Enumeration of Seidel matrices

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Overview

This talk is about the **real** equiangular lines problem.

Seidel matrices (review from previous talk)

$$S = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & -1 & 1 \\ 1 & -1 & 0 & -1 \\ 1 & 1 & -1 & 0 \end{bmatrix}$$

Definition

A symmetric matrix $S = S^T$ with 0s on the main diagonal and $\{-1, 1\}$ entries otherwise is called a Seidel matrix.

The group of signed permutation matrices act on Seidel matrices by $S \to PSP^{-1}$. The orbits are called switching classes.
One is interested in Seidel matrices up to this equivalence. In this talk: equivalence-free exhaustive generation is discussed.
The spectrum of S, $\Lambda(S)$ is the multiset of (real) eigenvalues $\{\lambda_1, \lambda_2, \ldots, \lambda_n\}$. We use the notation $\Lambda(S) := \{[\lambda_1]^{m_1}, \ldots, [\lambda_r]^{m_r}\}$.
The spectrum is an invariant up to switching.

Equiangular lines (review from previous talk)

Definiton

Let $d \geq 1$, and $n \geq 1$. A set of n lines, represented by unit vectors f_1, $\dots$, $f_n \in \mathbb{R}^d$ is called equiangular, if $|\langle f_i, f_j \rangle| = \alpha$ for all $i \neq j$.

Note for the pedantic: α is not really the angle, but let's not get lost in notation.

Equivalent descriptions:

- n equiangular lines in $\mathbb{R}^d$, as geometric objects
- unit norm columns of the $d \times n$ 'short-fat-matrix' F
- the $n \times n$ Gram matrix $G := F^T F$ of rank d with $G_{ii} = 1$ and $G_{ij} = G_{ji} = \pm\alpha$
- for $\alpha > 0$, $S := (G - I)/\alpha$ with smallest eigenvalue $\lambda_{\min} = -1/\alpha < 0$ of multiplicity $n - d$.

Note: Maximum number of lines: $N(d) \geq d + 1$ (take the simplex)

Very small Seidel matrices

Task

To generate ("visit") each equivalence class of Seidel matrices of order $n \geq 1$ exactly once. (Usually with additional constraints.)

Example: Seidel matrices for $n \leq 3$ (there are $2^{n(n-1)/2}$ of them)

$$S = \begin{bmatrix} 0 \end{bmatrix}, \qquad U = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \sim \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} = V.$$

$$X = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix} \sim \begin{bmatrix} 0 & -1 & 1 \\ -1 & 0 & -1 \\ 1 & -1 & 0 \end{bmatrix} \sim \begin{bmatrix} 0 & 1 & -1 \\ 1 & 0 & -1 \\ -1 & -1 & 0 \end{bmatrix} \sim \begin{bmatrix} 0 & -1 & -1 \\ -1 & 0 & 1 \\ -1 & 1 & 0 \end{bmatrix},$$

$$Y = \begin{bmatrix} 0 & -1 & -1 \\ -1 & 0 & -1 \\ -1 & -1 & 0 \end{bmatrix} \sim \begin{bmatrix} 0 & 1 & -1 \\ 1 & 0 & 1 \\ -1 & 1 & 0 \end{bmatrix} \sim \begin{bmatrix} 0 & -1 & 1 \\ -1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix} \sim \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & -1 \\ 1 & -1 & 0 \end{bmatrix}.$$

$$\Lambda(X) = \{[-1]^2, [2]^1\}, \qquad \Lambda(Y) = \{[-2]^1, [1]^2\}.$$

Historical and contemporary remarks

The number of inequivalent Seidel matrices quickly goes out of control.

n	#	Generated by
1	1	
2	1	
3	2	
4	3	
5	7	
6	16	
7	54	Van Lint, Seidel (1966, by hand)
8	243	
9	2.038	Bussemaker, Mathon, Seidel (1981)
10	33.120	Spence (early 1990s)
11	1.182.004	McKay (1990s)
12	87.723.296	Greaves, Koolen, Munemasa, Sz., 2014
13	12.886.193.064	Östergård and Sz., 2016
14	3.633.057.074.584	The number follows from Robinson's result

Seidel matrices and Euler graphs

Very roughly speaking generating the $n \times n$ Seidel matrices takes about the same effort as generating the graphs on $n - 1$ vertices. Radziszowski: "Graphs on 13 vertices are now accessible."

