 5:
Print CT

END.
```

References

1. Matthias Beck and Sinai Robins, *Dedekind sums: a combinatorial-geometric viewpoint*, Preprint (arXiv:math.NT/0112076), to appear in DIMACS: Series in Discrete Mathematics and Theoretical Computer Science (2002).
2. Peter J. Bickel and Kjell A. Doksum, *Mathematical statistics*, Holden-Day Inc., San Francisco, Calif., 1976, Basic ideas and selected topics, Holden-Day Series in Probability and Statistics. MR 56 #1513
3. R. Dedekind, *Erläuterungen zu den Fragmenten xxviii*, Collected works of Bernhard Riemann, Dover Publ., New York, 1953, pp. 466–478.
4. Karl Dilcher and Kurt Girstmair, *Dedekind sums and uniform distributions*, Amer. Math. Monthly **109** (2002), no. 3, 279–284.
5. F. Hirzebruch and D. Zagier, *The Atiyah-Singer theorem and elementary number theory*, Publish or Perish Inc., Boston, Mass., 1974, Mathematics Lecture Series, No. 3. MR 58 #31291
6. Donald E. Knuth, *The art of computer programming. Vol. 2*, second ed., Addison-Wesley Publishing Co., Reading, Mass., 1981, Seminumerical algorithms, Addison-Wesley Series in Computer Science and Information Processing. MR **83i:**68003
7. Samuel Kotz, Norman L. Johnson, and Campbell B. Read (eds.), *Encyclopedia of statistical sciences. Vol. 4*, John Wiley & Sons Inc., New York, 1983, Icing the tails to Limit theorems, Lecture Notes in Economics and Mathematical Systems, 192. MR **84k:**62001b
8. C. Meyer, *Über einige Anwendungen Dedekindscher Summen*, J. Reine Angew. Math. **198** (1957), 143–203. MR 21 #3396
9. L. J. Mordell, *Lattice points in a tetrahedron and generalized Dedekind sums*, J. Indian Math. Soc. (N.S.) **15** (1951), 41–46. MR 13,322b
10. Hans Rademacher and Emil Grosswald, *Dedekind sums*, The Mathematical Association of America, Washington, D.C., 1972, The Carus Mathematical Monographs, No. 16. MR 50 #9767

Department of Mathematical Sciences, Binghamton University (SUNY), Binghamton, NY 13902-6000, USA
E-mail address: matthias@math.binghamton.edu

Department of Mathematics, Temple University, Philadelphia, PA 19122, USA
E-mail address: srobins@math.temple.edu

Department of Mathematical Sciences, Binghamton University (SUNY), Binghamton, NY 13902-6000, USA
E-mail address: shelly@math.binghamton.edu