

THE MOTIF PROBLEM: GEOMETRIC REPRESENTATIONS OF SETS OF EQUIVALENCE RELATIONS

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A *motif* is a sequence of L points in \mathbb{R}^p satisfying certain equality conditions between specified coordinates, which are described by a *motif specification*. In this sense a motif is a geometric representation of p equivalence relations on subsets of $\{1, \dots, L\}$. The main problem considered here is to count the number of motifs that can be made using points from a given r -element subset of \mathbb{R}^p . Our principal results are as follows: The number of motifs is bounded above by $r^{\tau^*(H)}$, where $\tau^*(H)$ is an invariant called the fractional transversal number of a hypergraph, H , which is determined by the motif specification. On the other hand, we show that there are arbitrarily large subsets where the number of motifs is at least $(r/L)^{\tau^*(H)}$. We obtain more precise optimization results for two special types of motifs (*uniform* motifs and *single-starred* motifs). For uniform motifs, we show that our upper bound can be attained and characterize the subsets (called *grids*) which achieve the upper bound. We prove similar results for single-starred motifs, in which case sufficiently large subsets containing the maximum number of motifs must be contained in a union of a predetermined number of lines, the number depending only on the motif specification.

1. INTRODUCTION

We begin with an analysis of a special case of the motif problem which illustrates the counting problem that concerns us. For this introduction, let a *motif* be a quadruple of four points (a, b, c, d) in \mathbb{R}^3 that lie on pairwise non-adjacent vertices

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of a parallelepiped with edges parallel to the x -, y -, and z -axes, as shown in Figure 1. We allow the parallelepiped to be a reflection of the one shown here, or to be degenerate, so that the only constraint on a motif is that there are certain equality constraints between the coordinates of a , b , c , and d ; we require the x coordinates of a and c to be the same, the y coordinates of b and c to be the same, and so on, as shown in the table in Figure 1. (The term is not to be confused with the notion of motif as used in algebraic geometry.)

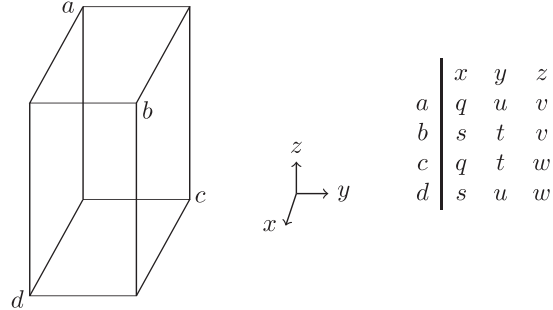


Figure 1. A motif.

Given a set \mathcal{S} of r distinct points in \mathbb{R}^3 , how many motifs can be made out of the points in \mathcal{S} ? We will show that there can be at most r^2 . Foliate \mathbb{R}^3 by planes parallel to the xy -plane, and suppose that there are n such planes, P_1, \dots, P_n , say, that contain points of \mathcal{S} , containing r_1, \dots, r_n points of \mathcal{S} , respectively. We may order the planes so that $r_1 \geq \dots \geq r_n > 0$. Now, in any motif, a and b must be contained in the same plane, P_i say, and c and d must be in the same plane, P_j , say. If $i \leq j$, then fix j , and observe that a and b are determined by c , d , and i ; there are then at most j ways of choosing i , and r_j^2 ways of choosing c and d , so our choice of j contributes at most jr_j^2 motifs. On the other hand, if $i > j$, fix i , and observe that c and d are determined by a , b , and j , and that there are at most $i - 1$ ways of choosing j , so our choice of i contributes at most $(i - 1)r_i^2$ motifs. Therefore, the total number of motifs possible is no more than

$$\begin{aligned} \sum_{1 \leq j \leq n} jr_j^2 + \sum_{2 \leq i \leq n} (i - 1)r_i^2 &= \sum_{1 \leq i \leq n} (2i - 1)r_i^2 \\ &\leq \sum_{1 \leq i \leq n} r_i(2r_1 + \dots + 2r_{i-1} + r_i) \\ &= (r_1 + \dots + r_n)^2 = r^2, \quad \text{as desired.} \end{aligned}$$

On the other hand, if we choose \mathcal{S} to be all points in a three-dimensional grid of A points by B points by C points, \mathcal{S} will have size $r = ABC$ and will admit $A^2B^2C^2 = r^2$ motifs. This shows that the upper bound r^2 is optimal.

In Section 2, we will generalize this definition by considering a motif to be a sequence of L points in \mathbb{R}^p satisfying certain coordinate equality conditions given

by a *motif specification*. For any motif specification, we define H , its associated hypergraph. In Theorem 5, we prove that the number of motifs that can be made from sequences of points taken from a given set \mathcal{S} of size r is bounded above by $r^{\tau^*(H)}$, where $\tau^*(H)$ is the fractional transversal number of H .

In Section 3, we define and study the class of *uniform* motifs, which are a subclass of those for which all edges of H are of the same size, n , say. In Theorem 7, we show that the maximum number of uniform motifs generated from a set \mathcal{S} of size r in \mathbb{R}^p is bounded above by $r^{L/n}$ and that, after normalization of the motif specification, this maximum is assumed if and only if \mathcal{S} is a *grid*, i.e., \mathcal{S} is of the form $\mathcal{S}_1 \times \cdots \times \mathcal{S}_q$, where $\mathcal{S}_i \subseteq \mathbb{R}^{p_i}$ for each $i = 1, \dots, q$, and p_1, \dots, p_q are as defined below in Section 3.

In Section 4, we define and study the special class of *single-starred* motifs. In Theorem 12, we show that the maximum number of single-starred motifs in a set \mathcal{S} of size r is asymptotic to $\mathcal{C}r^L$, where \mathcal{C} is a constant determined by the motif specification. If r is large enough, we also characterize the structure of the sets \mathcal{S} with a maximum number of motifs. We close the paper with some questions.

