An der Fakultät für Mathematik
der Otto-von-Guericke-Universität Magdeburg
zur Erlangung des akademischen Grades
Master of Science
angefertigte

Masterarbeit

Construction Methods for Gaussoids

vorgelegt am 23.08.2018 von
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Aktualisiert am 21.02.2019

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Contents

Notation

Throughout, N denotes a finite ground set with at least three elements. Elements $i, j, k, \ldots \in N$ are identified with singleton subsets of N. Juxtaposition abbreviates set union, so that $ijK = \{i\} \cup \{j\} \cup K \subseteq N$. The symmetric difference of two sets is $A \oplus B$. The powerset of N is denoted 2^N and the system of all k-element subsets is $\binom{N}{k}$. The cardinality of N is denoted by n and when the set ifself is of no particular relevance, we may suppose $N = [n] := \{1, \ldots, n\}$.

Given a symmetric matrix $(N \times N)$-matrix Σ, the *principal* minors are $p_I := \det \Sigma_{I,I}$ for $I \subseteq N$, where $p_\emptyset := 1$, and the *almost-princial* minors are $a_{ij|K} := \det \Sigma_{iK,jK}$ for $ij \in \binom{N}{2}, K \subseteq N \setminus ij$.

Parentheses are omitted wherever possible, including at the application of a function to its argument. Function application binds tighter than every operator, so $fc \nearrow c$ should be read as $f(c) \nearrow c$.

1 Introduction

Notions of *independence* appear in many branches of Mathematics and the theory of matroids ties seemingly unrelated independence concepts — or cryptomorphisms thereof — in areas as diverse as linear algebra, graph, lattice and field theory, combinatorial optimisation or the study of semimodular functions, into an axiomatic framework. However, matroids deal with a unary independence predicate "a subset I of the ground set N is independent" and does not capture the independence of random variables familiar from statistics, which is a binary relation: "the random variable X is independent of Y", or the more general ternary relation of *conditional independence*: "subsystems ξ_I and ξ_J of a vector ξ of random variables are (conditionally) independent, given the system ξ_K".

This thesis is concerned with *gaussoids*, a combinatorial structure which originates from probabilistic conditional independence relations among random variables with a joint regular Gaussian distribution; see [Stu05, Chapter 2] for a brief introduction. Thus these structures are concerned with the ternary kind of independence. Conditional independence, however, is not purely a probabilistic concept. Similarly to the multitude of unary independence relations in mathematical theories, ternary independence relations arise in different areas, such as probability and graph theory, relational databases or artificial intelligence [Pea88, PP85]. A unifying framework for these notions is provided by the semigraphoid axioms.

This introduction briefly traces the path from general conditional independence structures to localisable relations. The use of local relations is not merely a notational detail, but facilitates a geometric interpretation of conditional independence relations. Starting with Section 2 local relations are identified with collections of 2-dimensional faces of the N-dimensional cube. This association provides the idea underlying our main gaussoid construction method in Section 4.2. Therefore, it seems necessary to justify the transition to local relations before gaussoids can be introduced.

For a finite ground set N and mutually disjoint subsets I, J, K of N, the triple $(I, J|K)$ is a *(formal) conditional independence statement* or *CI statement* for short. $\mathcal{T}_N$ denotes the set of all such triples, its subsets are called *global CI relations*. A *global semigraphoid* S is a CI relation which satisfies the following axioms:

Triviality $(I, \emptyset|K)$,

Symmetry $(I, J|K) \Rightarrow (J, I|K)$,

Decomposition $(I, JL|K) \Rightarrow (I, L|K)$,

Weak union $(I, JL|K) \Rightarrow (I, J|KL)$, and

Contraction $(I, J|KL) \wedge (I, L|K) \Rightarrow (I, JL|K)$,

for all mutually disjoint sets I, J, K, L of N, where every CI statement $(I, J|K)$ appearing in the axioms is understood to be a short-hand for asserting its membership $(I, J|K) \in S$. In this way, the axioms are Boolean formulae whose set of variables is $\mathcal{T}_N$ and whose satisfying assignments are the global semigraphoids.

These axioms are satisfied by all probability distributions when the symbol $(I, J|K)$ is interpreted as probabilistic conditional independence. Notably, all axioms take the form of *inference rules*. Semigraphoids are a formal model for reasoning about CI inference.

A further property whose significance was highlighted by Matúš [Mat97] is *localisability*. To explain this term, the class of *elementary CI statements* $\mathcal{A}_N$ has to be introduced. It is the subset of $\mathcal{T}_N$ containing all $(I, J|K)$ where $I = i$ and $J = j$ are singleton sets. For the purpose of studying semigraphoids, by the Symmetry axiom, these two sets commute in a CI statement, so that $(i, j|K)$ might be regarded as a pair of sets $(ij|K)$ where ij is now a two-element set. Define $\mathcal{A}_N := \{(ij|K) : ij \in \binom{N}{2}, K \subseteq N \setminus ij\}$. A global relation $S \subseteq \mathcal{T}_N$ is *localisable* when it can be recovered from just its intersection with $\mathcal{A}_N$, in the following way:

$$(I, J|K) \in S \Leftrightarrow (I, J|K)_\star \subseteq S \cap \mathcal{A}_N,$$

where $(I, J|K)_\star := \{(ij|L) \in \mathcal{A}_N : i \in I, j \in J, K \subseteq L \subseteq IJK \setminus ij\}$. The operation of intersecting with $\mathcal{A}_N$ is referred to as *localisation*. Global semigraphoids are localisable [Mat92, Lemma 3]. This property conveniently reduces redundancy in semigraphoids and simplifies notation as well as axiomatisation. The subsets of $\mathcal{A}_N$ which are localisations of global semigraphoids — those sets will simply be called semigraphoids — can be axiomatised with just a single inference rule:

$$(ij|L) \in S \wedge (ik|jL) \in S \Rightarrow (ik|L) \in S \wedge (ij|kL) \in S$$

for all $ijk \in \binom{N}{3}$ and $L \subseteq N \setminus ijk$. In the remainder of this thesis, attention will be restricted to local relations, i.e. subsets of $\mathcal{A}_N$.

Gaussoids are a special type of semigraphoid featuring stronger inference rules. They were introduced by Lněnička and Matúš in [LM07] after preparatory work by Matúš [Mat05]. As their name suggests, they are inspired by regular Gaussian probability distributions. Suppose $\xi \sim \mathcal{N}(\mu, \Sigma)$ is distributed according to a multivariate regular Gaussian distribution with mean vector μ and positive-definite covariance matrix Σ. Its conditional independence model $\langle\!\langle \xi \rangle\!\rangle$ is the set of all CI statements which hold for ξ. It can be shown that in the regular Gaussian case, this model is encoded in the *almost-principal minors* of Σ:

$$(ij|K) \in \langle\!\langle \xi \rangle\!\rangle \Leftrightarrow \det \Sigma_{iK,jK} = 0,$$

where $\Sigma_{A,B}$ denotes the submatrix of Σ with rows indexed by A and columns indexed by B. Determinants of submatrices are commonly called *minors* of the matrix. A minor $\Sigma_{K,K}$ where rows and columns are indexed by the same set are *principal*, whereas a minor $\Sigma_{iK,jK}$ where row and column indices differ by just one element is *almost-principal*. Our notation $\mathcal{A}_N$ for elementary CI statements, following [BDKS17], derives from this instance.

In this way, one can define the CI model of a symmetric matrix Σ via $\langle\!\langle \Sigma \rangle\!\rangle := \{(ij|K) \in \mathcal{A}_N : \det \Sigma_{iK,jK} = 0\}$. Almost-principal minors are polynomials in the entries of the matrix, hence the question of which CI relations arise from regular Gaussian distributions becomes one of commutative algebra: "which sets of almost-principal minors of a positive-definite matrix can simultaneously vanish?" Due to this link, gaussoids received attention before or independent of their axiomatic definition [Mat05, Šim06, Sul09]. Matúš' fundamental result states

Theorem ([Mat05])**.** Let $\mathcal{K}, \mathcal{L} \subseteq \mathcal{A}_N$ and A a *complex* symmetric matrix with non-vanishing principal minors. The inference $\mathcal{K} \subseteq \langle\!\langle A \rangle\!\rangle \Rightarrow \mathcal{L} \cap \langle\!\langle A \rangle\!\rangle \neq \emptyset$ holds if and only if $f_{\mathcal{L}} \in \sqrt{I_{\mathcal{K}}}$.

Here, $f_{\mathcal{L}}$ is the product of all almost-principal minors indexed by $\mathcal{L}$, as a polynomial in the entries of a generic symmetric matrix, and $I_{\mathcal{K}}$ is a suitable ideal derived from $\mathcal{K}$, which incorporates the non-vanishing of principal minors. The "$\Rightarrow$" direction of this theorem requires Hilbert's Nullstellensatz, hence an algebraically closed field. However, the other direction holds for every field. By choosing $\mathcal{K}$ and $\mathcal{L}$ appropriately and proving the incidence of $f_{\mathcal{L}}$ to $\sqrt{I_{\mathcal{K}}}$, this theorem allows the deduction of four inference statements (G1)–(G4) which became the definition of gaussoid. Gaussoids arising from a positive-definite matrix were called *realisable* for contrast.

As briefly mentioned, results on gaussoids around the time when the gaussoid axioms were introduced concerned inference axioms for realisable gaussoids only. [LM07] enumerated the 3- and 4-gaussoids and classified them according to realisability. Following parallels to matroid theory, [BDKS17] introduced oriented, positive and valuated gaussoids, and, among other things, enumerated the 5-gaussoids using `SAT` solvers.

There was no general construction method for non-realisable gaussoids and no estimate on the asymptotic number of gaussoids or their share among all CI relations. These three points are addressed in this thesis.

The thesis is organised as follows. Section 2 introduces the gaussoid axioms, symmetries and gaussoid minors. N-gaussoids are viewed as sets of 2-dimensional faces of the N-dimensional cube and minors correspond to a slicing operation on this cube.

Section 3 surveys two sources of gaussoids: matrices with non-vanishing principal minors and undirected graphs. An exponential upper bound on the number of representable gaussoids, due to Peter Nelson, is proved. The "`N` Theorem" 3.5 about apr-sequences of gaussoids as well as a classification of simultaneously ascending and descending gaussoids in Theorem 3.10 are new.

Section 4 is based on a known result, Lemma 4.1, which states that N-gaussoids are exactly those CI relations whose proper minors are gaussoids themselves. Certain graphs $Q(N, k, p, q)$ are defined, whose connectivity encodes intersections of faces in the N-cube and their key figures are derived. It is shown that independent sets in these graphs generate a doubly exponential number of N-gaussoids. The same technique is used to obtain a relative upper bound on the number of gaussoids, too. In the last Section 4.4, the previous results are applied to the study of gaussoid closure. A minor-based algorithm to construct gaussoid closures is presented. Two examples of badly behaving CI relations are constructed: one with exponentially many closures in the input size, and one with an exponentially large closure.

2 Preliminaries

2.1 The gaussoid axioms

To abstract the conditional independence inference statements which hold for regular Gaussian distributions, Lněnička and Matúš [LM07] have introduced the notion of a *gaussoid*. A gaussoid is a combinatorial structure defined inference rules for the containment of squares.

Definition 2.1. A set $G \subseteq \mathcal{A}_N$ is an N*-gaussoid* if it satisfies the following axioms for all distinct $i, j, k \in N$ and $L \subseteq N \setminus ijk$:

$$(ij|L) \wedge (ik|jL) \Rightarrow (ik|L) \wedge (ij|kL), \tag{G1}$$
$$(ij|kL) \wedge (ik|jL) \Rightarrow (ij|L) \wedge (ik|L), \tag{G2}$$
$$(ij|L) \wedge (ik|L) \Rightarrow (ij|kL) \wedge (ik|jL), \tag{G3}$$
$$(ij|L) \wedge (ij|kL) \Rightarrow (ik|L) \vee (jk|L). \tag{G4}$$

The collection of N-gaussoids is denoted $\mathfrak{G}_N$.

These axioms are known as the semigraphoid axiom (G1), the intersection axiom (G2) and its converse (G3), and weak transitivity (G4) [LM07, BDKS17].

