Construction of Isomorphism Classes of Oriented Matroids

RALF GUGISCH
Mathematisches Institut, Universität Bayreuth
D–95440 Bayreuth, Germany
(ralf.gugisch@uni–bayreuth.de)

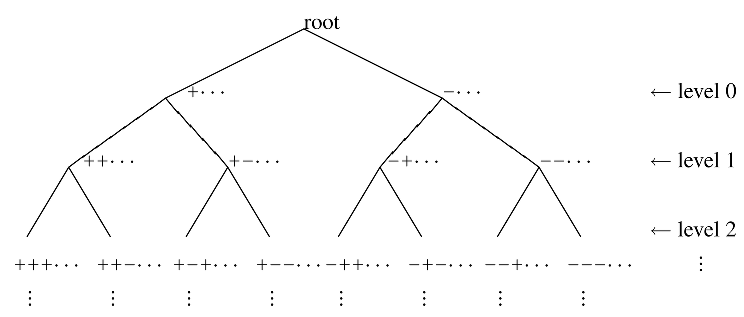
1. Introduction

We developed a generator for oriented matroids with prescribed underlying matroid. The oriented matroids are represented as chirotopes. (For some background information on oriented matroids, see the frame below.) The generation process and -output can be controlled via a variety of possible restrictions:

- The domain $D \subseteq n^k$ of the chirotope (i.e. the underlying matroid) is given as user input.
- Known orientations (besides the zeros) can be prescribed, too.
- There is the possibility to specify a list of forbidden circuits.
- You can specify a subset $R \subseteq n^k$ of relevant k-tuples, such that only partially defined chirotopes on R are generated. A partially defined chirotope $\chi_{\downarrow R}$ can be interpreted as the class of all chirotopes coinciding with $\chi_{\downarrow R}$ on R. Actually, the program generates a transversal of these classes.
- Different kinds of isomorphisms for oriented matroids can be combined arbitrarily: relabeling, negation and reorientation.
- For relabeling isomorphy, the acting group can be restricted to a subgroup G of the symmetric group.
- A group of relabeling automorphisms A can be prescribed, such that each generated solution has A as subgroup of its automorphism group.

2. The generator

The generator is implemented as backtrack algorithm:



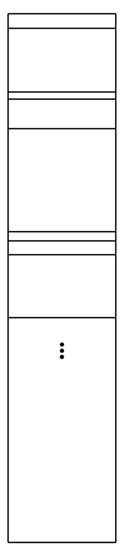
Principally, we generate all alternating functions $\chi : n^k \to \{0, \pm 1\}$ with prescribed domain $D \subseteq n^k$, but by pruning branches of the tree due to several further tests on each level, we ensure, that only chirotopes with the requested properties are reached at the last level.

On level i of the backtrack algorithm, the function value $\chi(\vec{a}^{(i)})$ for the ith ordered k-tuple $\vec{a}^{(i)} = (a_1^{(i)}, \dots, a_k^{(i)}) \in n^k$ is specified (using the reverse lexical order on k-tuples). Then, the following tests are performed:

- If the value $\chi(\vec{a})$ is known due to the generation input, then $\chi(\vec{a})$ is set accordingly, else, the two choices $\chi(\vec{a}) = +1$ and $\chi(\vec{a}) = -1$ are tried both during the backtracking.
- If a group of automorphisms is prescribed, we calculate the orbits on the k-tuples in advance. Then, after the first function value of an orbit is specified, the remaining values ensue.
- When generating up to negation, we can restrict the first otherwise freely choosable orientation to $+1$. This way, we generate exactly one candidate for each negation class.
- Similarly in the case when we generate up to reorientation: We fix up to n orientations to $+1$. The choosen k-tuples are the first ones affected by an reorientation of the points $1 \leq i \leq n$, respectively.
- Ensure, that we generate chirotopes only: For all ordered $k+2$-tuples $(x, y, a_1^{(i)}, \dots, a_k^{(i)})$, test the corresponding three-term Grassmann-Plücker relations. This way, each candidate χ reaching the last level fulfills all three-term Grassmann-Plücker relations and thus is a chirotope.
- In order to check the list of forbidden circuits, we calculate for each ordered $k+1$-tuple $(x, a_1^{(i)}, \dots, a_k^{(i)})$ the corresponding circuit.
- Whenever a sub-chirotope on $n' \leq n$ points is complete, test if the shortened chirotope $\chi_{\downarrow n'^k}$ is canonic up to relabeling (and reorientation and/or negation, if appropriate).

