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Computing distance-regular graph and association scheme parameters in SageMath with sage-drg

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Abstract. The sage-drg package for the SageMath computer algebra system has been originally developed for computation of parameters of distance-regular graphs. Recently, its functionality has been extended to handle general association schemes. The package has been used to obtain nonexistence results for both distance-regular graphs and *Q*-polynomial association schemes, mostly using the triple intersection numbers technique.

Povzetek. Paket sage-drg za program za simbolno računanje SageMath je bil prvotno razvit za namene računanja parametrov razdaljno regularnih grafov. Njegova funkcionalnost je bila nedavno razširjena s podporo za splošne asociativne sheme. Paket je bil uporabljen pri dokazovanju neobstoja tako razdaljno regularnih grafov kot tudi *Q*-polinomskih asociativnih shem, večinoma z uporabo tehnike računanja trojnih presečnih števil.

Keywords: association schemes, distance-regular graphs, Krein parameters, triple intersection numbers, symbolic computation

1 Introduction

Let *X* be a finite set of vertices and $\{R_0, R_1, ..., R_D\}$ be a set of non-empty subsets of $X \times X$ (i.e., binary relations on *X*). Let A_i denote the adjacency matrix of the graph (X, R_i) ($0 \le i \le D$). The pair $(X, \{R_i\}_{i=0}^D)$ is called a *(symmetric) association scheme* with *D* classes if the following conditions hold:

- (1) $A_0 = I_{|X|}$, which is the identity matrix of size |X|,
- (2) $\sum_{i=0}^{D} A_i = J_{|X|}$, which is the square all-one matrix of size |X|,
- (3) $A_i^{\top} = A_i \ (1 \le i \le D),$
- (4) $A_i A_j = \sum_{k=0}^{D} p_{ij}^k A_k$, where p_{ij}^k (the *intersection numbers*) are nonnegative integers ($0 \le i, j \le D$).



Figure 1: Examples of association schemes with 3 classes with the same parameters.

Let us now consider the examples given in Figure 1. For each of them, we define relations on their vertices. If u and v are vertices of the association scheme, we have $(u,v) \in R_0$ whenever u = v, $(u,v) \in R_1$ when there is an edge between u and v, $(u,v) \in R_2$ when u and v have the same color, and $(u,v) \in R_3$ if none of these apply. Note that in the two examples on the left, the lines represent cliques, so $(u,v) \in R_1$ holds whenever u and v are in the same row or column (but not both), while the two examples on the right are embedded on a torus (i.e., we identify parallel boundaries) and show actual edges between the vertices. We can easily verify that these examples satisfy the above conditions and thus represent association schemes with 3 classes. In fact, they all share the same intersection numbers.

$$(p_{ij}^{0})_{i,j=0}^{3} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 6 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 6 \end{pmatrix} \qquad (p_{ij}^{1})_{i,j=0}^{3} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 2 & 1 & 2 \\ 0 & 1 & 0 & 2 \\ 0 & 2 & 2 & 2 \end{pmatrix}$$
$$(p_{ij}^{2})_{i,j=0}^{3} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 2 & 0 & 4 \\ 1 & 0 & 2 & 0 \\ 0 & 4 & 0 & 2 \end{pmatrix} \qquad (p_{ij}^{3})_{i,j=0}^{3} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 2 & 2 & 2 \\ 0 & 2 & 0 & 1 \\ 1 & 2 & 1 & 2 \end{pmatrix}$$

Nonetheless, the four association schemes can be checked to be mutually non-isomor-

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phic.

Let us now return to general association schemes. The vector space \mathcal{M} over \mathbb{R} spanned by the matrices A_i ($0 \le i \le D$) forms an algebra (called the *Bose-Mesner algebra*), which has a second basis $\{E_0, E_1, \ldots, E_D\}$ consisting of projectors to the common eigenspaces of the matrices A_i ($0 \le i \le D$). These projectors follow a property dual to (4) above:

$$E_i \circ E_j = \frac{1}{|X|} \sum_{k=0}^{D} q_{ij}^k E_k \quad (0 \le i, j \le D).$$

Here, \circ represents entrywise matrix multiplication. The constants q_{ij}^k are called the *Krein parameters*. The Krein parameters thus have a role dual to the intersection numbers, although, unlike the latter, they are not required to be integral – however, by the *Krein condition*, they must always be nonnegative. The Krein parameters of an association scheme can be computed from its intersection numbers and vice-versa. In fact, we may do so for the association schemes from Figure 1 using sage-drg¹.