Before beginning an analysis of the gaussoid axioms, we introduce geometric parlance which is used throughout this thesis. The N*-cube* is the combinatorial hypercube Q_N as a graph whose vertices $\{\mathtt{0}, \mathtt{1}\}^N$ are the binary strings indexed by N with an edge between two vertices if and only if their Hamming distance equals 1. A *face* of the n-cube is a word in $\mathcal{F}^N := \{\mathtt{0}, \mathtt{1}, *\}^N$. The $*$ symbols are thought to indicate positions which vary between $\mathtt{0}$ and $\mathtt{1}$. If $w_* d$ denotes the number of $*$ symbols in a face d, then this varying generates $2^{w_* d}$ vertices in Q_N which span a $w_* d$-dimensional face of the N-cube as a polytope. Hence this number is called the *dimension* of that face and denoted $\dim d$; the set of all k-dimensional faces, or k*-faces*, is $\mathcal{F}_k^N$. Clearly the number of k-faces of the N-cube is $\binom{n}{k} 2^{n-k}$ and their counts sum up to exactly 3^n. The two- and three-dimensional faces are of principal importance. We refer to $\mathcal{A}_N := \mathcal{F}_2^N$ as the *squares* and to $\mathcal{C}_N := \mathcal{F}_3^N$ as the *cubes*. For contrast, Q_N will always be called "N-cube" or "hypercube", if the parameter N is obvious from context or insignificant.

The symbol $(I|K)$, for $I, K \subseteq N$ disjoint, describes an $|I|$-face by making all positions indexed by I into $*$ and all positions indexed by K into $\mathtt{1}$, leaving all others $\mathtt{0}$. Given a face $(I|K)$, we use $\tilde{K}$ to refer to $N \setminus IK$, i.e. the positions of the $\mathtt{0}$s. Given a face x, we denote the index sets of $*$s, $\mathtt{1}$s and $\mathtt{0}$s respectively by I_x, K_x and $\tilde{K}_x$. This correspondence between words and pairs of disjoint index sets is used wherever it simplifies notation. Thus we see that elementary CI statements $(ij|K)$ correspond to squares in the hypercube. Higher-dimensional faces of the N-cube become an important indexing tool for gaussoids in Section 4.

Returning to the gaussoid axioms, we note that each of them is a Boolean formula involving squares as variables, quantified over all ordered triples (i, j, k) and sets L. There are $4 \cdot 3! \binom{n}{3} \cdot 2^{n-3}$ axioms defining n-gaussoids. The pair of sets $(ijk|L)$ specifies a cube containing all the squares which appear in the axioms. The ordering on the set ijk permutes the axes of this cube. Figure 1 shows (G1)–(G4) in a Schlegel diagram of the ijk-cube.

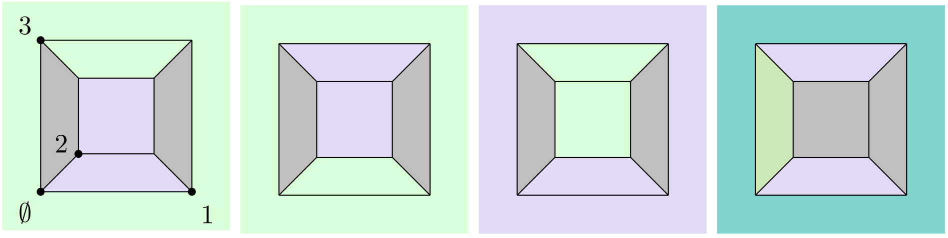
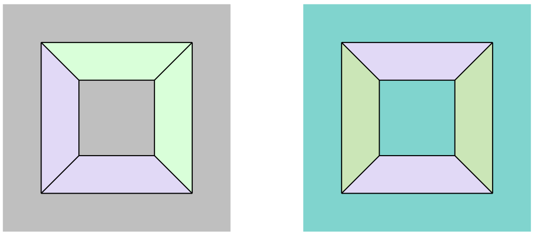


Figure 1: The four gaussoid axioms (G1)–(G4) as inference rules in Schlegel diagrams of the 3-cube for $(i, j, k) = (1, 2, 3)$, $L = \emptyset$. Purple denotes the premises and green the conclusions. The last axiom has alternative conclusions, which are colored in different shades of green.



(a) (b)

Figure 2: (a) Any "knee" in the cube is completed to the unique "belt" which contains it. (b) Two opposite squares are completed to (at least) one of the two belts which contain them.

It is instructive to write down all $4 \cdot 3! = 24$ axioms for $n = 3$ and simplify them. If the axioms are viewed as a set of rules on how to close a given set of squares to a gaussoid, they boil down to two pictorially simple rules depicted in Figure 2, up to symmetries of the cube. It is then easy to check that Figure 3 lists exactly the eleven 3-gaussoids.

The quantifiers around the gaussoid axioms make $\mathfrak{G}_N$ invariant under the action of the symmetric group $\mathfrak{S}_N$. This action furnishes a notion of isomorphy for gaussoids, as defined in [LM07], but extended to the more general hypercube setting as follows:

Definition 2.2. Two sets of faces are *isomorphic* if they lie in the same orbit of the $\mathfrak{S}_N$ action given on faces via $\sigma(I|K) := (\sigma I|\sigma K)$. This relation is denoted $\cong$.

The following lemma provides a practically useful necessary condition for (gaussoid) isomorphy. For 3-gaussoids it is also sufficient, that is, the isomorphy classes of gaussoids in Figure 3 correspond to the levels in the poset, with the exception of the singleton level, which splits into two further isomorphy classes.

Lemma 2.3. Besides the cardinality $|H|$, the vector $(|\{(I|K) \in H : |K| = k\}|)_{k \in [n]}$, called the *order histogram*, is an invariant of the isomorphy class of a set of faces H. $\square$

Definition 2.4. The *dual* or *opposite* of a face $(I|K)$ is $(I|K)^\circ := (I|\tilde{K}) = (I|N \setminus IK)$. The dual of $(ij|)$ is abbreviated to $(ij|*) := (ij|)^\circ = (ij|N \setminus ij)$. This definition is extended element-wise to sets of faces.

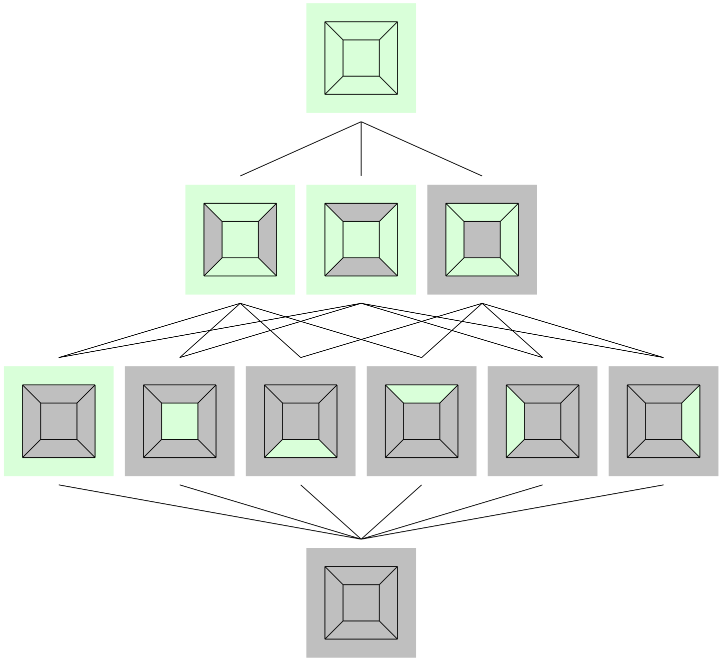


Figure 3: The eleven gaussoids on $n = 3$ arranged in a poset with respect to inclusion, from bottom up: the empty gaussoid, singletons, belts and the full gaussoid.

Duality is an involution on, and another symmetry of, gaussoids. Replacing every variable in (G1)–(G4) by its dual axiomatises the duals of gaussoids. Again by the $\forall$-quantifiers around the axioms, this is just a permutation of the axioms, which shows that gaussoids are indeed closed under duality. That duality is not a form of gaussoid isomorphy follows from Lemma 2.3.

2.2 The hypercube and minors

It is well-known that the set of faces of the hypercube, as a polytope, forms a join semi-lattice with respect to inclusion. It becomes a proper lattice if an artificial face $\emptyset$ is added in the obvious way as a smallest element. In this section, we present formal tools which facilitate proofs by calculation in this lattice as well as computer implementations.

Definition 2.5. (1) A face $(I|K)$ is *included* in another face $(I'|K')$, denoted $(I|K) \subseteq (I'|K')$, if the following conditions hold: (i) $I \subseteq I'$, (ii) $K \subseteq I'K'$, and (iii) $\tilde{K} \subseteq I'\tilde{K}'$.

(2) The *intersection* of faces is $(I|K) \cap (I'|K') := \sup\{d \in \mathcal{F}^N : d \subseteq (I|K) \wedge d \subseteq (I'|K')\}$ with respect to the lattice order $\subseteq$ on faces. By convention, if the set of faces under the sup is empty, the intersection is denoted $\emptyset \notin \mathcal{F}^N$. Two faces *intersect* when the intersection is not $\emptyset$.

(3) For a set $H \subseteq \mathcal{F}^N$, the set of faces which are included in some face $(I|K)$ is $H \cap (L|M) := \{d \in H : d \subseteq (I|K)\}$.

The intuitive validity of these definitions rests on the consistency of inclusion as defined above with the definition of inclusion in the face lattice. This is easily seen to hold as the properties listed in Definition 2.5 (1) ensure that $(I|K) \subseteq (I'|K')$ is equivalent to all extremal points of $(I|K)$, which are the vertices of Q_N obtained by varying the $*$ symbols indexed by I, lying in $(I'|K')$. This is enough since the faces of a polytope are convex.

The intersection of faces and its dimension can be described in this calculus of pairs of sets $(I|K)$ as follows:

Lemma 2.6. The intersection $(I|K) \cap (I'|K')$ is non-empty if and only if $K \subseteq I'K'$ and $K' \subseteq IK$. In this case it is given by $(I|K) \cap (I'|K') = (I \cap I'|KK')$. Assigning dimension $-\infty$ to $\emptyset$, one has in particular

$$\dim((I|K) \cap (I'|K')) = \begin{cases} -\infty, & (K \cap \tilde{K}')(K' \cap \tilde{K}) \neq \emptyset, \\ |I \cap I'|, & \text{else.} \end{cases}$$

Proof. Assume that $K \subseteq I'K'$ and $K' \subseteq IK$ hold and consider the face $s = (I \cap I'|KK')$. It is clear that $I_s = I \cap I'$ is contained in both I-sets. Since $K \subseteq I'K'$ and $K' \subseteq IK$, we see that $KK' \subseteq KKI \subseteq KI$ and $KK' \subseteq K'I'K' \subseteq K'I'$, so that $K_s = KK' \subseteq KI \cap K'I'$. Using $\tilde{K}' \cap (N \setminus K) = \tilde{K}'$ and $\tilde{K} \cap (N \setminus K') = \tilde{K}$ which are implied by the assumption, one can show that $\tilde{K}_s = \tilde{K}\tilde{K}'$, hence the containment in both $\tilde{K}$-sets is analogous to the K-sets. Thus s is contained in both $(I|K)$ and $(I|K')$. It is easy to see that there is only one face contained in both $(I|K)$ and $(I'|K')$ which achieves the maximal intersection dimension $|I \cap I'|$, namely $(I|K) \cap (I'|K')$. If $K \subseteq I'K'$ does not hold, then $K \cap \tilde{K}'$ is non-empty. Pick some $i \in K \cap \tilde{K}'$. A face s contained in both faces, if it exists, cannot have a `0` or $*$ at i because $i \in K$. It cannot have a `1` either because $i \in \tilde{K}'$. It follows that such a face s does not exist. The argument is analogous if $K' \subseteq IK$ is violated. □

Corollary 2.7. For $3 \leq k \leq m$, a k-face shares at most $\binom{k-1}{2}2^{k-3}$ squares with an m-face or is already included in it.

Proof. Let $(I|K)$ be a k-face and $(J|L)$ an m-face. If $(I|K)$ and $(J|L)$ do not intersect, they do not share a square and the statement holds. If they intersect, the intersection dimension is $|I \cap J|$. Since $k = |I| \leq |J| = m$, the intersection is at most k. If it is exactly k, then the intersection is $(I|K)$, hence $(I|K) \subseteq (J|L)$. Otherweise the intersection dimension is $\leq k-1$ and Q_{k-1} contains $\binom{k-1}{2}2^{k-3}$ squares. □

This result is especially useful in the case $k = 3$ where it reads "if a cube shares more than a single square with an m-face, then it is already contained in it". The constructions in Section 4 based on Lemma 4.1 frequently exploit this special case together with the fact that all singleton sets of squares are vacuously gaussoids. These results require the notion of *minor* of a gaussoid which we introduce next.

Minors are an important concept in matroid theory. When a simple matroid is represented as the geometric lattice of its flats, minors correspond to intervals in that lattice [Wel10, Theorem 4.4.3]. Our aim is to understand gaussoid minors analogously, by replacing the geometric lattice cryptomorphism with the set of squares in the hypercube and lattice interval with hypercube face. Our treatment focuses on sets of squares because they bear a meaning for conditional independence, but the results generalise to sets of faces of varying dimension.