We use the minimal lexicographic representation of a chirotope as canonic form, taking advantage of the principle of *orderly generation*. This allows to skip (huge!) branches of the backtrack tree whenever we recognize, that a candidate χ is not minimal.

On the other hand, the minimization is much more difficult than other canonization methods using *iterated classification*. The problem gets apparent, when the operating relabelling group gets big. The drastic influence of the size of the acting group on the generation time can best be shown by an example. Below, we show the computation times for orientations of some underlying matroids of rank 3 over 8 points. Compare the group sizes $|G|$ of the automorphism group of the underlying matroid with the relative generation time per found structure:



underlying matroid	orien-tations	time in seconds	time per structure	$\lvert G\rvert$
++	135	66	0.4889	40 320
0+++	589	5	0.0084	720
0000++	66	0.8	0.0121	576
0++++++++++++++++++0++++++++++++++++++++++++++++++++++++	273	1	0.0036	72
0++++++0++	953	1	0.0010	48
0++++++0+++0	85	0.5	0.0058	48
0++++++0++++++++++++++++++++++0+++++++++++++++++++++++++	128	0.4	0.0031	48
0++++++0++++++++++++++++++++++++++0+++++++++++++++++++++	582	0.3	0.0005	8
⋮				

altogether: 4890 oriented matroids of rank 3 over 8 points

Another approach using canonization via *iterated classification* and the *homomorphism principle* is in development.

3. Comparison

Our generator is with reservations comparable to the generator of L. Finschi [1], when generating without any restrictions. The reservations are, because Finschi generates all oriented matroids of rank k on n points, in contrast to our approach of generating all orientations of an underlying matroid, only. But as the generation of uniform structures consumes by far the most time, we can compare to the generation of these.

In the following table, we list for given rank k and number n of points the number of structures up to reorientation, negation and relabelling, both of uniform oriented matroids as generated by us – as well as of all oriented matroids, as given in [1]. The generation times are given beneath the corresponding numbers. (Beware, that the different generators ran on different computers.)

$k\backslash n$	2	3	4	5	6	7	8	9	10
2	1(1)	1(1)	1(1)	1(1)	1(1)	1(1)	1(1)	1(1) 1s(0s)	1(1) 4s(0s)
3		1(1)	1(2)	1(4)	4(17)	11(143) 3s(3s)	135(4890) 1.1m(2.2m)	4 382(461 054) 0.9h(3.6h)	312 356(95 052 532) 4.2t(72t)
4			1(1)	1(3)	1(12)	11(206) 8s(10s)	2628(181 472) 1h(4.1h)		
5				1(1)	1(4)	1(25) 2s(2s)	135(6029) 16.9m(48.3m)		
6					1(1)	1(5)	1(50) 55s(26s)	4382(508 321) 3.3t(∼10t)	
7						1(1)	1(6) 1s(0s)	1(91) 19.7m(9.9m)	
8							1(1)	1(7) 14s(0s)	1(164) 11.5h(4.8h)
9								1(1) 3s(0s)	1(8) 2.8m(0s)
10									1(1) 27s(0s)

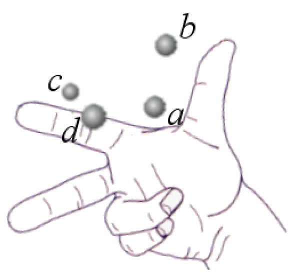
4. References

[1] L. Finschi. *A Graph Theoretical Approach for Reconstruction and Generation of Oriented Matroids*. PhD thesis, ETH Zrich, 2001.