2. MOTIFS AND MOTIF SPECIFICATIONS

We generalize the notion of motif to L -tuples of points in \mathbb{R}^p as follows: given positive integers L and p , call a *motif specification on p, L* a sequence π_1, \dots, π_p of partitions of subsets of $\{1, \dots, L\}$, together with constants $D_{im} \in \mathbb{R}$ for each pair (i, m) such that $i \in \{1, \dots, L\}$, $m \in \{1, \dots, p\}$, and i is in no block of π_m . A tuple $(f_1, \dots, f_L) \in (\mathbb{R}^p)^L$ will then be a *motif* (for that specification) if:

1. Whenever $i, j \in \{1, \dots, L\}$ are in the same block of π_m , for some $m \in \{1, \dots, p\}$, then $(f_i)_m = (f_j)_m$.
2. Whenever $i \in \{1, \dots, L\}$ is in no block of π_m , for some $m \in \{1, \dots, p\}$, then $(f_i)_m = D_{im}$.

Thus, a motif in \mathbb{R}^p is a geometric representation of p equivalence relations on subsets of $\{1, \dots, L\}$. As far as we can determine, this is the first time this notion has been introduced and studied.

Given a subset $\mathcal{S} \subseteq \mathbb{R}^p$ and a motif specification, we let $\mathcal{M}(\mathcal{S})$ be the number of motifs in \mathcal{S} , i.e., the number of L -tuples of elements of \mathcal{S} that are motifs. We want to know how large $\mathcal{M}(\mathcal{S})$ can be for a set \mathcal{S} of given size. To state and prove an estimate for this, we make the following definitions:

- Let the *hypergraph of a motif specification* be the hypergraph with vertex set $\{1, \dots, L\}$ and an edge for each block of each partition π_1, \dots, π_p , such that each edge is incident on the vertices that are elements of the corresponding block. The hypergraph may have loops, i.e., edges which are incident on just one vertex; also, different edges may be incident on the same set of vertices.

- Given a hypergraph H , let $V(H)$ be the set of its vertices and $E(H)$ be the set of its edges. We write $x \in e$ if the edge e is incident on the vertex x .
- [1] A hypergraph is *uniform* if all its edges have the same size.
- [3][1] A *fractional transversal* g of a hypergraph H is a function $g : V(H) \rightarrow \mathbb{R}_{\geq 0}$ such that $\sum_{x: x \in e} g(x) \geq 1$ for all $e \in E(H)$. We call $\sum_x g(x)$ the *total weight* of g .
- [3][1] The *fractional transversal number*, $\tau^*(H)$, of a hypergraph H is defined to be

$$\tau^*(H) := \min \left\{ \sum_x g(x) \mid g \text{ a fractional transversal of } H. \right\}$$

- [3][1] A *fractional matching* f of a hypergraph H is a function $f : E(H) \rightarrow \mathbb{R}_{\geq 0}$ such that $\sum_{e: x \in e} f(e) \leq 1$ for all $x \in V(H)$. We call $\sum_e f(e)$ the *total weight* of f . (The function f may assign different weights to different edges which are incident on the same set of vertices.)
- [3][1] The *fractional matching number*, $\nu^*(H)$, of a hypergraph H is defined to be

$$\nu^*(H) := \max \left\{ \sum_e f(e) \mid f \text{ a fractional matching of } H. \right\}$$

- Given any $m > 0$ and a function $F : \mathbb{R}^m \rightarrow \mathbb{R}$ which is nonzero only at finitely many places in \mathbb{R}^m , write $*$ for an argument of F in order to denote summing over that argument:

$$G(*) = \sum_{a \in \mathbb{R}} G(a),$$

$$F(*, *, c) = \sum_{a, b \in \mathbb{R}} F(a, b, c), \quad \text{etc.}$$

Given a hypergraph H and a function $g : V(H) \rightarrow \mathbb{R}_{\geq 0}$, duplicating an edge in H does not add a new constraint which g must satisfy to be a fractional transversal, but adds a copy of an existing constraint. This does not change the minimum possible total weight of g , so, if the hypergraph H' is obtained from H by omitting duplicate edges, then $\tau^*(H') = \tau^*(H)$. Similarly, in a fractional matching f of a hypergraph H , moving weight between multiple edges which are incident on the same set of vertices does not change the total weight of f , and also does not change whether f is a fractional matching. Therefore, a maximum total weight fractional matching can always be constructed which has zero weight on all but one edge of every set of multiple edges, and, if the hypergraph H' is obtained from H by omitting duplicate edges, then $\nu^*(H') = \nu^*(H)$.

Theorem 1. [3][1] *For all hypergraphs H , $\tau^*(H) = \nu^*(H)$. Also, if a fractional transversal and fractional matching of H have the same total weight w , then $w = \tau^*(H) = \nu^*(H)$.*

Proof. If M is the incidence matrix of H , $\tau^*(H)$ is the optimal value for the linear programming problem of minimizing $\mathbf{1}^T \mathbf{x}$, where $\mathbf{x} \geq 0$ and $M\mathbf{x} \geq \mathbf{1}$. Also, $\nu^*(H)$ is the optimal value for the linear programming problem of maximizing $\mathbf{1}^T \mathbf{y}$, where $\mathbf{y} \geq 0$ and $M^T \mathbf{y} \leq \mathbf{1}$. However, these problems are dual, so they have the same optimal value and $\tau^*(H) = \nu^*(H)$. The second claim now follows from the definitions of τ^* and ν^* . \square

In the case of our introductory example, $L = 4$ and $p = 3$, and the motif specification uses partitions $\pi_1 = \{\{1, 3\}, \{2, 4\}\}$, $\pi_2 = \{\{1, 4\}, \{2, 3\}\}$, and $\pi_3 = \{\{1, 2\}, \{3, 4\}\}$. The hypergraph H is therefore a complete graph on 4 vertices, and one fractional transversal of H is the function g_0 that takes all vertices to $1/2$. Similarly, one fractional matching of H is the function f_0 that takes all edges to $1/3$. Since these have the same total weight, 2, we see that $\tau^*(H) = \nu^*(H) = 2$, and that g_0 and f_0 are optimal.