First, we review definitions of minors found in the literature. Minors for arbitrary CI structures have been studied for example in [Mat97]. There, a *minor* of a CI structure is obtained by definition by choosing two disjoint sets $L, M \subseteq N$ and performing *restriction* to LM followed by *contraction* by $N \setminus L$, which are in symbols:

$$\begin{aligned} \mathrm{contr}_L A &= \{(ij|K) \in \mathcal{A}_L : (ij|K(N \setminus L)) \in A\} \subseteq \mathcal{A}_L, \\ \mathrm{restr}_L A &= A \cap \mathcal{A}_L \subseteq \mathcal{A}_L. \end{aligned}$$

Minors of gaussoids were also defined explicitly in [BDKS17] using statistical terminology with an emphasis on the parallels to matroid theory. A minor is every set of squares arising from a gaussoid via any sequence of *marginalisation* and *conditioning*:

$$\begin{aligned} \mathrm{marg}_L A &= \{(ij|K) \in A : L \subseteq N \setminus ijK\} \subseteq \mathcal{A}_{N \setminus L}, \\ \mathrm{cond}_L A &= \{(ij|K) \in \mathcal{A}_{N \setminus L} : (ij|KL) \in A\} \subseteq \mathcal{A}_{N \setminus L}. \end{aligned}$$

One observes that these operations are indeed dual to the ones defined by Matúš: $\mathrm{cond}_L = \mathrm{contr}_{N \setminus L}$ and $\mathrm{marg}_L = \mathrm{restr}_{N \setminus L}$. Furthermore, either operation can be the identity, $\mathrm{restr}_N = \mathrm{id}$ and $\mathrm{contr}_N = \mathrm{id}$. Finally, the two sets L and M in Matúš' definition of minor can be decoupled like this: $\mathrm{contr}_L \mathrm{restr}_{LM} = \mathrm{restr}_L \mathrm{contr}_{N \setminus M}$. It follows that both notions of minor coincide.

A face $(L|M)$ of the N-cube is canonically isomorphic to the L-cube by deleting from the N-cube $\{0, 1\}^N$ all coordinates outside of L. It is clear that this deletion operation is a lattice isomorphism $\mathcal{F}^N \cap (L|M) \leftrightarrow \mathcal{F}^L$. Let this canonical isomorphism be denoted by $\pi_{(L|M)}$. We would like to interpret the minor $\mathrm{restr}_L \mathrm{cond}_M$ as an operation in the hypercube.

Proposition 2.8. Let $A \subseteq \mathcal{A}_N$, then $\mathrm{restr}_L \mathrm{cond}_M A = \pi_{(L|M)}(A \cap (L|M))$.

Proof. Take $(ij|K') \in \mathrm{restr}_L \mathrm{cond}_M A$. ij and K' can be seen as subsets of N and then satisfy $ijK' \subseteq L$ and $(ij|K'M) \in A$. From this it is immediate that $ij \subseteq L$ and $K'M \subseteq LM$. Furthermore, $N \setminus ijK'M = (N \setminus ijK') \cap (N \setminus M) \subseteq \widetilde{LM}$, hence $(ij|K'M) \subseteq (L|M)$ and $(ij|K') \in \pi_{(L|M)}(A \cap (L|M))$.

In the other direction, suppose that $(ij|K') \in \pi_{(L|M)}(A \cap (L|M))$ and let $(ij|K)$ be its preimage under $\pi_{(L|M)}$. Then $(ij|K) \in A \cap (L|M)$ and it follows $ij \subseteq L$, $K \subseteq LM$ and also $M \subseteq K$ because $\tilde{K} \subseteq \widetilde{LM}$. Thus K decomposes into $K = K'M$ where naturally $K' \cap M = \emptyset$. This proves that $(ij|K') \in \mathrm{restr}_L \mathrm{cond}_M A$. □

Proposition 2.8 shows that faces of the hypercube provide a geometric intuition and a compact encoding of established definitions of minor. The following definition introduces notation reflecting this as well as an opposite operation called *embedding*, which mounts a set of squares from the I-cube into an $|I|$-dimensional face of a higher hypercube.

Definition 2.9. (1) For a set $A \subseteq \mathcal{A}_N$ and $(I|K) \in \mathcal{F}^N_k$, the $(I|K)$-*minor* of A is the set $A \searrow (I|K) := \pi_{(I|K)}(A \cap (I|K)) \subseteq \mathcal{A}_I$. A k-*minor* is an $(I|K)$-minor with $|I| = k$.

(2) For a set $A \subseteq \mathcal{A}_I$ and $(I|K) \in \mathcal{F}^N_k$, the *embedding* of A *into* $(I|K)$ is the preimage $A \nearrow (I|K) := \pi^{-1}_{(I|K)} A \subseteq \mathcal{A}_N$.

Some theorems in matroid theory are devoted to the characterisation of certain classes of matroids — or the impossibility thereof — in terms of forbidden and compulsory minors. We give the corresponding definitions for CI structures now. Gaussoids will be examined from this point of view in Section 4.

Definition 2.10. (1) A class $\mathfrak{A} \subseteq 2^{\mathcal{A}_n}$ of sets of squares is *minor-closed* if with $A \in \mathfrak{A}$ all minors of A belong to $\mathfrak{A}$.

(2) A set of squares X is a *forbidden minor* for a minor-closed class $\mathfrak{A}$ if it is minimal with the property that it does not belong to $\mathfrak{A}$, in the sense that all its proper minors do belong to $\mathfrak{A}$.

(3) If there is a forbidden k-minor for some k, then all non-forbidden k-minors are called *compulsory k-minors* for the class $\mathfrak{A}$.

The following algebraic relations involving the operations introduced in this section are an easy exercise and their proofs are omitted.

Lemma 2.11. Let A be a set of squares, d a face and $\sigma \in \mathcal{S}_N$ a permutation. Then the following hold: (1) $\sigma A \searrow \sigma d = \sigma(A \searrow d)$, and (2) $A^\circ \searrow d^\circ = (A \searrow d)^\circ$. $\square$

We conclude this section with two trivial observations about embeddings and minors. The first states that a family of sets of squares in various lower-dimensional hypercubes can be simultaneously embedded into the N-cube in a unique way, provided that the faces into which they are embedded are sufficiently far apart as to not intersect in any face of dimension ≥ 2. The second result states that a set of squares of the hypercube can be recognised by an array of its minors, provided that the faces which encode the minors cover all squares of the hypercube. Both statements are used extensively in the recursive construction of gaussoids in Section 4.

Lemma 2.12. (1) Let $(d_m)_{m \in M} \subseteq \mathcal{F}^N$ be a family of faces of dimension at least 2 no two of which share a square. Then every mapping $\alpha : M \mapsto 2^{\mathcal{A}_{I_{d_m}}}$ lifts uniquely to a set of squares $A := \bigsqcup_{m \in M} \alpha d_m \nearrow d_m \subseteq \mathcal{A}_N$.

(2) Let $(d_m)_{m \in M}$ be a family of faces such that every square of the hypercube is contained in at least one of them. Then a set $A \subseteq \mathcal{A}_n$ is determined by the family $(H \searrow d_m)_{m \in M}$. $\square$

3 Gaussoids in mathematical structures

3.1 Realisable gaussoids

The interest in gaussoids originally arose from the study of CI inference among N jointly regular Gaussian random variables. Conditional independence in this important class of distributions can be characterised in terms of vanishing almost-principal minors of the positive-definite covariance matrix. Based on this algebraic understanding, Matúš [Mat05] proved a general inference rule for the set of vanishing almost-principal minors of a symmetric positive-definite matrix, and, more generally, a symmetric complex matrix with non-vanishing principal minors, from which the gaussoid axioms (G1)–(G4) could be deduced.

Definition 3.1. An N-gaussoid G is *realisable* if there is a positive-definite $(N \times N)$-matrix A over $\mathbb{R}$ such that $G = \langle\!\langle A \rangle\!\rangle := \{(ij|K) \in \mathcal{A}_N : \det A_{iK,jK} = 0\}$. In this case, the matrix A is called a *realisation* of G.

The definition of realisable gaussoids stems from the special significance of positive-definite matrices in statistics. A more general definition uses matrices over an arbitrary field. The proof of Matúš' Theorem, quoted in the Introduction, generalises to symmetric matrices with non-vanishing principal minors over an arbitrary algebraically closed field. Since every field is contained in an algebraically closed field, this is enough to infer that the gaussoid axioms are fulfilled by the vanishing set of almost-principal minors of such matrices.

Definition 3.2. An N-gaussoid G is *representable over a field* $\mathbb{F}$ if there is a symmetric $(N \times N)$-matrix A over $\mathbb{F}$ with non-vanishing principal minors such that $G = \langle\!\langle A \rangle\!\rangle$. In this case, the matrix A is called an $\mathbb{F}$*-representation* of G. G is *representable* if it is $\mathbb{F}$-representable for some field $\mathbb{F}$.

Gaussoids obey some of the inference rules for the vanishing almost-principal minors of a suitable matrix, that is to say: every set of vanishing almost-principal minors of such a matrix is a gaussoid, but the converse does not hold. Indeed, one can show that the share of representable gaussoids among all gaussoids quickly tends to zero when the dimension n increases. This result was suggested by Peter Nelson [Nel]. The first part of the proof is

Lemma 3.3. Let $G = \langle\!\langle A \rangle\!\rangle$ be an $\mathbb{F}$-representable $[n]$-gaussoid. Then the $(n \times 2n)$-matrix $[I_n|A]$, where I_n is the $n \times n$ identity matrix, defines via its columns an $\mathbb{F}$-representable matroid M over $[2n]$. The mapping $G \mapsto M$ is injective.

Proof. The rank of $B := [I_n|A]$ is clearly n, thus the matroid M is determined by its non-vanishing maximal minors, as they indicate precisely the bases. The gaussoid G is determined indirectly by the *non*-vanishing almost-principal minors of A. The proof consists of providing a map from $(ij|K)$ to an n-element subset L of $[2n]$ such that the $(ij|K)$-almost-principal minor of A is equal to the maximal minor with columns L of B, up to a sign.

Define the set $L := ([n] \setminus iK) \cup (j + n) \cup (K + n)$, where $S + n$ is an element-wise translation. We show that $\det A_{iK,jK} = \pm \det B_{[n],L}$ using Laplace expansions of the columns $L \cap [n]$. At the beginning, we have a submatrix of B with row indices $[n]$ and column indices $L = ([n] \setminus iK) \cup (j+n) \cup (K+n)$. Since the $([n],[n])$-submatrix of B hosts the identity matrix, Laplace expansion of a column $k \in [n]$ possibly changes a sign in front of the determinant and deletes row and column k. After performing all the Laplace expansions for columns $L \cap [n]$, the rows which are left are $[n] \setminus (L \cap [n]) = iK$ and the columns $L \setminus (L \cap [n]) = (j+n) \cup (K+n)$. Thus this submatrix is exactly $A_{iK,jK}$ and the determinants coincide modulo sign. □

This implies a singly exponential upper bound on the number of representable gaussoids, via a result by Nelson [Nel18], which states that the number of representable matroids on $[n]$, for $n \geq 12$, is upper-bounded by $2^{n^3/4}$. In Section 4.3 we derive a doubly exponential lower bound for the number of all gaussoids to complete the proof of

Corollary 3.4. The share of representable n-gaussoids among all n-gaussoids tends to zero, as $n \to \infty$, at least as quickly as $2^{cn^3 - c'n2^n}$ for positive constants c, c'. □

Having established that the representable, and in particular realisable, gaussoids are relatively few, we turn to results on the difficulty of finding representations of a gaussoid.

The realisability of a given N-gaussoid G is equivalent to the existence of a matrix $\Sigma = (\sigma_{ij})$ over $\mathbb{R}$, whose principal and almost-principal minors we denote by p_I and $a_{ij|K}$ respectively, which satisfies the system of equations, inequations and strict inequalities

$$\begin{aligned} \sigma_{ij} &= \sigma_{ji}, && \forall\, i,j \in N, \\ p_I &> 0, && \forall\, \emptyset \subsetneq I \subseteq N, \\ a_{ij|K} &= 0, && \forall\, (ij|K) \in G, \\ a_{ij|K} &\neq 0, && \forall\, (ij|K) \in \mathcal{A}_n \setminus G. \end{aligned}$$

The set of matrices fulfilling these conditions is the *realisation space* of G. All expressions which are constrained in the above system are polynomials in the entries of Σ, hence the realisation space is a semi-algebraic set. The problem of deciding whether a semi-algebraic set is empty or not is a decision problem in the *existential theory of the reals*, which known to be decidable but `NP`-hard [BPCR16, Remark 13.10].