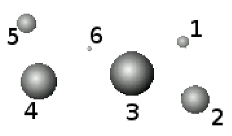
[2] R. Gugisch. *Konstruktion von Isomorphieklassen orientierter Matroide*. PhD thesis, University of Bayreuth, 2005.

Oriented Matroids, Chirotopes and Affine Point Configurations

One occurence of oriented matroids is in connection with affine configurations of a set of points in euclidian d-dimensional space. To any sequence of $d+1$ affinely independent points is assigned an orientation (positive or negative). For example, one can decide if four points in space are positively oriented by the common "right-hand rule".



By this concept we can assign to any sequence of n points an *orientation function* $\chi : n^{d+1} \to \{0, \pm 1\}$, where a function value of 0 means, that the corresponding $d+1$-tuple of points lies in a hyperplane. Obviously, χ is alternating. We can write the function as sequence of its function values at the ordered $d+1$-tuples. (We use the reverse lexical order for listing the tuples.) As example, here is an orientation function of 6 points in space:



$$\begin{array}{l} \scriptstyle 1234\ 1235\ 1245\ 1345\ 2345\ 1236\ 1246\ 1346\ 2346\ 1256\ 1356\ 2356\ 1456\ 2456\ 3456 \\ \chi = \ ++0\ --++0\ -++0\ +++ \end{array}$$

Orientation functions fulfill an oriented version of the base exchange axiom, the so called binary Grassmann-Plücker relations:

For any $\vec{a}, \vec{b} \in n^{d+1}$, the following holds:

$$\chi(\vec{a}) \cdot \chi(\vec{b}) = 1 \Longrightarrow$$
$$\exists i \in \{0, \dots, d\} : \chi(b_i, a_1, \dots, a_d) \cdot \chi(b_0, \dots, \underset{\substack{\uparrow \\ i\text{th position}}}{a_0}, \dots, b_d) = 1\,. \qquad \text{(GP)}$$

In general, alternating, non-trivial (i.e. not constantly zero) functions $\chi : n^k \to \{0, \pm 1\}$ fulfilling (GP) are called *chirotopes* of rank k. Thus, the orientation function of a sequence of points in d-dimensional euklidean space is a chirotope of rank $d+1$.

Note, that not each chirotope is an orientation function. We call chirotopes being the orientation function of an affine point configuration *affinely realizable*. The decision, if a chirotope is affinely realizable and of finding a realization is a problem of its own, shown to be NP-hard.

A chirotope implies a huge amount of further structure which is embraced in the concept of *oriented matroids*.

One such induced structure consists of the (oriented) *circuits*: A pair (C^+, C^-) of two disjunct subsets of n is called a circuit, if there exists an ordered $k+1$-tuple $(c_0, \dots, c_k) \supseteq C^+ \cup C^-$, such that for $i = 0, \dots, k$:

$$\chi(c_0, \dots, c_{i-1}, c_{i+1}, \dots, c_k) = \begin{cases} +\epsilon \cdot (-1)^i & \text{, if } c_i \in C^+ \\ -\epsilon \cdot (-1)^i & \text{, if } c_i \in C^- \\ 0 & \text{, else.} \end{cases}$$

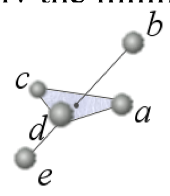
(with $\epsilon \in \pm 1$). Thus, all circuits of an oriented matroid can be obtained from the chirotope by checking all ordered $k+1$-tuples.

We write circuits as signed sets, i.e. we attach the appropriate sign to the elements of C^+ resp. C^-. For example,

$$\{+1, -3, +4, -6\} \text{ and } \{+2, -3, +4, +5, -6\}$$

are two circuits of the chirotope given above.

In an affine point configuration, two disjunct subsets of points whose convex hulls intersect are called a radon partition. The circuits of the assigned chirotope are exactly the minimal radon partitions.