We can now prove an upper bound on $\mathcal{M}(\mathcal{S})$. We use the following two inequalities from the literature.

Lemma 2 (Hölder's inequality). *Let $m \geq 0$ and $n > 0$, and suppose that we are given mn nonnegative real numbers x_{ij} , $i = 1, \dots, m$, $j = 1, \dots, n$, and n positive real numbers h_1, \dots, h_n such that $h_1 + \dots + h_n = 1$. Then*

$$\sum_{1 \leq i \leq m} x_{i1}^{h_1} x_{i2}^{h_2} \cdots x_{in}^{h_n} \leq \left(\sum_{1 \leq i \leq m} x_{i1} \right)^{h_1} \cdots \left(\sum_{1 \leq i \leq m} x_{in} \right)^{h_n}.$$

Also, equality holds if and only if either the vector $(x_{ij})_{1 \leq i \leq m}$ is zero for some j or the vectors $(x_{i1})_{1 \leq i \leq m}, \dots, (x_{in})_{1 \leq i \leq m}$ are all proportional.

Proof. This is [2, Theorem 11]; or, use [4, Problem 9.1] and induce on n .

Lemma 3. *Let $m \geq 0$, and suppose that we are given $r > 1$ and m nonnegative real numbers, x_1, \dots, x_m . Then*

$$x_1^r + \cdots + x_m^r \leq (x_1 + \cdots + x_m)^r.$$

Proof. [2, Theorem 19] If $x_1 = \cdots = x_m = 0$, the result is clear. Otherwise, both sides are homogeneous in x_1, \dots, x_m of degree r , so by rescaling we may assume that $x_1 + \cdots + x_m = 1$. Then, for each i , $x_i^r \leq x_i \leq 1$, so $x_1^r + \cdots + x_m^r \leq x_1 + \cdots + x_m = 1$, as desired. \square

Take 0^0 to be 1.

Lemma 4. *Given some $n > 0$, functions $F_1, \dots, F_n : \mathbb{R} \rightarrow \mathbb{R}_{\geq 0}$ each of which is nonzero at most at only finitely many places, and exponents $h_1, \dots, h_n \geq 0$ such that $h_1 + \dots + h_n \geq 1$, then*

$$\sum_{a \in \mathbb{R}} F_1(a)^{h_1} \dots F_n(a)^{h_n} \leq F_1(*)^{h_1} \dots F_n(*)^{h_n}.$$

Proof. Zero exponents do not contribute to the product on either side, so discard them, and assume that $h_i > 0$ for all i . Then, in the case where $\sum_i h_i = 1$, the inequality is Lemma 2. Otherwise, it follows from applying the $\sum_i h_i = 1$ case to the functions $F_1^{h_1+\dots+h_n}, \dots, F_n^{h_1+\dots+h_n}$ and exponents $h_1/(h_1 + \dots + h_n), \dots, h_n/(h_1 + \dots + h_n)$ and then applying Lemma 3 with $r = h_1 + \dots + h_n$.

Theorem 5. *Given any motif specification on p, L , let H be its hypergraph, and let \mathcal{S} be a subset of \mathbb{R}^p with size r . Then $\mathcal{M}(\mathcal{S}) \leq r^{\tau^*(H)}$.*

Proof. Let $I : \mathbb{R}^p \rightarrow \{0, 1\}$ be the indicator function of \mathcal{S} . Fix a motif specification. Any motif can then be written as an L by p matrix of coordinates whose entries are variables and constants, where there is one variable for each block of each π_i , and the constants are the D_{im} 's, placed in the appropriate spots of the matrix. For instance, for the motif specification used in the introduction, the matrix will be a 4 by 3 matrix containing six variables, as shown on the right-hand side of Figure 1. In general, we may suppose that we use variables v_1, \dots, v_n , and we can then write the number of motifs in \mathcal{S} as

$$(1) \quad \mathcal{M}(\mathcal{S}) = \sum_{v_1, \dots, v_n \in \mathbb{R}} I(R_1) \dots I(R_L),$$

where R_1, \dots, R_L are p -tuples of variables and constants obtained from reading off the rows of the matrix. Now, taking the number 0 or 1 and raising it to an arbitrary nonnegative power will not decrease it. So, from (1), we find that the number of motifs in \mathcal{S} is no more than

$$(2) \quad Y = \sum_{v_1, \dots, v_n \in \mathbb{R}} I(R_1)^{g(1)} \dots I(R_L)^{g(L)},$$

where g is an optimal fractional transversal of H . For example, using the matrix in Figure 1 and the optimal fractional transversal g_0 mentioned above, (2) will take the form

$$Y = \sum_{q, s, t, u, v, w \in \mathbb{R}} I(q, u, v)^{1/2} I(s, t, v)^{1/2} I(q, t, w)^{1/2} I(s, u, w)^{1/2}.$$

Now, observe that any given variable in the sum (2) corresponds to an edge, e , say, of H , and that the sum of the exponents of the $I(R_i)$'s in which this variable

appears equals $\sum_{x: x \in e} g(x)$, which, by the definition of a fractional transversal, is at least 1. We can therefore apply Lemma 4 to eliminate the sum over this variable, replacing it by $*$ wherever it appears. This will not decrease the value of (2). In the case given in Figure 1, for example, we observe that

$$\sum_q I(q, u, v)^{1/2} I(q, t, w)^{1/2} \leq I(*, u, v)^{1/2} I(*, t, w)^{1/2}$$

and so

$$Y \leq \sum_{s, t, u, v, w \in \mathbb{R}} I(*, u, v)^{1/2} I(s, t, v)^{1/2} I(*, t, w)^{1/2} I(s, u, w)^{1/2}.$$

If we repeat this operation until all variables are removed, we will find that

$$Y \leq I(R'_1)^{g(1)} \dots I(R'_L)^{g(L)},$$

where each R'_i is a p -tuple each of whose elements is either a constant or $*$. Since each $I(R'_i)$ can be no bigger than r , this shows that \mathcal{S} has no more than $r^{\tau^*(H)}$ motifs, as desired. \square

We can also prove a lower bound which shows that in infinitely many cases, this upper bound is best possible, up to a constant factor.