sage:	import drg		
sage:	p = [[1, 0],	0, 0], [0, 6, 0, 0], [0, 0, 3, 0], [0, 0	0, 0, 6]],
:	[[0, 1,	0, 0], [1, 2, 1, 2], [0, 1, 0, 2], [0, 2]	2, 2, 2]],
:	[[0, 0,	1, 0], [0, 2, 0, 4], [1, 0, 2, 0], [0, 4]	4, 0, 2]],
:	[[0, 0,	0, 1], [0, 2, 2, 2], [0, 2, 0, 1], [1, 2]	2, 1, 2]]]
sage:	<pre>scheme = drg.</pre>	ASParameters(p)	
sage:	scheme.kreinP	arameters()	
0: [1	0 0 0] 1:	[0 1 0 0] 2: [0 0 1 0] 3: [0 0 0	1]
[0]	6 0 0]	[1 2 1 2] [0 2 0 4] [0 2 2 2	2]
[0]	0 3 0]	[0 1 0 2] [1 0 2 0] [0 2 0	1]
[0]	0 0 6]	[0 2 2 2] [0 4 0 2] [1 2 1 2	2]

We notice that the Krein parameters match the intersection numbers, showing that our schemes are *formally self-dual*.

A standard problem in the theory of association scheme is that of existence and classification: given a parameter set, does such an association scheme exist? If so, is it unique? Can all examples be constructed? A parameter set is said to be *feasible* if no condition is known that would rule out its existence. For more about association schemes, see Bannai & Ito [1].

A special class of association schemes is that of *P*-polynomial (or metric) association schemes. An association scheme is said to be *P*-polynomial whenever $A_i = v_i(A_1)$, where v_i is a polynomial of degree i ($0 \le i \le D$), for some ordering of its relations. Equivalently, the relation R_i corresponds to being at distance i in the graph (X, R_1) . These graphs are precisely the *distance-regular graphs*, which have been extensively studied, and for which many tables of feasible parameters have been compiled [2, 3, 4, 6]. All

¹The outputs have been condensed for brevity.

the parameters of a *P*-polynomial association scheme can be computed from a subset of its intersection numbers, namely $b_i = p_{1,i+1}^i$ ($0 \le i \le D - 1$) and $c_i = p_{1,i-1}^i$ ($1 \le i \le D$). These are usually written as the *intersection array* { $b_0, b_1, \ldots, b_{D-1}; c_1, c_2, \ldots, c_D$ }.

Dually, we may define a class of *Q*-polynomial (or cometric) association schemes as those for which $E_i = v_i^*(E_1)$, where v_i^* is a polynomial (for entrywise multiplication) of degree i ($0 \le i \le D$), for some ordering of its eigenspaces. Similarly as for *P*-polynomial schemes, the parameters of a *Q*-polynomial association scheme can be computed from a subset of its Krein parameters, namely $b_i^* = q_{1,i+1}^i$ ($0 \le i \le D - 1$) and $c_i^* = q_{1,i-1}^i$ ($1 \le i \le D$). These are usually written as the *Krein array* { $b_0^*, b_1^*, \ldots, b_{D-1}^*; c_1^*, c_2^*, \ldots, c_D^*$ }. Unlike for the *P*-polynomial association schemes, no general combinatorial characterization is known for *Q*-polynomial schemes. Although it was already Delsarte [8] who noticed that many *Q*-polynomial association schemes are related to combinatorial designs, they have only received considerable attention in the past few years [7, 11, 13, 14, 16, 17]. Williford [23] has also published a list of feasible parameters for certain types of *Q*-polynomial association schemes with few classes.

2 The sage-drg package

As the name suggests, the sage-drg package [21] has been developed by the author to support his research in distance-regular graphs. Recently, the functionality of the package has been extended to support general association schemes. It is written as an extension for the SageMath computer algebra system [19], which is free open-source software written in the Python programming language [18], with many functionalities deriving from other free open-source software, such as Maxima [15], which is used for symbolic computation, or the GLPK [12] and CBC [9] linear programming solvers. The sage-drg package is thus also free open-source software available under the MIT license, written in the Python programming language, making use of the SageMath library.