Another way to learn something about representable gaussoids is to group almost-principal minors of a symmetric matrix over $\mathbb{F}$ by the size of their submatrices, called the *order* of the minor, and to reduce each group to just the information whether <u>`N`</u>one, <u>`S`</u>ome (but not all) or <u>`A`</u>ll of its almost-principal minors vanish. The string of $n-1$ letters from the alphabet $\{\texttt{N}, \texttt{S}, \texttt{A}\}$ which is defined in this way, for increasing order $1 \leq k \leq n-1$, is called the *apr-sequence* of the matrix. It was introduced recently by Fallat and Martínez-Rivera [FM18]. This sequence can be defined analogously for a gaussoid G, where the order of a square $(ij|K)$ is $|K|+1$ and the k-th letter is `N` if G contains *all*, `S` if G contains some (but not all), or `A` if G contains none of the squares $(ij|K)$ with $|K| = k-1$. This definition is consistent with the apr-sequence of a represting matrix, if G is representable.

One result regarding apr-sequences is the so-called `NN` Theorem, which states that if the apr-sequence of a symmetric matrix contains two successive `N`s, then all the following letters must be `N`. For the apr-sequences of gaussoids, an even stronger "`N` Theorem" follows easily from the gaussoid axioms.

Theorem 3.5. The apr-sequence of a gaussoid G contains the letter `N` if and only if it consists entirely of `N`s. In other words, the only gaussoid whose apr-sequence contains `N` is the full gaussoid.

Proof. Suppose that the `N` is at position ℓ with $1 \leq \ell \leq n-2$. We show that the next letter is `N`. Let $(ij|kL)$ be an arbitrary square of order $\ell+1$. Then $(ij|L)$ and $(ik|L)$ are squares of order ℓ and hence contained in G. Axiom (G3) implies that $(ij|kL)$ belongs to G. If `N` is at position ℓ for $2 \leq \ell \leq n-1$, then it follows analogously using (G2) that the previous letter is also `N`. □

Besides the realisable gaussoids, $\mathbb{R}$- and $\mathbb{C}$-representable ones were discussed to some extent in [Mat05] and then in [BDKS17]. The apr-sequences in [FM18] are treated over arbitrary fields and no assumption is made about the principal minors. As far as the author is aware, $\mathbb{F}$-representable gaussoids for $\mathbb{F}$ of positive characteristic have not been investigated directly. In the following, we restrict attention to realisable gaussoids, too.

Realisable gaussoids are a fairly robust class with respect to the operations on gaussoids introduced in Section 2. For a permutation $\sigma \in \mathcal{S}_N$, one can check that $\sigma\langle\!\langle A\rangle\!\rangle = \langle\!\langle \sigma A \sigma^T\rangle\!\rangle$, where σ is also used on the right-hand side to denote its permutation matrix. Duality corresponds to inversion of the matrix and it is shown in [BDKS17, Proposition 2.6] how a representation of a minor can be derived by successive deletions of rows and columns and taking Schur complements. All these operations preserve positive definiteness. Thus a realisation of a gaussoid can be converted effectively into a realisation for: any member of its isomorphy class, its dual or any of its minors.

All minors of a realisable gaussoid are realisable, hence the class of realisable gaussoids is minor-closed. The opposite of this is not true, i.e. there exist non-realisable gaussoids all of whose minors are realisable — the forbidden minors for this class. A characterisation of realisable 4-gaussoids was carried out by Lněnička and Matúš [LM07, Corollary 5]; they give five additional "higher" inference axioms in the 4-cube, proving that 629 of 679 gaussoids on $n = 4$ are realisable. Since all 3-gaussoids are realisable, the forbidden 4-minors for realisability are exactly the 50 non-realisable 4-gaussoids. Moreover, [Šim06, Theorem 3.2] exhibits an infinite list of forbidden minors. Thus new non-realisable gaussoids with all realisable proper minors appear in arbitrarily large dimension. The gaussoid axioms (G1)–(G4) refer only to variables i, j, k which are the axes of a particular cube $(ijk|L)$. To express this restriction, we say that gaussoids are *axiomatised in cubes*. Since the number of realisable N-gaussoids is finite, they can, for fixed N, be finitely axiomatised in the N-cube. Sullivant [Sul09] showed that new CI inferences always arise in larger hypercubes and that some of them cannot be axiomatised in smaller hypercubes. There is therefore no finite complete list of axioms in a hypercube for the class of realisable gaussoids.

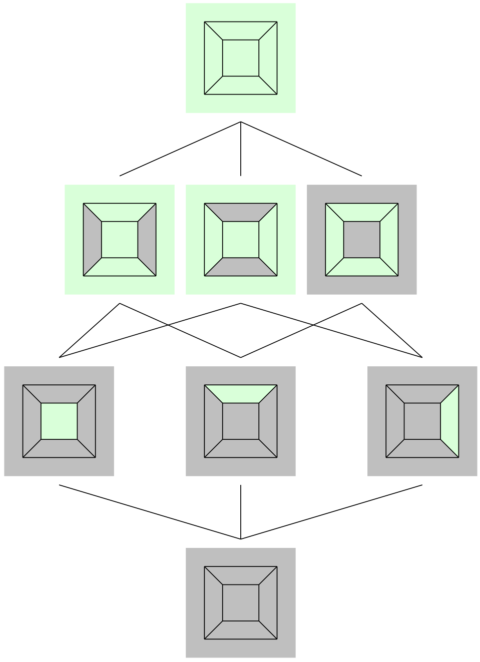


Figure 4: The sub-poset of Figure 3 consisting of the eight separation graphoids on $n = 3$. Three singletons are missing because of the ascension axiom. The duals of separation graphoids have the other half of the singletons and are otherwise the same.

3.2 Graphical gaussoids

Another class of CI models arises from simple undirected graphs by *separation* of two vertices, also known as the global Markov property in undirected graphical models, which appears here localised [Mat97] to single vertices i and j:

Definition 3.6. Let G be a simple undirected graph with vertex set N and $(ij|K) \in \mathcal{A}_N$. The set K *separates* vertices i and j in G if every path connecting i and j contains a vertex in K. The corresponding CI structure

$$\langle\!\langle G \rangle\!\rangle := \{(ij|K) \in \mathcal{A}_N : K \text{ separates } i \text{ and } j\}$$

is a *separation graphoid*.

In contrast to the class of realisable gaussoids, separation graphoids can be characterised by axioms and this was carried out in [Mat97, Section 4]:

Theorem 3.7. The separation graphoids on N are exactly the sets of squares obeying, for all distinct $i, j, k \in N$ and $L \subseteq N \setminus ijk$:

$$(ij|kL) \wedge (ik|jL) \Rightarrow (ij|L) \wedge (ik|L), \tag{G2}$$
$$(ij|L) \Rightarrow (ik|L) \vee (jk|L), \tag{G4'}$$
$$(ij|L) \Rightarrow (ij|kL). \tag{A}$$

In other words, they fulfill (G2), a stronger version of (G4) and the *ascension axiom* (A). □

Under the ascension axiom, (G4) and (G4') are equivalent. Axiom (G3) is trivially implied by (A), and (G2) together with (A) imply (G1). Thus separation graphoids might also be called *ascending gaussoids* or *graphical gaussoids*.

Figure 4 shows the separation graphoids on $n = 3$. By their axiomatisation, they are minor-closed. It is known that there are exactly $2^{\binom{n}{2}}$ separation graphoids on $[n]$. The argument is simple but provides some insight into the information encoded into separation graphoids.

Proposition 3.8. The separation graphoids on N are in bijection with the simple undirected graphs on vertices N. There are exactly $2^{\binom{n}{2}}$ of them.

Proof. Every graph G defines a distinct separation graphoid S, so it suffices to show that G can be reconstructed from the CI relation S. Since S is ascending, it is $(ij|L) \in S$ for some L if and only if $(ij|*) \in S$. But $(ij|*) \notin S$ means that there exists a path between i and j which does not use any vertex in $N \setminus ij$. Such a path must be an edge between i and j. Conversely, if this edge exists, it constitutes a path which avoids every subset of $N \setminus ij$. Thus, the set of edges of G can be reconstructed by testing $(ij|*) \in S$. □

Remark 3.9. The proof shows that there is an edge between i and j if and only if $(ij|*) \notin \langle\!\langle G \rangle\!\rangle$. The other extremal CI statements $(ij|)$ certify that every path between i and j contains no vertex, i.e. that there is no path in G between i and j. Thus the CI relation directly keeps track of edges and connected components.

Separation graphoids have even more structure. [BDKS17, Theorem 5.6] shows that they are exactly the supports of *positive gaussoids*, a type of "gaussoid with coefficients" analogous to positroids in matroid theory, and realisable. A realisation can be found in terms of the graph's adjacency matrix [LM07, Theorem 1].

The duals of ascending gaussoids are descending gaussoids. Indeed duality permutes (G1)–(G4) under their quantifiers. The dual of axiom (A) is $(ij|N\setminus ijL) \Rightarrow (ij|N\setminus ijkL)$ which, under $\forall$-quantifiers, is equivalent to

$$(ij|kL) \Rightarrow (ij|L). \tag{D}$$

There exist many examples which confirm the intuition that separation gaussoids are not closed under duality. Theorem 3.10 provides a characterisation of the intersection of separation graphoids and their duals which serves as a high-level proof of this.

Separation graphoids, or ascending gaussoids, can be equivalently defined by $(ij|K) \in \langle\!\langle G \rangle\!\rangle$ if and only if i and j are in different connected components of the graph $G \setminus K$, where the set of vertices K and all incident edges are removed from G. Dually, one finds that $(ij|K) \in \langle\!\langle G \rangle\!\rangle^\circ$ if and only if i and j are in different connected components of the induced subgraph $G[ijK]$.

This settles the action of duality on separation graphoids. Isomorphy is, as with representable gaussoids, easy: a permutation $\sigma \in \mathfrak{S}_n$ achieves a relabeling of the vertices, $\sigma\langle\!\langle G \rangle\!\rangle = \langle\!\langle \sigma G \rangle\!\rangle$. [Mat97, Lemma 3] describes procedures for modifying a graph, using vertex deletion and the insertion of small cliques, to obtain graphical representations of its minors. This shows that separation graphoids and their duals are effectively closed under isomorphy and minors.

n	Gaussoids	$\mathbb{C}$-representable	Realisable	Ascending/ Descending	Self-dual	Ascending $\cap$ Descending
3	11	11	11	8	5	5
4	679	679	629	64	39	15
5	60 212 776	$\geq$ 39 775 176 $\leq$ 55 489 560	$\leq$ 43 276 644	1 024	8 276	52
6	—	—	—	32 768	16 045 982 029	203
n	—	$\geq 2^{\frac{1}{2}n(n-1)}$ $\leq 2^{2n^3}$	$\geq 2^{\frac{1}{2}n(n-1)}$ $\leq 2^{2n^3}$	$2^{\frac{1}{2}n(n-1)}$	—	Bell_n

Table 1: Exact counts and bounds on various types of gaussoids.

The class of simultaneously ascending and descending gaussoids has a rich structure: besides fulfilling (A) and (D), all of them are self-dual and realisable. They arise from partitions of the ground set.

Theorem 3.10. The simultaneously ascending and descending N-gaussoids are in bijection with the partitions of N. Hence their cardinality is given by the Bell numbers.

Proof. Let G be an ascending and descending gaussoid. If any $(ij|K)$ is in G, then $(ij|L) \in G$ for all $L \subseteq N \setminus ij$, that is, G is determined by all $(ij|) \in G$. Then we may view G as a subset of N^2 which, due to its origin in $\mathcal{A}_N$, does not contain (i,i) for every i but is symmetric in that $(i,j) \in G$ implies $(j,i) \in G$. Gaussoid axioms (G1)–(G3) are trivial in the presence of ascension and descension axioms, and (G4) becomes $(ij|) \Rightarrow (ik|) \vee (jk|)$. To summarise, among all subsets of N^2, G obeys exactly the following axioms for all distinct i, j, k:

$$(i,i) \notin G,$$
$$(i,j) \notin G \Rightarrow (j,i) \notin G,$$
$$(i,k) \notin G \wedge (j,k) \notin G \Rightarrow (i,j) \notin G.$$

Thus G is the complement of an equivalence relation on N. ☐

Corollary 3.11. The number of realisable self-dual n-gaussoids grows at least as fast as the Bell numbers. ☐

#`SAT` solvers were employed in [BDKS17] to count the models of axiom systems related to gaussoids. The idea is that ordinary n-gaussoids are defined by their $4 \cdot 3!\binom{n}{3} \cdot 2^{n-3}$ axioms. When seen as a large conjunction of Boolean formulae in the $\binom{n}{2}2^{n-2}$ variables $(ij|K) \in \mathcal{A}_n$, the assignments to these variables which satisfy the formula describe exactly the n-gaussoids. A #`SAT` solver takes a Boolean formula as input and outputs the number of satisfying assignments. Every gaussoidal structure which can be axiomatised can be counted this way.