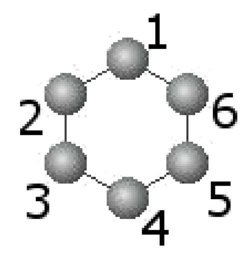


$$\{+a, -b, +c, +d, -e\}$$

Note, that an affinely realizable chirotope cannot have positive circuits, i.e. circuits (C^+, C^-) with $C^- = \emptyset$.

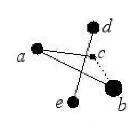
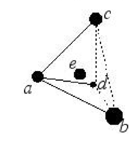
From each oriented matroid, we get an unoriented matroid, the so called *underlying matroid*, by taking the domain of the chirotope. The oriented matroid is called *uniform*, if the underlying matroid is uniform, i.e. if the chirotope has no zero function values.

Application in Chemical Conformation Analyis: The Example Cyclohexane



- The molecular graph has as automorphism group the dihedral group D_6 with 12 elements.
- Assuming that any 4 atoms are affinely independent, we prescribe the domain $D := n^4$.
- Generating all isomorphism classes of uniform chirotopes on 6 points with D_6 as acting group results in *386* solutions.

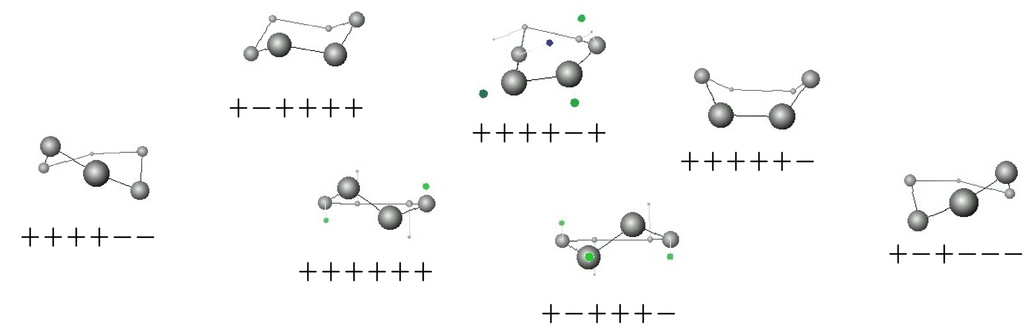
1234	1235	1245	1345	2345	1236	1246	1346	2346	1256	1356	2356	1456	2456	3456
+	+	+	+	+	+	+	+	+	+	+	+	+	+	+
+	+	+	+	+	+	+	+	+	+	+	+	+	+	−
+	+	+	+	+	+	+	+	+	+	+	+	+	−	−
+	+	+	+	+	+	+	+	+	+	+	+	−	+	+
+	+	+	+	+	+	+	+	+	+	+	+	−	−	+
⋮														

- We prescribe a list of forbidden circuits reflecting some mathematical and chemical knowledge.
  - positive circuits are not affinely realizable.
  - this situation can be avoided by excluding the circuit $(+a, +b, +c, -d, -e)$: 
  - this situation can be avoided by excluding the circuit $(+a, +b, +c, +d, -e)$: 

  By excluding forbidden circuits, we reduce the number of solutions to *162*.
- Chemical molecules are mutable. We specify a set of relevant atom-quadrupels, whose orientations remain invariant under chemical intramolecular motions, and obtain *13* partially defined chirotopes.

1234	1235	1245	1345	2345	1236	1246	1346	2346	1256	1356	2356	1456	2456	3456
+				+	+				+			+		+
+				+	+				+			+		−
+				+	+				+			−		+
+				+	+				+			−		−
+				+	+				−			+		+

- Only for *7* of these, we found a realization.



- Thereof, *4* orientation patterns lead to a chemical stable conformation.
- Repeating the generation up to negation leads to *3* orientation patterns, reflecting the fact, that two of the found conformations are mirror images of each other.