Theorem 6. *Given any motif specification on p, L , let H be its hypergraph. Then, for all $N > 0$, there exists a subset \mathcal{S} of \mathbb{R}^p such that the size, r , of \mathcal{S} is at least N , and $\mathcal{M}(\mathcal{S}) \geq (r/L)^{\nu^*(H)}$.*

Proof. Let f be an optimal fractional matching of H . We may assume all of the values of f are rational, since we are taking the minimum of a linear function with rational coefficients over a rational polytope. If $f(e) = 0$ for all edges e of H , then $\nu^*(H) = 0$ and the theorem is trivial, since it reduces to saying that there exist arbitrarily large sets with at least one motif. Otherwise, f has at least one positive value. Let $d > 0$ be a common multiple of the denominators of all positive values of f , and write down the L by p matrix of coordinates, as we did in Theorem 5. Now, fix a positive integer M , and let each variable v in the matrix of coordinates run over $M^{df(e)}$ values, where e is the edge of H corresponding to v . The number of values taken on by the row of the matrix corresponding to the vertex x will then be $M^{d \sum_{e: x \in e} f(e)}$, which, by the definition of a fractional matching, is at most M^d . Therefore, taking the set of all possible rows of the matrix will construct a set \mathcal{S} with size at most LM^d . Also, we must have $\sum_{e: x \in e} f(e) = 1$ for at least one vertex x , since if not, we could increase any $f(e)$ slightly and still have a fractional matching, contradicting optimality of f . It follows that the size of \mathcal{S} must be at least M^d . Finally, the number of motifs in \mathcal{S} is at least $M^{d \sum_e f(e)} = M^{d\nu^*(H)}$. Letting M become large completes the proof.

REMARK. Start with the matrix of coordinates used in Theorems 5 and 6, and make a tableau by leaving the constants in the matrix unchanged, but replacing each variable v with the indeterminate $X_{f(e)}$, where e is the edge of H corresponding to v , and f is some optimal fractional matching of H . Then it follows from the proof of Theorem 6 that Theorem 6 may be improved by replacing L with L' , where L' is the number of distinct rows in the tableau.

3. UNIFORM MOTIFS AND GRIDS

Suppose that the motif specification contains no constants and that its hypergraph is uniform, i.e., all blocks in all partitions have the same size, n , say. We may then reorder the coordinates of \mathbb{R}^p so as to place each set of identical partitions in the specification into a contiguous range; let there be q such ranges, with lengths, in order, p_1, \dots, p_q ($p_1 + \dots + p_q = p$).

Theorem 7. *Let a motif specification on p, L have no constants and a uniform hypergraph, with edge size n , and let its coordinates be ordered as above. Then, for all $r \geq 0$, the maximum number of motifs in a subset \mathcal{S} of \mathbb{R}^p of size r is always $r^{L/n}$, and this maximum is attained iff \mathcal{S} is a grid, i.e., \mathcal{S} is of the form*

$$(3) \quad \mathcal{S}_1 \times \dots \times \mathcal{S}_q, \text{ where } \mathcal{S}_i \subseteq \mathbb{R}^{p_i} \text{ for each } i = 1, \dots, q.$$

Proof. If $\pi_i = \pi_j$, then coordinates i and j of \mathbb{R}^p can be lumped together and treated as a single coordinate. Doing this repeatedly, we reduce to the case where $q = p$ and $p_1 = \dots = p_q = 1$.

If we let g have value $1/n$ on each vertex, then g is a fractional transversal of the hypergraph H of the motif specification. Also, if we let f have value $1/p$ on each edge, then f is a fractional matching of H . However, f and g both have weight L/n . It follows that $\tau^*(H) = \nu^*(H) = L/n$. Now, if we let \mathcal{S} contain r points which have all coordinates zero except the first, the first coordinate ranging over $1, \dots, r$, then \mathcal{S} will have exactly $r^{L/n}$ motifs. Together with Theorem 5, this proves that the maximum number of motifs in a set of size r is $r^{L/n}$.

If \mathcal{S} is of the form (3), then write down the L by p matrix of coordinates referred to in Theorem 5. We can obtain a motif in \mathcal{S} by, for each i , substituting an arbitrarily chosen element of \mathcal{S}_i for each variable in column i . If each set \mathcal{S}_i has size r_i ($i = 1, \dots, p$), it follows that \mathcal{S} contains at least

$$\prod_{1 \leq i \leq p} r_i^{L/n} = \left(\prod_{1 \leq i \leq p} r_i \right)^{L/n} = r^{L/n}$$

motifs. It remains to prove that any set which attains the maximum number of motifs for its size is of the form (3).

Suppose that \mathcal{S} is a set which attains the maximum number of motifs for its size, and let \mathcal{S} have indicator function $I : \mathbb{R}^p \rightarrow \mathbb{R}$. We may assume that \mathcal{S} is nonempty, as otherwise the result is trivial. Now, as in the proof of Theorem 5, we

construct a chain of inequalities starting from $\mathcal{M}(\mathcal{S})$ and ending at $r^{L/n}$. To have $r^{L/n}$ motifs in \mathcal{S} , all these inequalities must be equalities. Looking at the matrix of coordinates, we see that a new inequality appears in the chain whenever we remove a variable and replace it by $*$. Since we can choose to remove the variables in any order, it follows that we must have

$$(4) \quad \sum_z I(R_1)^{1/n} \cdots I(R_L)^{1/n} = I(R'_1)^{1/n} \cdots I(R'_L)^{1/n},$$

whenever R_1, \dots, R_L result from taking the rows of the matrix of coordinates and substituting each variable by either a real number, $*$, or the variable z , and the R'_i 's are derived from the R_i 's by substituting $*$ for z .