The ascending or descending gaussoids as well as the gaussoids which are both simultaneously are characterised in Proposition 3.8 and Theorem 3.10 respectively. Self-dual gaussoids can be axiomatised by adding the implication $(ij|K) \Rightarrow (ij|N \setminus ijK)$, for all $ij \in \binom{N}{2}$ and $K \subseteq N \setminus ij$, to the list of gaussoid axioms and running a #`SAT` solver on the resulting formula.

Jörn Papenbroock [Pap] reported the bounds for $\mathbb{C}$-representable 5-gaussoids as an intermediate result of his work on [BDKS17, Challenge 8.5]. He uses a computer algebra system to compute the ideal of almost-principal minors which are contained in a given gaussoid G, in a polynomial ring whose variables are the entries of a generic symmetric matrix. Then this ideal is successively saturated with respect to the ideal of every principal minor and every almost-principal minor outside of G. This method either produces an empty variety which certifies non-representability over $\mathbb{C}$ or a non-empty variety in which a generic point is a $\mathbb{C}$-representation of G.

The upper bound on realisable 5-gaussoids was obtained from a #`SAT` solver using the higher axioms for 4-realisability of [LM07] to axiomatise 5-gaussoids all of whose 4-minors (and trivially 3-minors) are realisable. This is an upper bound since the class of realisable gaussoids is minor-closed.

#`SAT` computations were performed using Marc Thurley's `sharpSAT` [Thu06]. The methods and results reported here will become available at www.gaussoids.de.

4 The recursive construction of gaussoids

4.1 Minor puzzles

One corollary to the gaussoid axioms is that the compulsory 3-minors of gaussoids are exactly the 3-gaussoids, since the $(ijk|L)$-minor of a gaussoid satisfies exactly the axioms (G1)–(G4) in the ijk-cube. The following lemma proves and extends this observation to k-minors for all $3 \le k \le n$. This property also holds for other local CI structures, such as semi-, pseudo- and ordinary graphoids [Mat97, Proposition 1] as well as separation graphoids, for the same reason, namely that they are axiomatised in cubes.

Lemma 4.1. Let $G \subseteq \mathcal{A}_N$ and $3 \le k \le n$. Then G is an n-gaussoid if and only if $G \searrow d$ is a k-gaussoid for every $d \in \mathcal{F}_k^N$.

Proof. First consider the case $k = 3$. The axioms in Definition 2.1 are quantified over arbitrary cubes $(ijk|L)$ together with an order on ijk, and each axiom refers to squares inside the cube $(ijk|L)$ only. No matter the order of ijk, owing to Lemma 2.11 (1), the axioms state precisely that this 3-minor is a 3-gaussoid.

The case of $k > 3$ is reduced to the statement for $k = 3$. Indeed all 3-minors are gaussoids if and only if all 3-minors of k-minors are gaussoids, because those two collections of minors are made from the same set of cubes of the n-cube. □

As a consequence, we see that the class of gaussoids is minor-closed and that the k-gaussoids are its compulsory k-minors, for all $k \ge 3$. Forbidden and compulsory minors supplement the axiomatic definition with a recursive one.

With Lemma 4.1, the construction of an n-gaussoid can be seen as a high-dimensional self-similar puzzle. The puzzle pieces are lower-dimensional gaussoids, as many of each as needed, which are to be embedded into faces of the n-cube. The difficulty comes from the fact that every square is shared by $\binom{n-2}{k-2}$ k-faces. The gaussoids must be chosen so that all of them agree on whether a shared square is an element of the n-gaussoid under construction or not. There are cases where k-gaussoids simply do not fit together in neighbouring k-faces. Furthermore, Example 4.3 exhibits a pair of n-gaussoids which, when embedded into opposite n-faces of the $(n+1)$-cube, do not permit fitting gaussoids to be assigned to all the other n-faces. At the point the failure becomes apparent, a share of $\frac{2|\mathcal{F}_2^n|}{|\mathcal{F}_2^{n+1}|} = 1 - \frac{2}{n+1}$ of all squares have already been assigned to. Consequently, even though pieces appear to fit together locally, the puzzle might not work out globally.

Lemma 2.12 (2) states that a collection of faces which cover all squares of the hypercube are enough to identify a set of squares via minors. But it is not sufficient for attesting gaussoidity to verify that all minors given by a set of faces which cover all squares are compulsory. For example, consider the set of cubes $\mathcal{C}_n \setminus c_0$ with an ignored cube $c_0 \in \mathcal{C}_n$. This set certainly covers all squares but a set of squares, which is not a gaussoid, can be constructed such that all c-minors for $c \in \mathcal{C}_n \setminus c_0$ are gaussoids. The set $H \nearrow c_0 \subseteq \mathcal{A}_n$ is not a gaussoid if $H \subseteq \mathcal{A}_3$ is not a 3-gaussoid, as certified by the minor $H = (H \nearrow c_0) \searrow c_0$. All other 3-minors are either singletons or the empty gaussoid by Corollary 2.7, which are vacuously gaussoids.

As a first application of this Lemma 4.1, we prove that the number of gaussoids grows at least exponentially.

Theorem 4.2. There are two disjoint embeddings of n-gaussoids into $(n+1)$-gaussoids, hence $|\mathfrak{G}_{n+1}| \geq 2|\mathfrak{G}_n|$.

Proof. The opposite n-faces $d = \mathtt{0}{*}^n$ and $d^\circ = \mathtt{1}{*}^n$ of the $(n+1)$-cube do not intersect, thus, by Lemma 2.12 (1), every pair in the set $\{(G, \emptyset) : G \in \mathfrak{G}_n\} \cup \{(\emptyset, G) : G \in \mathfrak{G}_n\}$ lifts to a set of squares of the $(n+1)$-cube. Let H denote one such set. We apply Lemma 4.1 with $k = 3$ to see that it is a gaussoid. Any cube $c \in \mathcal{C}_{n+1}$ lies either completely in d, completely in d° or is of the form $c = {*}x$ where $w_* x = 2$. In the first case, and analogously the second, the c-minor is a gaussoid because $H \searrow c = (H \searrow d) \searrow c$ and $H \searrow d$ is a gaussoid. In the last case, c shares exactly one square, $\mathtt{0}x$, with d and one, $\mathtt{1}x$, with d°. Since only one square of the c-face belongs to a face to which a non-empty gaussoid was assigned, the c-minor $H \searrow c$ is empty or at most a singleton, hence trivially a gaussoid. This concludes the proof that H is a gaussoid.

Apart from counting $(\emptyset, \emptyset)$ twice, all these gaussoids are distinct as an obvious consequence of Lemma 2.12 (2). The lack of one gaussoid from counting $(\emptyset, \emptyset)$ twice can be fixed by observing that the full set of squares $\mathcal{A}_{n+1}$ is a gaussoid as well and does not arise from any pair in the above construction. $\square$

It is worthwhile to consider improvements to this theorem. Since the two opposite faces $d = \mathtt{0}{*}^n$ and $d^\circ = \mathtt{1}{*}^n$ do not intersect, it seems possible to assign arbitrary pairs $(G, G') \in \mathfrak{G}_n^2$ to those faces. It cannot be expected that $G \nearrow d \sqcup G' \nearrow d^\circ$ is already a gaussoid, but if a sufficient number of these pairs allow extension to unique gaussoids, one would obtain a doubly exponential lower bound on the number of gaussoids. After G and G' have been prescribed into the $(n+1)$-cube, one has to examine the cubes outside of d and d°, which are of the form ${*}x$ with $w_* x = 2$. The set of these cubes, denoted $\mathcal{B}_{n+1}$, is in canonical bijection to $\mathcal{A}_n$. Each cube $c \in \mathcal{B}_{n+1}$ shares exactly one square with each of d and d°, namely $\mathtt{0}x$ and $\mathtt{1}x$, and these squares oppose each other in c. We say that a square in d or d° is *activated* if the prescribed n-gaussoid contains the square and *deactivated* if it does not. The other squares, outside of d and d° are initially *undecided*. There are then three cases for the activation status of the two squares in c whose possible extensions by the laws depicted in Figure 2 partition the set of 3-gaussoids:

none of them is activated this is already the empty gaussoid and possible extensions are the four singletons activating each of the non-prescribed squares, or their union, which is the unique belt avoiding the prescribed squares,

exactly one of them is activated this is already a gaussoid and there is no possible proper extension as every 3-gaussoid with more than one activated square contains the opposite of every activated square, which is forbidden here,

both of them are activated this is not a gaussoid and the possible extensions are each of the two belts through the prescribed squares and their union, which is the full gaussoid.

Every square on d or d° belongs to a single cube in $\mathcal{B}_{n+1}$ and every other square is shared by $(n-1)$ cubes in $\mathcal{B}_{n+1}$, and, again, the extensions picked for the cubes in $\mathcal{B}_{n+1}$ must all agree on the activation status of their shared squares. This is non-trivial and one can find a number of pairs of n-gaussoids to embed into d and d° which do not permit any gaussoid extension.

Example 4.3. For the n-face $d = 0{*}^n$, consider the set $H := a \nearrow d \sqcup \mathcal{A}_n \nearrow d^\circ$ for the full n-gaussoid $\mathcal{A}_n$ and a singleton $a \in \mathcal{A}_n$. We show that there exists no gaussoid $H' \supseteq H$ such that $H' \searrow d = a$ and $H' \searrow d^\circ = \mathcal{A}_n$.

To simplify notation, we may assume that $***0^{n-2}$ is the cube in $\mathcal{B}_{n+1}$ in which the singleton activates a square, namely $\mathtt{0}{*}{*}\mathtt{0}^{n-2}$. Since the opposite square $\mathtt{1}{*}{*}\mathtt{0}^{n-2}$ is activated from the full gaussoid, at least one of ${*}{*}\mathtt{00}^{n-2}$ or ${*}\mathtt{0}{*}\mathtt{0}^{n-2}$ must be activated by axiom (G4). By symmetry, we may assume that it is the former. Since $n \geq 3$, this square lies inside another cube, ${*}{*}\mathtt{0}{*}\mathtt{0}^{n-3}$, where $\mathtt{1}{*}\mathtt{0}{*}\mathtt{0}^{n-3}$ is activated by the full gaussoid in d°. The two activated faces in that cube intersect in an edge, hence form a knee, which in turn forces the activation of the square opposite to $\mathtt{1}{*}\mathtt{0}{*}\mathtt{0}^{n-3}$, contradicting the assignment of just a singleton to d.

While some pairs yield no gaussoid extension, others yield multiple, but it is not obvious whether a doubly exponential lower bound can be achieved. Instead of analysing the inter-dependencies of squares in $\mathcal{B}_{n+1}$, the next two sections derive a lower bound on the size of sets of cubes which are sufficiently independent in the n-cube so that puzzling arbitrary gaussoids into them does not create the need to check for agreement on squares.

4.2 The graphs $Q(N, k, p, q)$

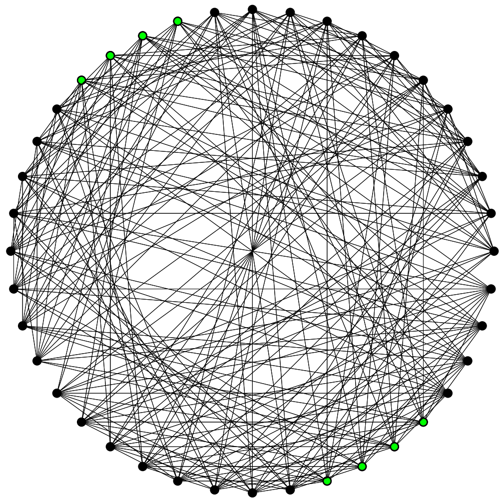
The technique developed in this section is used in the next section to derive a doubly exponential lower bound and a doubly exponential relative upper bound, whose order is optimal, on the number of gaussoids.

Definition 4.4. Let $Q(N, k, p, q)$, for $n \geq k \geq p \geq q$, be the undirected simple graph with vertex set $\mathcal{F}_k^N$ and an edge between $d, f \in \mathcal{F}_k^N$ if and only if there is a p-face s such that $\dim(d \cap s) \geq q$ and $\dim(f \cap s) \geq q$.