Once the package is installed and loaded into SageMath, the DRGParameters class can be used to represent parameter sets of distance-regular graphs. To instantiate such an object, an intersection array can be passed to its constructor in the form of two lists or tuples of the same length.

```
sage: from drg import DRGParameters
sage: syl = DRGParameters([5, 4, 2], [1, 1, 4])
sage: syl
Parameters of a distance-regular graph with intersection array
{5, 4, 2; 1, 1, 4}
```

For parameter sets of *Q*-polynomial association schemes, the QPolyParameters class can be used to instantiate objects from Krein arrays.

```
sage: from drg import QPolyParameters
sage: m11 = QPolyParameters([10, 242/27, 11/5], [1, 55/27, 44/5])
sage: m11
Parameters of a Q-polynomial association scheme with Krein array
{10, 242/27, 11/5; 1, 55/27, 44/5}
```

Given these arrays, the remaining parameters can be computed.

<pre>sage: syl.pTable()</pre>																
0:	Γ	1	0	0	0]	1:	[0 1	0	0]							
	Ε	0	5	0	0]		[1 0	4	0]							
	Ε	0	0	20	0]		[0 4	8	8]							
	Γ	0	0	0	10]		[0 0]	8	2]							
2:	[0	0	1	0]	3:	[0	0	0	1]						
	Ε	0	1	2	2]		[0	0	4	1]						
	Ε	1	2	11	6]		[0	4	12	4]						
	[0	2	6	2]		[1	1	4	4]						
<pre>sage: syl.kreinParameters()</pre>																
0:	Ε	1	0	0	0]					1:	Γ	0	1	0	0]	
	Ε	0	16	0	0]						Γ	1	44/5	22/5	9/5]	
	Ε	0	0	10	0]						[0	22/5	2	18/5]	
	[0	0	0	9]						[0	9/5	18/5	18/5]	
2:	Ε		(0	0		1		0]	3:	[0	0	0	1]	
	[(0 17	76/25	16/5	5 14	4/2	25]		[0	16/5	32/5	32/5]	
	[1	16/5	4	4	9,	/5]		[0	32/5	2	8/5]	
	Г		(0 14	44/25	9/!	5 3	6/	25]		Γ	1	32/5	8/5	0]	

The package also supports variables in the parameters.

The parameter sets can be checked for feasibility. Note that many more feasibility conditions are known for *P*-polynomial schemes than for general or *Q*-polynomial schemes.

```
sage: f1.check_feasible() # no error, parameter set is feasible
sage: f2.check_feasible()
...
InfeasibleError: nonexistence by JurišićVidali12
```

A more detailed description of the usage of the package is given in [20].

3 Nonexistence results

The package can also be used to compute *triple intersection numbers* of an association scheme, i.e., counts of vertices in given relations to a chosen triple of vertices. Unlike the intersection numbers, which are constants with regard to the choice of two vertices in a given relation and the relations to each of them, triple intersection numbers may depend on the particular choice of the triple and not only the relations between them. Still, in some cases, equations can be obtained from the Krein condition [5] which limit the possible values of triple intersection numbers, sometimes down to a manageable number of solutions.

In the paper introducing the package [22], the author has used it to compute triple intersection numbers for a family of feasible intersection arrays of distance-regular graphs and three more sporadic cases, each time obtaining a contradiction, thus concluding the nonexistence of the corresponding graphs. In a subsequent collaboration with Gavrilyuk and Suda [10], the same technique has been used to show nonexistence for a family of feasible Krein arrays of *Q*-polynomial association schemes derived from a class of putative tight 4-designs, thus also showing their nonexistence and closing a long-standing problem in design theory.

Gavrilyuk and the author have also used the package to show nonexistence of many feasible examples of *Q*-polynomial association schemes appearing in the tables by Williford [23] (paper still in preparation). Although it was enough, in most cases, to observe that there are no solutions for triple intersection numbers corresponding to a particular triple of vertices, a few cases required further checks which showed that the obtained solutions were inconsistent, and thus corresponding association schemes cannot exist. Integer linear programming facilities provided by SageMath have been employed to efficiently generate the needed solutions to either derive a contradiction or arrive to a set of solutions which are consistent with each other.

To obtain the above results, the newly added features of sage-drg have been used extensively. More than 2000 lines of code (nearly half of the existing codebase) have been written or rewritten to support general association schemes (and, in particular,

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Q-polynomial association schemes) and to implement a generator of integral solutions of systems of linear inequalities, which was used to search for contradictions as described above. Altogether, the results imply nonexistence for 133 sets of parameters of association schemes listed in tables of feasible parameters, and four infinite families of parameter sets.

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