We prove that there is a constant $C > 0$ (namely $C = I(*, \dots, *) = r$), and functions $F_1, \dots, F_p : \mathbb{R} \rightarrow \mathbb{R}_{\geq 0}$, each zero except at finitely many points, such that

$$(5) \quad I(b_1, \dots, b_p) = CF_1(b_1) \cdots F_p(b_p), \quad \text{for all } b_1, \dots, b_p \in \mathbb{R}.$$

We will do this by inducing on s to prove the statement that, for all $s = 0, \dots, p$,

$$(6) \quad I(b_1, \dots, b_s, *, \dots, *) = CF_1(b_1) \cdots F_s(b_s), \quad \text{for all } b_1, \dots, b_s \in \mathbb{R},$$

for functions F_1, \dots, F_p which we construct in the course of the induction.

If $s = 0$, this is clear, with the given value of C , since there are no functions F_i . Otherwise, assume that (6) has been proved for $s = t - 1$. We wish to prove it for $s = t$. Fix some c_1, \dots, c_{t-1} such that $I(c_1, \dots, c_{t-1}, *, \dots, *) > 0$, and set

$$F_t(z) := \frac{I(c_1, \dots, c_{t-1}, z, *, \dots, *)}{I(c_1, \dots, c_{t-1}, *, *, \dots, *)}, \quad z \in \mathbb{R}.$$

We now induce secondarily on the number of coordinates j in $\{1, \dots, t-1\}$ for which $b_j \neq c_j$. Let this number be m . We have already proved (6) for $s = t$ and $m = 0$. Suppose that it has been proved for $s = t$ and $m = 0, \dots, m' - 1$. We wish to prove it for $s = t$ and $m = m'$. Fix some b_1, \dots, b_{t-1} which differ from the c_i 's in exactly m' places. Assume that $I(b_1, \dots, b_{t-1}, *, \dots, *) > 0$; if not, by (6) for $s = t - 1$, at least one of $F_1(b_1), \dots, F_{t-1}(b_{t-1})$ must be zero, so both sides of (6) are zero and we are done. Pick some $i \in \{1, \dots, t-1\}$ for which $b_i \neq c_i$, and set $b'_j = b_j$ if $j \neq i$ and $j \in \{1, \dots, t-1\}$, $b'_i = c_i$. We now fill in the matrix of coordinates with four different possibilities for a row:

$$\begin{aligned} R''_1 &= (b_1, \dots, b_{t-1}, z, *, \dots, *), \\ R''_2 &= (b'_1, \dots, b'_{t-1}, z, *, \dots, *), \\ R''_3 &= (b_1, \dots, b_{t-1}, *, *, \dots, *), \quad \text{and} \\ R''_4 &= (b'_1, \dots, b'_{t-1}, *, *, \dots, *). \end{aligned}$$

The rows are determined as follows. By assumption, $\pi_i \neq \pi_t$, so we can find some u and v which are in the same block of π_t but different blocks of π_i . We set $R_w := R''_1$

for each row w such that w is in the same block of π_t as u and v , and w is in the same block of π_i as u ; $R_w := R_2''$ for each row w such that w is in the same block of π_t as u and v , but w is not in the same block of π_i as u ; $R_w := R_3''$ for each row w such that w is not in the same block of π_t as u and v , but w is in the same block of π_i as u ; and $R_w := R_4''$ in rows w such that w is not in the same block of π_t as u and v , and w is not in the same block of π_i as u . We then apply (4). We observe that by assumption and by (6) for $s = t - 1$, $F_j(b_j) > 0$ and $F_j(c_j) > 0$ for $j = 1, \dots, t - 1$, so $I(R_3'') > 0$ and $I(R_4'') > 0$. We can therefore remove factors of $I(R_3'')^{1/n}$ and $I(R_4'')^{1/n}$ whenever they appear on both sides of (4), leaving the equality

$$(7) \quad \sum_z I(R_1'')^{x/n} I(R_2'')^{(n-x)/n} = I(R_3'')^{x/n} I(R_4'')^{(n-x)/n} \\ = \left(\sum_z I(R_1'') \right)^{x/n} \left(\sum_z I(R_2'') \right)^{(n-x)/n}.$$

Here, x is the number of indices w such that u and w are in the same blocks of π_i and π_t ; it follows that there are $n - x$ indices w such that u and w are in the same block of π_t but different blocks of π_i . By construction, $0 < x < n$. Now, (7) is an example of the case of Lemma 2 in which equality holds, so, since we know that the vectors $(I(b_1, \dots, b_{t-1}, z, *, \dots, *))_z$ and $(I(b'_1, \dots, b'_{t-1}, z, *, \dots, *))_z$ are both nonzero, they must be proportional. Therefore,

$$(8) \quad \frac{I(b_1, \dots, b_{t-1}, z, *, \dots, *)}{I(b_1, \dots, b_{t-1}, *, *, \dots, *)} = \frac{I(b'_1, \dots, b'_{t-1}, z, *, \dots, *)}{I(b'_1, \dots, b'_{t-1}, *, *, \dots, *)}, \quad \text{for all } z \in \mathbb{R}.$$

Since (6) has been proved for $s = t$ and $m = m' - 1$, the right-hand side of (8) must equal $F_t(z)$. Then from (8) and (6) for $s = t - 1$, it follows that (6) holds for $s = t$ with the given b_1, \dots, b_{t-1} , and $b_t = z$ arbitrary. Since b_1, \dots, b_{t-1} were chosen arbitrarily with $m = m'$, this completes the secondary induction, and hence the overall induction.

Setting $s = p$ in (6), we conclude that (5) holds. Therefore, \mathcal{S} is a grid, as desired.

4. SINGLE-STARRED MOTIFS

We now discuss another case where we can determine the asymptotic behavior of the maximum number of motifs in a set of given size. Call a motif specification on p, L *single-starred* if it contains no constants, and, for each $i = 1, \dots, L$, there exists a unique j such that π_j contains the block $\{i\}$. In this case, any fractional transversal g of the hypergraph H of the specification must have $g(i) \geq 1$ for all $i = 1, \dots, L$; since this condition is also sufficient to make g a fractional transversal, we see that $\tau^*(H) = L$ and that an optimal fractional transversal must have $g(i) = 1$ for all i .