Pictorially, an edge exists between k-faces d and f when there is a p-dimensional "bridge" which requires q anchor dimensions on either side. For suitable choices of p and q, the faces in independent sets in these graphs will be just far enough away from each other in the hypercube to allow the compatible assignment of arbitrary k-gaussoids to them. The proof is then analogous to Theorem 4.2. Before we can execute this plan, a study of these graphs is necessary. The main result of this section is

Theorem 4.5. The graph $Q(N, k, p, q)$ is transitive, hence regular. It is complete if and only if $n + q \leq p + k$. The degree of any vertex can be calculated as follows:

$$\deg Q(N, k, p, q) = -1 + \sum_{m,j\ (\dagger)} \binom{k}{j} 2^{k-j} \binom{n-k}{k-j} \binom{n-2k+j}{m},$$


(a) $Q(5,3,2,2)$

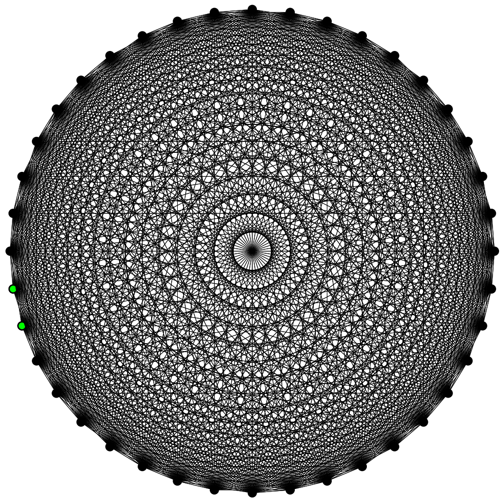

(b) $Q(5,3,3,2)$

Figure 5: Two graphs of the form $Q(5,3,p,q)$. Both are regular graphs with 40 vertices. (a) has $p = q = 2$ and degree 12, and (b) has $p = 3, q = 2$ and degree 38. Green vertices exhibit a maximal independent set.

where the sum extends over pairs $(m, j) \in [n-k] \times [k]$ which satisfy the feasibility and connectivity conditions

$$n - 2k + j \geq m \quad \wedge \quad p \geq m + 2q - \min\{q, j\}. \tag{†}$$

Proof. The textbook proof for the transitivity of the hypercube Q_n found in [GR01, Lemma 3.1.1] extends in the following way. For $\pi \in \mathcal{S}_N$ and $X \subseteq N$, define the mapping $\phi = \phi_{\pi,X} : (J|L) \mapsto \pi(J|(X \setminus J) \oplus L)$. This map is a translation mod 2 in the $(L \cup \tilde{L})$-cube inside the N-cube, followed by a permutation of the N-cube, hence a bijection. It is clear that for any pair of faces there is a mapping of this form which carries one to the other. To see that ϕ is an automorphism, it suffices to prove that $\phi(d \cap f) = \phi d \cap \phi f$. Because ϕ preserves dimension, it then follows that if d and s share a q-face, then ϕd and ϕs share a q-face as well. Applying this observation twice, namely to d, s and s, f, in the situation where d and f are connected by a p-face s shows that ϕ preserves edges in $Q(N, k, p, q)$. The critical property that ϕ commutes with intersection is proved in Lemma 4.6.

The characterisation of completeness rests on Lemma 4.7. Using the gap function ρ_q defined there, it is shown that $\rho_q(d, f) \leq p$ is equivalent to the adjacency of d and f in $Q(N, k, p, q)$ and that adjacency is inherited along decreasing gap. Since $Q(N, k, p, q)$ is regular, it is complete if and only if some vertex is adjacent to all others. For that to happen, the vertex must be adjacent to one which has the largest gap to it. As shown in the lemma, the maximum of ρ_q is $n - k + q$ and hence completeness is equivalent to $n - k + q \leq p$.

The exact degree also follows from Lemma 4.7. Since the graph is regular, we may fix any vertex d and count the adjacent faces f by their parameters $m = |(K_d \oplus K_f) \setminus I_d I_f|$ and $j = |I_d \cap I_f|$ relative to d. A priori, m ranges in $[n-k]$ and j ranges in $[k]$, but not all of their combinations allow f to be a k-face which is adjacent to d. First, we determine the pairs (m, j) for which an adjacent k-face exists and then count how many of them exist for fixed parameters. Let $(m, j) \in [n-k] \times [k]$ be given. When $j \in [k]$ is small, few $*$ symbols are shared between d and the hypothetical face f. For the $*$s of f to share exactly j $*$s with d, it must hold that $n \geq 2k - j$. Once this is given, a k-face f can be constructed if and only if the non-shared $*$s of size $k - j$ leave enough `0`s and `1`s available to create the prescribed disagreement of size m between the two faces. As an inequality this means $n - k \geq m + (k - j)$, or $n - 2k + j \geq m$. Together with $m \geq 0$, this inequality already entails the condition $n \geq 2k - j$ imposed by the choice of j. Thus it is sufficient to require only $n - 2k + j \geq m$, which is the left half of (†). Given a k-face f with parameters m and j, the existence of an edge between d and f in $Q(N, k, p, q)$ further imposes the condition Lemma 4.7 (1), which is the right half of (†).

Now let d be a fixed k-face and let $(m, j) \in [n-k] \times [k]$ satisfy (†). We count the possibilities to construct a k-face f with parameters m and j. There are $\binom{k}{j}$ ways to place the j $*$ symbols shared by d and f. On the remaining $k - j$ positions where d has $*$s, f can hold anything but $*$s without affecting the intersection dimension, so there are 2^{k-j} independent choices. f is now defined on all positions in I_d. There are $k - j$ $*$s which have to be placed in $K_d \tilde{K}_d$ in order to make f a k-face and there are $\binom{n-k}{k-j}$ choices. After this choice, I_f is fully defined and we may only place `0`s and `1`s anymore in the set $N \setminus I_d I_f$ where d has only `0`s and `1`s as well. Among the remaining $n - 2k - j$ positions, a set of size m must be chosen, where f is already determined by having to differ from d. On the remaining $n - 2k - j - m$ positions, f is determined by having not to differ from d. Note that the feasibility of all the choices enumerated above is guaranteed by (†). They sum up to

$$\sum_{m,j\ (\dagger)} \binom{k}{j} 2^{k-j} \binom{n-k}{k-j} \binom{n-2k+j}{m},$$

and since d is not adjacent to itself, which is uniquely described by the feasible parameters $j = k$ and $m = 0$, we have to subtract 1 from this sum, which concludes the proof, barring the two lemmata. □

Lemma 4.6. Let $\phi = \phi_{\pi,X}$ as defined above. Assume $\emptyset \neq s = d \cap f$, then $\phi s = \phi d \cap \phi f$.

Proof. Using Lemma 2.6, it is easy to see that if d and f intersect, then ϕd and ϕf intersect. We prove that the two components of ϕs coincide with the description of $\phi d \cap \phi f$ given in that lemma. The assumption that d and f intersect in s provides:

$$I_s = I_d \cap I_f, \tag{1}$$

$$K_s = K_d \cup K_f, \quad \tilde{K}_s = \tilde{K}_d \cup \tilde{K}_f, \tag{2}$$

$$K_d \subseteq I_f \cup K_f, \quad K_f \subseteq I_d \cup K_d. \tag{3}$$

The first component of ϕs is: $\pi I_s = \pi(I_d \cap I_f) = \pi I_d \cap \pi I_f = I_{\phi d} \cap I_{\phi f} = I_{\phi d \cap \phi f}$. The second component requires a lengthier calculation involving only the facts cited above and elementary laws of set operations. □

Lemma 4.7. For two k-faces d, f of the hypercube, define $\rho_q(d,f) := m + 2q - \min\{q,j\}$, where $m = |(K_d \oplus K_f) \setminus I_d I_f|$ and $j = |I_d \cap I_f|$. The following hold:

(1) $\rho_q(d,f) \le p$ holds if and only if d and f are adjacent in $Q(N,k,p,q)$,

(2) the range of ρ_q is $[q, n-k+q]$,

(3) ρ_q is strictly isotone with respect to q, i.e. $\rho_q < \rho_{q+1}$,

(4) for $d, d', f \in \mathcal{F}_k^n$ with $\rho_q(d,d') \le \rho_q(d,f)$, if d and f are adjacent in $Q(N,k,p,q)$, then so are d and d'.

Proof. Given two k-faces d and f, the ground set N splits into three sets: (i) $(K_d \oplus K_f) \setminus I_d I_f$ of cardinality m where both have `0` and `1` symbols only but differ, (ii) $I_d \cap I_f$ of cardinality j of shared $*$ symbols, and (iii) everything else, i.e. positions where `0` and `1` patterns agree or where `0` and `1` in one face are against $*$ in the other. In order to connect two k-faces in $Q(N,k,p,q)$, there needs to be a p-face which intersects either of them in at least q dimensions. Such a face necessarily has to cover the set of size m with $*$s, as it will not intersect both of them simultaneously with any other choice. Conversely, once m is covered, a 0-dimensional intersection with both faces is ensured by placing `0`s and `1`s appropriately. To achieve a q-dimensional intersection, q-many $*$s have to be placed on I_d and I_f each. By using the j shared $*$s, one needs at least $2q - \min\{q,j\}$ further $*$s to construct a connecting p-face. Thus $\rho_q(d,f)$ is the minimum dimension p necessary to connect d and f in $Q(N,k,p,q)$. This proves claim (1).

It is clear that ρ_q is minimal when m is minimal and j is maximal. This can be achieved simultaneously by choosing $f = d$ and there we have $\rho_q(d,d) = q$. Now consider the dual face $d^\circ = (I_d, N \setminus K_d I_d)$ of d. The gap is $\rho(d,d^\circ) = |N| - |I_d| + 2q - \min\{q, |I_d|\} = n - k + q$ assuming d is a vertex of $Q(N,k,p,q)$ where in particular $|I_d| = k \ge q$. Increasing this value would require reducing j since m is already maximal. Un-sharing $*$s with d consumes positions inside the block of `0`s and `1`s in d of size $n-k$ which reduces m by an equal amount. Hence $n-k+q$ is maximal. Furthermore, by varying m but keeping $j = k$, all values in the range $[q, n-k+q]$ can be attained, proving claim (2).

Claim (3) follows from a straightforward calculation:

$$\begin{aligned}\rho_{q+1}(d,f) - \rho_q(d,f) &= 2 - (\min\{q+1,j\} - \min\{q,j\}) \\ &= \begin{cases} 2, & j \le q, \\ 1, & j \ge q+1. \end{cases}\end{aligned}$$

In particular, this inequality reinforces that $\rho_q(d,f) \le p$ characterises the existence of a p-face which shares *at least* a q-dimensional intersection with both d and f, hence the presence of an edge in $Q(N,k,p,q)$.

In the situation of claim (4), since d and f are adjacent in $Q(N,k,p,q)$, we have $\rho_q(d,d') \le \rho_q(d,f) \le p$ by (1). Applying the same property in reverse proves the claim. □

While the formula given in Theorem 4.5 is easy to evaluate, it is not "closed enough" to be useful in its generality for the applications of $Q(N,k,p,q)$ to the construction of gaussoids. Instead, we compute the degree explicitly for parameters which fit our needs:

Corollary 4.8. (1) $Q(n, 3, 2, 2)$ is complete for $n \leq 3$. Otherwise its degree is $6(n-3) \leq 6(n-2)$.

(2) $Q(n, 3, 3, 2)$ is complete for $n \leq 4$. Otherwise its degree is $12(n-3)(n-4) + 7(n-3) \leq 12(n-1)(n-2)$. □

4.3 Bounds on the number of gaussoids

As briefly outlined before Theorem 4.5, we can use independent sets in $Q(N, k, p, q)$ to construct gaussoids and also non-gaussoids. The central technique is presented in

Proposition 4.9. Let $\mathcal{F}$ be an independent set in $Q(N, k, 3, 2)$, then the following inequality holds: $|\mathfrak{G}_n| \geq |\mathfrak{G}_k|^{|\mathcal{F}|}$.

Proof. Let $d, f \in \mathcal{F}$. Since $\mathcal{F}$ is independent, there is no $c \in \mathcal{C}_n$ which shares a square with d and with f. Since d as a k-face with $k \geq 3$ contains a cube, this implies that d and f do not share a square. Thus an assignment $\alpha : \mathcal{F} \to \mathfrak{G}_k$ lifts to a set of squares $G := \bigsqcup_{d \in \mathcal{F}} \alpha d \nearrow d \subseteq \mathcal{A}_N$. The mapping $\alpha \mapsto G$ is injective.

To see that G is a gaussoid, we examine its 3-minors. Let $c \in \mathcal{C}_n$ be arbitrary. In case c is fully contained in some $d \in \mathcal{F}$, then clearly $G \searrow c = (\alpha d \nearrow d) \searrow c = \alpha d \searrow c \in \mathfrak{G}_3$ since $\alpha d \in \mathfrak{G}_k$. Otherwise, because of Corollary 2.7, c can share at most one square with any face in $\mathcal{F}$. If it shares no square with any element of $\mathcal{F}$, then $G \searrow c$ is empty, hence a gaussoid. If it shares a square with some face in $\mathcal{F}$, it cannot share a square with any other element of $\mathcal{F}$ because $\mathcal{F}$ is an independent set in $Q(N, k, 3, 2)$. In this case, $G \searrow c$ is a singleton and hence a gaussoid. □

Proposition 4.10. Let $\mathcal{F}$ be an independent set in $Q(N, k, 2, 2)$ and denote by c the maximum size of a collection of mutually range-disjoint injections of $\mathfrak{G}_k$ into $2^{\mathcal{A}_k} \setminus \mathfrak{G}_k$. Then $\frac{2^{|\mathcal{A}_n|}}{|\mathfrak{G}_n|} \geq c^{|\mathcal{F}|}$.