For a single-starred specification, write down the matrix of coordinates used in Theorems 5 and 6, and make a tableau by replacing each variable corresponding to a block of size 1 with *. By assumption, there will be exactly one * in each row. Each assignment v of values to the remaining variables then determines $f_1(v), \dots, f_L(v)$ in $(\mathbb{R} \cup \{*\})^p$, given by reading off the rows of the tableau. Let k be the number of variables remaining. By choosing an ordering of the variables, we may think of v as being a member of \mathbb{R}^k .

Let $M_1(L) := L(L^L + 1)$, and let $M(L) := (2M_1(L))^{L-1}L^2 + 1$; we have $M(L) \geq M_1(L)$ for all L . We now make the following definitions:

- A point $v \in \mathbb{R}^k$ is a *center* of a set $\mathcal{S} \subseteq \mathbb{R}^p$ with size r and indicator function $I : \mathbb{R}^p \rightarrow \{0, 1\}$ if at least $L-1$ of $I(f_1(v)), \dots, I(f_L(v))$ are at least $r/M(L)$.
- A point $v \in \mathbb{R}^k$ is a *hypercenter* of a set $\mathcal{S} \subseteq \mathbb{R}^p$ with size r and indicator function $I : \mathbb{R}^p \rightarrow \{0, 1\}$ if all of $I(f_1(v)), \dots, I(f_L(v))$ are at least $r/M_1(L)$.
- A point $w \in \mathbb{R}^p$ is said to be *of the form* $x \in (\mathbb{R} \cup \{*\})^p$ if, for each $i = 1, \dots, p$ such that x_i is not *, $w_i = x_i$.
- A point $w \in \mathbb{R}^p$ is *in line with* a point $v \in \mathbb{R}^k$ if it is of the form $f_i(v)$, for some $i \in \{1, \dots, L\}$.

It follows that every hypercenter of \mathcal{S} is also a center of \mathcal{S} .

For a single-starred motif specification, let C_1, \dots, C_q be the columns of the tableau where a * occurs, and let $\alpha_1 > 0, \dots, \alpha_q > 0$ be the number of *s occurring in columns C_1, \dots, C_q , respectively. Observe that $q \leq L$ and that $\alpha_1 + \dots + \alpha_q = L$. Set

$$\mathcal{C} := \frac{\alpha_1^{\alpha_1} \cdots \alpha_q^{\alpha_q}}{L^L}.$$

We have $\mathcal{C} \geq L^{-L}$.

Lemma 8. *For each single-starred motif specification on p, L , there is some function ϕ such that $\phi(r) \rightarrow 0$ as $r \rightarrow \infty$ and such that, for any r , there exists a set $\mathcal{S} \subseteq \mathbb{R}^p$ of size r with at least $\mathcal{C}(1 + \phi(r))r^L$ motifs.*

Proof. For any nonnegative integer N , we can construct a set \mathcal{S} of size LN by, for each $i = 1, \dots, q$, taking $\alpha_i N$ points which have all coordinates 0 except their C_i th, which ranges over $\{1, \dots, \alpha_i N\}$. There are then at least

$$(\alpha_1 N)^{\alpha_1} \cdots (\alpha_q N)^{\alpha_q} = \mathcal{C}(LN)^L$$

motifs in \mathcal{S} . To construct a set of arbitrary size, r say, we can set $N := \lfloor r/L \rfloor$ and pad out \mathcal{S} until we get a set of size r with at least $\mathcal{C}(L \lfloor r/L \rfloor)^L$ motifs. Since $(L \lfloor r/L \rfloor)/r \rightarrow 1$ as $r \rightarrow \infty$, this completes the proof.

Lemma 9. *For each single-starred motif specification on p, L , there exists r_0 such that whenever $r \geq r_0$ and $\mathcal{S} \subseteq \mathbb{R}^p$ of size r has the maximum number of motifs possible for a set of its size, then \mathcal{S} has a hypercenter.*

Proof. Let $I : \mathbb{R}^p \rightarrow \{0, 1\}$ be the indicator function of \mathcal{S} . Then

$$(9) \quad \mathcal{M}(\mathcal{S}) = \sum_{v \in \mathbb{R}^k} I(f_1(v)) \cdots I(f_L(v)).$$

If \mathcal{S} has no hypercenter, we know that for each v , there is some i with $I(f_i(v)) \leq r/M_1(L)$, so (9) can be no more than

$$\frac{r}{M_1(L)} \sum_{1 \leq i \leq L} \sum_{v \in \mathbb{R}^k} \prod_{j \neq i} I(f_j(v)).$$

However, each variable must occur at least twice in the tableau, so for each i , after deleting row i , each variable must still occur at least once. It follows that for each i ,

$$(10) \quad \sum_{v \in \mathbb{R}^k} \prod_{j \neq i} I(f_j(v)) \leq I(*, \dots, *)^{L-1} = r^{L-1}$$

and therefore \mathcal{S} has no more than $Lr^L/M_1(L)$ motifs. However, by Lemma 8, there exists a set of size r with at least $L^{-L}(1 + \phi(r))r^L$ motifs, and if we pick r_0 large enough, we will have $L^{-L}(1 + \phi(r)) > (1 + L^L)^{-1}$ for all $r \geq r_0$. This contradicts the assumption that \mathcal{S} had the maximum number of motifs.