Proof. The proof is analogous to Proposition 4.9 but uses the independent set to perturb any gaussoid injectively into $c^{|\mathcal{F}|}$ non-gaussoids. Again, since $q = 2$ and $\mathcal{F}$ is independent, an assignment $\alpha : \mathcal{F} \to 2^{\mathcal{A}_k}$ lifts uniquely via $\nearrow$ to a subset of $\mathcal{A}_N$. Let $\{f_i\}_{i \in [c]}$ be a set of range-disjoint injections as indicated in the claim. Consider the maps $\alpha' : \mathcal{F} \to [c]$. To each $G \in \mathfrak{G}_n$ associate $H_{\alpha'} := \bigsqcup_{d \in F} f_{\alpha' d}(G \searrow d) \nearrow d \subseteq \mathcal{A}_N$.

Because the ranges of f_is are disjoint, the mapping $(G, \alpha') \mapsto H_{\alpha'}$ is injective. None of the sets $H_{\alpha'}$ is a gaussoid since any $d \in \mathcal{F}$ certifies $H_{\alpha'} \searrow d = f_{\alpha' d}(G \searrow d) \notin \mathfrak{G}_k$. □

Remark 4.11. The proofs of Propositions 4.9 and 4.10 exploit two properties of the class $\bigcup_{n \geq 3} \mathfrak{G}_n$ of gaussoids: (1) they have a recursive puzzle property, Lemma 4.1, which is strictly stronger than being minor-closed, and (2) the empty set and all singletons on $n = 3$ are gaussoids. The same technique does not work for realisable gaussoids because they lack property (1) and not for separation graphoids because they lack property (2), and indeed Section 3 shows that these two classes cannot have a doubly exponential lower bound on their size.

We apply these propositions for $k = 3$. To find fairly large independent sets in $Q(n, 3, 3, 2)$ and $Q(n, 3, 2, 2)$, we can use Brooks' Theorem [Lov75] and the degree bounds from Corollary 4.8. By the former, since the graphs are connected, have degree at least 3 but are not complete, there exists a proper $\deg Q(n, 3, 3, 2)$-coloring of $Q(n, 3, 3, 2)$, which shows the existence of an independent set, as one color class of this coloring, whose size is at least that of an average color class:

$$\frac{|\mathfrak{F}_3^n|}{\deg Q(n,3,3,2)} \geq \frac{n(n-1)(n-2)}{6 \cdot 12(n-1)(n-2)} 2^{n-3} = \frac{n}{6^2} 2^{n-4} = \frac{n}{9} 2^{n-6}.$$

For $Q(n, 3, 2, 2)$, we find analogously

$$\frac{|\mathfrak{F}_3^n|}{\deg Q(n,3,2,2)} \geq \frac{n(n-1)(n-2)}{6 \cdot 6(n-2)} 2^{n-3} = \frac{n(n-1)}{6^2} 2^{n-3} = \frac{n(n-1)}{9} 2^{n-5}.$$

The obtained quantities can be rounded upwards to integers. Not doing so still gives a lower bound on the size of an independent set. Proposition 4.9 hence shows, using $|\mathfrak{G}_3| = 11$ and $\log_2 11 \geq 3$, that there are at least $11^{\frac{n}{9}2^{n-6}} \geq 2^{\frac{n}{3}2^{n-6}}$ n-gaussoids. Similarly, Proposition 4.10 with $c = \left\lfloor \frac{64-11}{11} \right\rfloor = 4$ gives an upper bound on the ratio of n-gaussoids of $4^{\frac{n(n-1)}{9}2^{n-5}} = 2^{\frac{n(n-1)}{9}2^{n-4}}$. Thus we have proved

Theorem 4.12. For $n \geq 5$, the number of n-gaussoids is bounded by $2^{\frac{1}{3}n2^{n-6}} \leq |\mathfrak{G}_n| \leq 2^{|\mathcal{A}_n|}/2^{\frac{4}{9}n(n-1)2^{n-6}}$. □

These bounds are bad for small n. They apply, even though the statement of the theorem does not reveal this, for $n < 5$ too. We contrast them below with the exact numbers of n-gaussoids from Table 1 for $n \leq 5$. The bounds are rounded to integers and far-away bounds displayed in exponential notation with truncated mantissa:

$$\begin{gathered} 2 \leq 11 \leq 50, \\ 2 \leq 679 \leq 665 \cdot 10^4, \\ 2 \leq 60\,212\,776 \leq 555\,249\,992 \cdot 10^{14}. \end{gathered}$$

The relative upper bound in Theorem 4.12 implies that the expected running time of a randomised algorithm for generating gaussoids, by guessing sets of squares uniformly and checking the gaussoid axioms on them, is at least doubly exponential in n.

Remark 4.13. Improvements on the constants from Brooks' Theorem are possible using methods of coding theory and combinatorics. Observe that sets of vertices in the graphs $Q(N, k, p, q)$ are special languages over the ternary alphabet $\{\mathtt{0}, \mathtt{1}, *\}$, in which every word must contain the $*$ symbol exactly k times. However, notions of coding theory, such as Hamming distance, do not directly relate to the interpretation of the graph. The $*$ symbol expresses varying between $\mathtt{0}$ and $\mathtt{1}$ and should not contribute to a notion of distance between faces, hence one defines the projection $E_{d,f}$ for two k-faces d, f which deletes from its input word all positions in $I_d I_f$. $E_{d,f}d$ and $E_{d,f}f$ are words over $\{\mathtt{0}, \mathtt{1}\}$. The Hamming distance of their projections is an appropriate measure of distance between words in our situation. This quantity appeared already in Lemma 4.7 as $m := |(K_d \oplus K_f) \setminus I_d I_f| = w_{\mathtt{1}}(E_{d,f}d \oplus E_{d,f}f)$, where the last term is the classical Hamming distance over $\{\mathtt{0}, \mathtt{1}\} \cong \mathbb{F}_2$.

For example, consider $d, f \in \mathcal{F}_3^n$ as vertices in $Q(n,3,3,2)$. By Lemma 4.7, two sufficient conditions for them not being connected by an edge are: (a) $j = 3$ and $m \geq 2$, or (b) $j = 0$ and m arbitrary. The case of $j = 3$ means $I_d = I_f$. It is an easy exercise to construct a binary code $\mathcal{D}_{n-3}$ of length $n-3$ and minimum distance 2 which has the maximum cardinality 2^{n-4} for its prescribed minimum distance. The set $\mathcal{F}_0 := \{***x : x \in \mathcal{D}_{n-3}\}$ is then independent in $Q(n,3,3,2)$ of size 2^{n-4}. Denoting by cyr_k the cyclic right-shift of a word by k symbols: $\mathrm{cyr}(x'x_1 \dots x_k) := x_1 \dots x_k x'$, we construct $\mathcal{F} := \bigcup_{k=0}^{\lfloor n/3 \rfloor - 1} \mathrm{cyr}_{3k} \mathcal{F}_0$ which remains independent because $j = 0$ for every pair of faces which come from different shifts of $\mathcal{F}_0$. This independent set has a cardinality of $\left\lfloor \frac{n}{3} \right\rfloor 2^{n-4}$. Constructing an independent set in $Q(n,3,2,2)$ leads to similar combinatorial challenges.

We leave further improvements of the constants for future work and instead concentrate on the polynomial order of n in the exponent in both bounds. Substituting the size $|\mathcal{A}_n| = \binom{n}{2} 2^{n-2}$ in the relative upper bound gives an interval for the absolute number of n-gaussoids for $n \geq 5$, which shows that $\log |\mathfrak{G}_n| \in \Omega(n2^n) \cap \mathcal{O}(n^2 2^n)$. It seems difficult to find better bounds on the polynomial order of n in the two interval endpoints. We conclude this section by showing that the linear order lower bound is indeed the limit of the independent set construction in $Q(n,3,3,2)$. The *independence number* αG of a graph G is the maximal size of an independent set in G. Similarly, the *clique number* ωG is the maximal size of a clique in the graph G. Since $Q(n,3,3,2)$ is transitive, the following inequality holds [GR01, Lemma 7.2.2]:

$$\alpha Q(n,3,3,2) \leq \frac{|\mathcal{F}_3^n|}{\omega Q(n,3,3,2)}.$$

Since $|\mathcal{F}_3^n| \in \Theta(n^3 2^n)$, it suffices to find a clique of size $\Omega(n^2)$ in every $Q(n,3,3,2)$. Take the set of cubes $\mathcal{J} := \{(1ij|) : ij \in \binom{[n] \setminus 1}{2}\}$. This set has cardinality $\binom{n-1}{2} \in \Theta(n^2)$ and any two elements $d = (1ij|)$, $f = (1kl|)$ in it are connected by an edge in $Q(n,3,3,2)$, since $\rho_2(d,f) = m + 2 \cdot 2 - \min\{2, j\} = 4 - \min\{2, j\} \leq 3$ with $m = 0$ and $j \geq 1$.

4.4 On the problem of gaussoid closure

In this section, we apply some of the earlier results and construction methods to present badly behaving examples related to gaussoid closure.

A fundamental operation for many kinds of mathematical structures is that of *closure*, i.e. to find the smallest or freest object from a certain class which contains a given object, such as the smallest linear subspace of a vector space containing a set of vectors. The class of n-gaussoids is not closed under union, for example, as suggested by their interpretation as *inference* structures; indeed, the union of two distinct singletons in the same 3-face is never a gaussoid. A notion of gaussoid closure could be applied in this case to get a replacement for the union — the smallest set of squares containing both gaussoids, which is itself a gaussoid. The common definition of a closure takes the intersection of all extensions of the given object, but this does not work for gaussoids, because they are not closed under intersection. This is a consequence of the two alternatives in the gaussoid axiom (G4): the intersection of any two distinct belts in the set of 3-gaussoids produces a 2-element set of squares in the 3-cube, which is not a gaussoid. This phenomenon is unlike other CI inference structures such as semigraphoids, which, by their axioms, are closed under intersection and hence have a closure operator.

Definition 4.14. For a set of squares $A \subseteq \mathcal{A}_n$, a gaussoid $G \supseteq A$ is a *gaussoid extension* of A. If G is additionally inclusion-minimal among all gaussoid extensions, it is a *gaussoid closure*.

The following example shows that there is indeed no unique gaussoid closure. Neither the isomorphy class nor the number of squares must coincide for two different gaussoid closures of a set of squares.

Example 4.15. (a) Consider the set of squares $A = \{\mathtt{**000}, \mathtt{**100}, \mathtt{*01*0}, \mathtt{1*00*}\}$. The first two squares oppose each other in the cube $\mathtt{***00}$ and hence fulfill the premise of axiom (G4). One of the alternatives mandated by this axiom lies in the same cube as $\mathtt{*01*0}$ and the other in the same cube as $\mathtt{1*00*}$. By repeated application of the gaussoid axioms, or Algorithm 1 introduced below, one finds that A has two minimal gaussoid extensions. To display them, we list their squares in groups corresponding to the 3-minors, repeating squares for each cube they appear in. Singleton and empty minors are omitted from the listing.

$$
\begin{aligned}
G_1 = \\
\underline{\mathtt{***00}} &: \mathtt{**000}, \mathtt{**100}, \mathtt{0**00}, \mathtt{1**00}, \\
\underline{\mathtt{***01}} &: \mathtt{**001}, \mathtt{**101}, \mathtt{0**01}, \mathtt{1**01}, \\
\underline{\mathtt{**1*0}} &: \mathtt{**100}, \mathtt{**110}, \mathtt{*01*0}, \mathtt{*11*0}, \\
\underline{\mathtt{**00*}} &: \mathtt{**000}, \mathtt{**001}, \mathtt{0*00*}, \mathtt{1*00*}, \\
\underline{\mathtt{**10*}} &: \mathtt{**100}, \mathtt{**101}, \mathtt{0*10*}, \mathtt{1*10*}, \\
\underline{\mathtt{0**0*}} &: \mathtt{0**00}, \mathtt{0**01}, \mathtt{0*00*}, \mathtt{0*10*}, \\
\underline{\mathtt{1**0*}} &: \mathtt{1**00}, \mathtt{1**01}, \mathtt{1*00*}, \mathtt{1*10*},
\end{aligned}
\qquad
\begin{aligned}
G_2 = \\
\underline{\mathtt{***00}} &: \mathtt{**000}, \mathtt{**100}, \mathtt{*0*00}, \mathtt{*1*00}, \\
\underline{\mathtt{***10}} &: \mathtt{**010}, \mathtt{**110}, \mathtt{*0*10}, \mathtt{*1*10}, \\
\underline{\mathtt{**0*0}} &: \mathtt{**000}, \mathtt{**010}, \mathtt{*00*0}, \mathtt{*10*0}, \\
\underline{\mathtt{**1*0}} &: \mathtt{**100}, \mathtt{**110}, \mathtt{*01*0}, \mathtt{*11*0}, \\
\underline{\mathtt{**00*}} &: \mathtt{**000}, \mathtt{**001}, \mathtt{0*00*}, \mathtt{1*00*}, \\
\underline{\mathtt{*0**0}} &: \mathtt{*0*00}, \mathtt{*0*10}, \mathtt{*00*0}, \mathtt{*01*0}, \\
\underline{\mathtt{*1**0}} &: \mathtt{*1*00}, \mathtt{*1*10}, \mathtt{*10*0}, \mathtt{*11*0}.
\end{aligned}
$$

Both gaussoids contain 15 squares but they are not isomorphic by Lemma 2.3 because G_1 has five distinct squares with $|K| = 2$ but G_2 has only three.