Lemma 10. *For each single-starred motif specification on p, L , there exists r_0 such that whenever $r \geq r_0$ and $\mathcal{S} \subseteq \mathbb{R}^p$ of size r has the maximum number of motifs possible for a set of its size, then all points in \mathcal{S} are in line with some center.*

Proof. If $L = 1$, all points in \mathbb{R}^k are centers, so the result is trivial. We may therefore assume that $L \geq 2$. Let $I : \mathbb{R}^p \rightarrow \{0, 1\}$ be the indicator function of \mathcal{S} . If we remove one point, w , from \mathcal{S} , then $I(f_i(v))$ does not decrease if the coordinate vector of w is not of the form $f_i(v)$, and decreases by 1 if the coordinate vector is of the form $f_i(v)$. Therefore, after removing w , the number of motifs in \mathcal{S} can decrease by at most

$$Y := \sum_{1 \leq i \leq L} \sum_{v \in \mathcal{T}_i} \prod_{j \neq i} I(f_j(v)),$$

where \mathcal{T}_i is the set of points $v \in \mathbb{R}^k$ for which w is of the form $f_i(v)$. If w is not in line with any center, there are no centers in $\mathcal{T}_1 \cup \cdots \cup \mathcal{T}_L$, so for any i and $v \in \mathcal{T}_i$, there must be some $i' \neq i$ with $I(f_{i'}(v)) < r/M(L)$. Therefore,

$$Y \leq \frac{r}{M(L)} \sum_{1 \leq i \neq i' \leq L} \sum_{v \in \mathcal{T}_i} \prod_{j \notin \{i, i'\}} I(f_j(v)).$$

However, when we sum over $v \in \mathcal{T}_i$, we are only summing over variables which do not occur in the i th row of the tableau, so after deleting the i th and i' th rows, each variable summed over must still occur at least once. Therefore,

$$\sum_{v \in \mathcal{T}_i} \prod_{j \notin \{i, i'\}} I(f_j(v)) \leq I(*, \dots, *)^{L-2} = r^{L-2}$$

and so we have decreased the number of motifs in \mathcal{S} by at most $(L^2/M(L))r^{L-1}$. Now, if we take r_0 to be at least as large as in Lemma 9, then \mathcal{S} must have a hypercenter, v_0 , say, and after deleting w , each of $I(f_1(v_0)), \dots, I(f_L(v_0))$ must be at least $(r/M_1(L)) - 1$. If we take r_0 to be at least as large as $2M_1(L)$, adding w back to be in line with v_0 will then increase the number of motifs in \mathcal{S} by at least $((r/M_1(L)) - 1)^{L-1} \geq (r/(2M_1(L)))^{L-1}$. Since $M(L) > (2M_1(L))^{L-1}L^2$, this means that moving w to be in line with a hypercenter increases the number of motifs in \mathcal{S} . This contradicts the assumption that \mathcal{S} had the maximum number of motifs.

Lemma 11. *For each single-starred motif specification on p, L , a set \mathcal{S} can have at most $LM(L)^{L-1}$ centers.*

Proof. Let the subset \mathcal{S} of \mathbb{R}^p have size r . For each center v , there is some i such that $I(f_j(v)) \geq r/M(L)$ for all $j \neq i$. Fix i . Then, for each $j \neq i$, if we sum $I(f_j(v))$ over the variables occurring in the j th row of the tableau, we will get r . Therefore, there can be at most $M(L)$ assignments of values to the variables in the j th row of the tableau for which $I(f_j(v)) \geq r/M(L)$. Recalling that, after deleting row i , each variable must still occur at least once, it follows that after fixing i , there are at most $M(L)^{L-1}$ possibilities for v . \mathcal{S} therefore has at most $LM(L)^{L-1}$ possible centers.

Theorem 12. *For each single-starred motif specification on p, L , as r becomes large, the maximum number of motifs in a set $\mathcal{S} \subseteq \mathbb{R}^p$ of size r is asymptotic to Cr^L . Also, there is some r_0 such that if $r \geq r_0$, then a set \mathcal{S} of size r with a maximum number of motifs for its size must have exactly one center, which must also be a hypercenter, and all points in \mathcal{S} must be in line with the center. In addition, the points in \mathcal{S} must fall into q lines, ℓ_1, \dots, ℓ_q , say, where each ℓ_i is given by fixing all coordinates except the C_i th.*

Proof. We have already proved that Cr^L is an asymptotic lower bound in Lemma 8. We now need to prove that it is also an asymptotic upper bound, and that optimal sets \mathcal{S} have the desired form.

Let r_0 be at least as large as required in Lemmas 9 and 10, and let \mathcal{S} be a set of size $r \geq r_0$ with a maximum number of motifs for its size. As usual, the number of motifs in \mathcal{S} is

$$\sum_{v \in \mathbb{R}^k} I(f_1(v)) \cdots I(f_L(v)).$$

We may bound this sum above by the sum of $L+1$ pieces; the first piece, Z_1 , will be given by summing over all v where $f_1(v) \neq f_i(v')$ for all centers v' and $i = 1, \dots, L$, the second piece, Z_2 , by summing over all v where $f_2(v) \neq f_i(v')$ for all centers v' and $i = 1, \dots, L$, and so on, up to the L th piece, Z_L , which is given by summing over all v where $f_L(v) \neq f_i(v')$ for all centers v' and $i = 1, \dots, L$. The last piece, Z_{L+1} , is computed by summing over all v where, for each $j = 1, \dots, L$, there is some center v' and $i \in \{1, \dots, L\}$ for which $f_j(v) = f_i(v')$.

To bound the first piece, observe that if $f_1(v) \neq f_i(v')$, then there are either no points whose coordinate vectors are both of the form $f_1(v)$ and $f_i(v')$ (in the case where the $*$ is in the same position in $f_1(v)$ and $f_i(v')$) or at most one point (in the case where the $*$ is in different positions in $f_1(v)$ and in $f_i(v')$.) Also, by Lemma 10, every point in \mathcal{S} is of the form $f_i(v')$, for some i and some center v' . Then, summing over i and v' and using Lemma 11, we see that $I(f_1(v)) \leq L^2 M(L)^{L-1}$, so by (10), the first piece of the sum is no more than $L^2 M(L)^{L-1} r^{L-1}$. We can bound the 2nd through L th pieces in the same way, so

$$(11) \quad \mathcal{M}(\mathcal{S}) \leq Z_1 + \cdots + Z_{L+1} \leq Z_{L+1} + L^3 M(L)^{L-1} r^{L-1}.$$

For $j = 1, \dots, L$, let $\sigma_j \in \{1, \dots, q\}$ be such that there is a $*$ in row j and column C_{σ_j} of the tableau, and for each $i = 1, \dots, q$, let \mathcal{S}_i be the set of points of \mathcal{S} whose coordinate vectors are of the form $f_j(v)$, for some center v of \mathcal{S} , and some j with $\sigma_j = i$. For $i = 1, \dots, q$, we let \mathcal{S}_i have indicator function I_i and size r_i . By Lemma 10, all points in \mathcal{S} must be in line with some center, so $\mathcal{S} = \cup_{1 \leq i \leq q} \mathcal{S}_i$. Now, if there is a point w which is in $\mathcal{S}_i \cap \mathcal{S}_{i'}$, for some $i \neq i'$, then w is of the form $f_j(v)$ and also of the form $f_{j'}(v')$, for some centers v and v' of \mathcal{S} . Every coordinate of w except the C_i th is determined by v and j , and every coordinate of w except the $C_{i'}$ th is determined by v' and j' . Then, since $i \neq i'$, w is determined by v, v', j , and j' . Since \mathcal{S} can have at most $LM(L)^{L-1}$ centers, there are at most $L^4 M(L)^{2L-2}$ possibilities for w . Therefore,

$$(12) \quad r_1 + \cdots + r_q \leq r + L^5 M(L)^{2L-2}.$$

Z_{L+1} is defined by summing $I(f_1(v)) \cdots I(f_L(v))$ over all v where, for each $j = 1, \dots, L$, there is some center v' and i with $f_j(v) = f_i(v')$. For this equality to occur, the $*$ must occur in the same position in $f_i(v')$ and $f_j(v)$, so σ_i must equal σ_j . It follows that, in the defining sum for Z_{L+1} , $I(f_j(v))$ can only count points in \mathcal{S}_{σ_j} and so

$$(13) \quad Z_{L+1} \leq \sum_{v \in \mathbb{R}^k} I_{\sigma_1}(f_1(v)) \cdots I_{\sigma_L}(f_L(v)),$$

and relaxing coordinate equality constraints in the tableau gives the inequality

$$(14) \quad \sum_{v \in \mathbb{R}^k} I_{\sigma_1}(f_1(v)) \cdots I_{\sigma_L}(f_L(v)) \leq \left(\sum_{x_1} I_{\sigma_1}(x_1) \right) \cdots \left(\sum_{x_L} I_{\sigma_L}(x_L) \right),$$

where, for each i , x_i is summed over all elements of $(\mathbb{R} \cup \{*\})^p$ which contain exactly one $*$, in coordinate C_{σ_i} . However, the right-hand side of this inequality is just

$$\prod_{1 \leq i \leq L} r_{\sigma_i} = \prod_{1 \leq j \leq q} r_j^{\alpha_j}$$

and therefore from (13) and (14) we get

$$(15) \quad Z_{L+1} \leq \prod_{1 \leq j \leq q} \alpha_j^{\alpha_j} \prod_{1 \leq j \leq q} (r_j / \alpha_j)^{\alpha_j}.$$

The asymptotic upper bound $\mathcal{C}r^L$ now follows immediately from (11), (12), (15), and the inequality

$$\prod_{1 \leq j \leq q} (r_j/\alpha_j)^{\alpha_j} \leq \left(\frac{r_1 + \cdots + r_q}{\alpha_1 + \cdots + \alpha_q} \right)^{\alpha_1 + \cdots + \alpha_q},$$

which is an application of the weighted arithmetic-geometric inequality (see [2, Theorem 9], or [4, Problem 2.3].)

By Lemma 9, we already know that \mathcal{S} has a hypercenter, v_0 , say, and by Lemma 10, we know that all its points are in line with some center. It remains to show that \mathcal{S} has only one center, and that its points fall into q lines as claimed. However, if \mathcal{S} had a center, v' , say, not equal to v_0 , then v' and v_0 would have to assign some variable a different value. Since each variable occurs in at least two rows of the matrix of coordinates, there must therefore be some i for which $I(f_i(v')) \geq r/M(L)$ and $f_i(v') \neq f_i(v_0)$. Now, the term

$$I_{\sigma_1}(f_1(v_0)) \cdots I_{\sigma_{i-1}}(f_{i-1}(v_0)) I_{\sigma_i}(f_i(v')) I_{\sigma_{i+1}}(f_{i+1}(v_0)) \cdots I_{\sigma_L}(f_L(v_0))$$

will occur on the right-hand side but not the left-hand side of (14), and it will have value at least $(r/M(L))(r/M_1(L))^{L-1}$; this means that the left- and right-hand sides of (15) must differ by at least $r^L/(M(L)M_1(L)^{L-1})$. By our asymptotic estimate, this will prevent \mathcal{S} from containing the maximum possible number of motifs, if we take r_0 sufficiently large. We conclude that \mathcal{S} must have only one center, v_0 . Finally, if there are i and j for which $\sigma_i = \sigma_j$ but $f_i(v_0) \neq f_j(v_0)$, the term

$$I_{\sigma_1}(f_1(v_0)) \cdots I_{\sigma_{i-1}}(f_{i-1}(v_0)) I_{\sigma_i}(f_j(v_0)) I_{\sigma_{i+1}}(f_{i+1}(v_0)) \cdots I_{\sigma_L}(f_L(v_0))$$

will occur on the right-hand side but not the left-hand side of (14), and it will have value at least $(r/M_1(L))^L$. As before, this will prevent \mathcal{S} from containing the maximum possible number of motifs. Therefore, we conclude that the set $\{f_1(v_0), \dots, f_L(v_0)\}$ has only q distinct elements, one with a * in position C_i for $i = 1, \dots, q$. Then, since every point in \mathcal{S} must be in line with the unique center, v_0 , every point in \mathcal{S} must have coordinate vector matching one of these q distinct elements. This establishes the only remaining claim.

5. CONCLUSION

To finish, we ask two questions:

1. For a general motif specification, what is the asymptotic behavior of the maximum number of motifs in a set of given size?
2. For motif specifications with no constants and uniform hypergraph, sets with the maximum number of motifs for their size are always grids. Also, for single-starred motif specifications, large enough sets with the maximum possible

number of motifs for their size are always the union of q lines. Are large sets with the maximum possible number of motifs for their size always unions of a small number of grids?

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