(b) The previous example can be modified slightly to yield a counterexample to the conjecture that all gaussoid closures might have the same cardinality. Starting with $A = \{\mathtt{**000}, \mathtt{**100}, \mathtt{1*00*}\}$, one obtains the two minimal extensions

$$
\begin{aligned}
G_1 = \\
\underline{\mathtt{***00}} &: \mathtt{**000}, \mathtt{**100}, \mathtt{0**00}, \mathtt{1**00}, \\
\underline{\mathtt{***01}} &: \mathtt{**001}, \mathtt{**101}, \mathtt{0**01}, \mathtt{1**01}, \\
\underline{\mathtt{**00*}} &: \mathtt{**000}, \mathtt{**001}, \mathtt{0*00*}, \mathtt{1*00*}, \\
\underline{\mathtt{**10*}} &: \mathtt{**100}, \mathtt{**101}, \mathtt{0*10*}, \mathtt{1*10*}, \\
\underline{\mathtt{0**0*}} &: \mathtt{0**00}, \mathtt{0**01}, \mathtt{0*00*}, \mathtt{0*10*}, \\
\underline{\mathtt{1**0*}} &: \mathtt{1**00}, \mathtt{1**01}, \mathtt{1*00*}, \mathtt{1*10*},
\end{aligned}
\qquad
\begin{aligned}
G_2 = \\
\underline{\mathtt{***00}} &: \mathtt{**000}, \mathtt{**100}, \mathtt{*0*00}, \mathtt{*1*00}, \\
\underline{\mathtt{**00*}} &: \mathtt{**000}, \mathtt{**001}, \mathtt{0*00*}, \mathtt{1*00*}.
\end{aligned}
$$

G_1 contains twelve distinct squares, but G_2 only seven.

Given a set of squares A, its closures, like all sets of squares, are completely described by their 3-minors. By Lemma 4.1, every 3-minor $M \searrow c$ of a closure M of A contains a 3-gaussoid which extends $A \searrow c$. This suggests Algorithm 1 to list all closures by iteratively closing 3-minors. It employs a subroutine VIOLATED, which lists all 3-faces c such that $A \searrow c \notin \mathfrak{G}_3$, and a subroutine CLOSURES3, which lists all closures of the given set of squares of the 3-cube. Both of these can be implemented using tables. SMALL-EXTENSIONS computes a list of gaussoid extensions of its argument A', not all of which are necessarily minimal. The **output** instruction adds a set of squares to the output list which is returned at the end. CLOSURES performs a post-processing step, by computing the minima of the output list in the $\subseteq$-poset of gaussoids. The extension of A' to $A' \cup (g \nearrow c)$ in line 5 corresponds to the simultaneous application of multiple gaussoid axioms in the c-cube.

Algorithm 1 The gaussoid closure algorithm.

```
1: function SMALL-EXTENSIONS(A′)
2:     output A′ if VIOLATED(A′) = ∅
3:     c ← pick VIOLATED(A′)
4:     for each g ← CLOSURES3(A′ ↘ c) do
5:         output all SMALL-EXTENSIONS(A′ ∪ (g ↗ c))
6:     end for
7: end function
8:
9: function CLOSURES(A)
10:     O ← SMALL-EXTENSIONS(A)
11:     output all ⊆-minimal elements of O
12: end function
```

Proposition 4.16. The routine CLOSURES in Algorithm 1 computes the minimal gaussoid extensions of a set of squares A.

Proof. First observe that only sets of squares without a violated cube are output. By Lemma 4.1, these are gaussoids. Furthermore, every recursive argument to SMALL-EXTENSIONS is an extension of A and every element in the output list is an extension of the argument A'. Hence the output list contains only gaussoid extensions of the original input A. Then it suffices to show that the output list of SMALL-EXTENSIONS contains all minimal gaussoid extensions. If this is the case, then the output of the post-processing step in CLOSURES is clearly the set of all minimal extensions, i.e. closures, only.

Let M be a minimal extension of A. Since M is a gaussoid extending A, all violated cubes in A must be fixed in M, by assigning extending 3-gaussoids to them. Let c be the violated cube which is picked in line 3. Then $\mathfrak{G}_3 \ni M \searrow c \supseteq A \searrow c$ and one of the iterations of 4 gives a gaussoid g with $A \searrow c \subseteq g \subseteq M \searrow c$. Thus M is still a minimal extension of $A \cup (g \nearrow c)$.

Using this invariant, we see that there is a path through the tree of recursive calls of SMALL-EXTENSIONS such that the set A'_k which is passed to the k-th call satisfies $A \subseteq A'_k \subseteq M$. This path stops eventually when A'_{k_0} becomes a gaussoid. Since this is a gaussoid extension of A contained in a minimal gaussoid extension M, it must be $A'_{k_0} = M$, which shows that M is indeed in the output list. □

The post-processing step in Closures is necessary. Some choices of g for c in line 4 might lead to violations elsewhere in the hypercube which feed back and cause c to be violated again. A cube which was violated twice has to be assigned the full 3-gaussoid the second time. The following example shows that in this way the full n-gaussoid can be put into the output list of Small-Extensions, even though it is not a minimal extension.

Example 4.17. We start from $A_0 = \mathcal{A}_3 \nearrow d \sqcup \mathcal{A}_3 \nearrow d^\circ$ for $d = 0{*}{*}{*}$, i.e. two full 3-gaussoids assigned to opposing 3-faces of the 4-cube and add some other squares, which correspond to choices which Algorithm 1 could have made on input A_0. The bigger set A specified below has the advantage that it leads to the desired phenomenon in a single step.

$$
\begin{aligned}
A = &\\
\underline{\texttt{0***}} &: \texttt{0**0}, \texttt{0**1}, \texttt{0*0*}, \texttt{0*1*}, \texttt{00**}, \texttt{01**},\\
\underline{\texttt{1***}} &: \texttt{1**0}, \texttt{1**1}, \texttt{1*0*}, \texttt{1*1*}, \texttt{10**}, \texttt{11**},\\
\underline{\texttt{***0}} &: \texttt{*0*0}, \texttt{*1*0}, \texttt{0**0}, \texttt{1**0},\\
\underline{\texttt{***1}} &: \texttt{*0*1}, \texttt{*1*1}, \texttt{0**1}, \texttt{1**1},\\
\underline{\texttt{**0*}} &: \texttt{*00*}, \texttt{*10*}, \texttt{0*0*}, \texttt{1*0*},\\
\underline{\texttt{**1*}} &: \texttt{0*1*}, \texttt{1*1*},\\
\underline{\texttt{*0**}} &: \texttt{*0*0}, \texttt{*0*1}, \texttt{*00*}, \texttt{00**}, \texttt{10**},\\
\underline{\texttt{*1**}} &: \texttt{*1*0}, \texttt{*1*1}, \texttt{*10*}, \texttt{01**}, \texttt{11**}.
\end{aligned}
$$

As can be seen from this listing, the $\texttt{**1*}$-minor of A is violated, as it contains only two squares. Since the squares oppose each other, this cube can be closed in two different ways. The first adds the two squares $\texttt{*01*}, \texttt{*11*}$ to this face which just completes the two 5-element minors and produces a gaussoid. The other alternative is adding $\texttt{**10}, \texttt{**11}$. Observe that the addition of $\texttt{**10}$ makes $\texttt{***0}$ into a 5-element minor and similarly for $\texttt{**11}$ and the $\texttt{***1}$. This set can only be closed to the full gaussoid.

This shows that Small-Extensions, when run with input A will add a non-full gaussoid as well as the full gaussoid to the output list. Clearly, the full gaussoid is not a minimal extension when another extension exists, hence proving the need for the poset minisation in Closures.

The gaussoid closures are highly non-unique. The next example shows that exponentially many minimal gaussoid extensions are possible.

Example 4.18. Let $\mathcal{F}$ be an independent set in $Q(n, 3, 3, 2)$, then we can assign a set of two opposing squares in the 3-cube to every 3-face in $\mathcal{F}$. By Lemma 2.12 (1), this assignment lifts to a subset of $\mathcal{A}_n$. In every 3-face indexed by $\mathcal{F}$, there are two minimal gaussoid extensions. All of the $2^{|\mathcal{F}|}$ possible choices lead to gaussoids, by examination of their 3-minors similar to the proof of Proposition 4.9. Because they are pairwise incomparable, it follows that all of them are minimal extensions.

The gaussoid closure can become surprisingly large as well.

Example 4.19. As a consequence of Theorem 3.5, as soon as all squares of a particular order are selected into a set of squares, its gaussoid closure is the full gaussoid. The number of squares of order k is $\binom{n}{2}\binom{n-2}{k-1}$ and this quantity is minimised for $k = 1$. Thus the set of squares of order 1, which has cardinality $\binom{n}{2}$, closes to the full gaussoid, which has cardinality $\binom{n}{2}2^{n-2}$.

Example 4.19 exhibits an input set such that for every input square, 2^{n-2} output squares are generated. It follows that the size of a gaussoid closure is not bounded polynomially in the input size. Example 4.18 shows that the number of gaussoid closures can be exponential in the input number of squares. The instances coming from large independent sets also serve as examples of large inputs which do not close to the full gaussoid.

5 Conclusion and future work

The results in this thesis roughly fall into three categories, according to how they were obtained. Section 2 introduced a calculation tool for faces of the hypercube and proofs were largely based on calculation. The proofs in Section 3, with the exception of Lemma 3.3, employed manipulations of axiom systems, notably the `N` Theorem 3.5 and the characterisations of ascending and simultaneously ascending and descending gaussoids Proposition 3.8 and Theorem 3.10. And finally Section 4 was based on minors and embeddings, their hypercube interpretation and consequently combinatorics of the hypercube. The last section applied the construction methods to produce badly behaving examples for the operation of gaussoid closure.

The association of gaussoids with sets of squares was fruitful in this regard, as it inspired the graphs $Q(N, k, p, q)$ as gaussoid construction devices. A branch of future work, following matroid theory, should investigate cryptomorphic definitions and operations for combining gaussoids to extend this toolset. [BDKS17] provides an alternative gaussoid definition to this end via combinatorial compatibility with certain quadratic trinomials which are derived from the edges inside cubes of the hypercube. This leads to *gaussoids over hyperfields* in the sense of Baker and Bowler [BB16] whose study was initiated in [BDKS17].

It was shown that the logarithm of the number of n-gaussoids is asymptotically between $n2^n$ and $n^2 2^n$. I conjecture that the polynomial order of n is closer to 2 than 1. The exponent 1 is the limit of what an independent set in $Q(n, 3, 3, 2)$ can achieve. Further work might go into varying the parameter k as well or coming up with less wasteful indexing structures for “safe” minors to assign to than independent sets.

Concerning axiomatic methods, a proper model-theoretic foundation for the *first-order language of gaussoids* is required to formulate and prove (non-)axiomatisability results for certain properties of gaussoids. Some work in this direction for graphoids was done in [CSBLLM16].

Furthermore, representability over finite fields remain to be investigated. The apr-sequences of gaussoids which were introduced ad-hoc in Section 3.1 likewise.

Acknowledgement

I would like to thank Thomas Kahle and Bernd Sturmfels for introducing me to the fascinating topic of gaussoids and independence structures and their support in my pursuit of it.

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Erklärung

Hiermit erkläre ich, dass ich die vorliegende Arbeit selbstständig und ohne Benutzung anderer als der angegebenen Quellen und Hilfsmittel angefertigt habe.

Ort, Datum, Unterschrift