Theorem[Mallows–Sloane, 1975]

The number of Seidel matrices up to equivalence equals to the number of Euler graphs up to graph isomorphism.

Euler graph: every vertex degree is even, but not necessarily connected.

- Explicit, computable formula is available (Robinson 1969).
- When n is odd, then every Seidel equivalence class contains a unique Euler graph. Therefore if $\Gamma_i, i \in I$ are pairwise nonisomorphic Euler graphs, with adjacency matrices $A_i, i \in I$, then $S_i := J - 2A_i - I$ are pairwise inequivalent Seidel matrices.
- The previous correspondence fails to hold for n even (already for $n = 4$), nevertheless, the number of objects agree.

Generation of combinatorial objects I

Recorded objects approach – this is what everyone knows.

- Step 0: Let $\mathcal{X}_n$ be a complete set of representatives of order n.
- Step 1: generate a superset $\mathcal{Y} \supseteq \mathcal{X}_{n+1}$ containing at least one representative (essentially, given $\mathcal{X}_n$, augment each element $X \in \mathcal{X}_n$ "in all possible ways").
- Step 2: remove duplicates from $\mathcal{Y}$ by comparing its elements with each other.

Bottleneck: needs a master "list of inequivalent objects". Not suitable for parallel computation. Not suitable to deal with cases where the number of elements of $\mathcal{X}_{n+1}$ is "large".

In terms of Seidel matrices, you append a new row and column in every possible way.

Generation II

Orderly generation. Idea: designate a "canonical" object $\varrho(S)$ for each equivalence class, and organize the search to visit these. Do this in a way so that equivalent augmented objects come from the same canonical parent.

- Step 0: Let $\mathcal{X}_n$ be a complete set of **canonical** representatives of order n.
- Step 1: for each $X \in \mathcal{X}_n$ generate a superset $Y(X)$ containing at least one representative of those matrices with ancestor X.
- Step 2: keep the canonical matrices only.

In terms of Seidel matrices, one suitable choice for ϱ is (for $n \geq 2$):

$$[\varrho(S)_{21}\varrho(S)_{31}\varrho(S)_{32}\dots\varrho(S)_{n(n-1)}] =$$

$$\max\{[Z_{21}Z_{31}Z_{32}Z_{41}Z_{42}Z_{43}\dots Z_{n1}\dots Z_{n(n-1)}]\colon Z = PSP^{-1}\}.$$

Conceptual/programming bottleneck: generating permutations with restricted prefixes. Knuth's Algorithm X does this.

Generation III

Canonical augmentation. Idea: keep an object only if the augmentation step itself is canonical.
In practice: associate a graph to the combinatorial objects, apply canonical labeling to the graph, and only keep an augmented graph if the newly appended vertex gets smallest canonical label*.

For the pedantic*: if the newly appended vertex is in the very same vertex orbit as the one with smallest canonical label.

- Step 0: Let $\mathcal{X}_n$ be a complete set of representatives of order n.
- Step 1: for each $X \in \mathcal{X}_n$ generate a superset $Y(X)$ containing at least one representative of those matrices with ancestor X. Keep only those which come from a canonical augmentation.
- Step 2: remove duplicates from $Y(X)$ by comparing its elements with each other.

Conceptual bottleneck: essentially unreadable literature. People from CS background make hardly any effort to document things pedantly, as... people from math background will not care anyways.

Example

Let's have

$$S = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}$$

Append a new row with coordinates $[1, 1, -1, 0]$, $[1, -1, 1, 0]$, $[-1, 1, 1, 0]$, respectively.

- In orderly generation only the choice $[1, 1, -1, 0]$ is accepted.
- With canonical augmentation – depending on how the labelling is done – either all three cases survive the tests (and then they are compared later), or none of them. In this latter case the Seidel matrix is discovered starting from $-S$ upon augmenting with $[1, 1, 1, 0]$.

Technically, you really need a graph here to perform a canonical labeling...

A graph representation of Seidel matrices

The goal is to encode S as a graph $X(S)$ such that if $S_1 \sim S_2$ then $X(S_1)$ and $X(S_2)$ are isomorphic as graphs.

Graph representation of $n \times n$ Seidel matrices

Let S be $n \times n$. We create a graph $X(S)$ on $3n$ vertices in the following way: a row $r_i, i \in \{1, \ldots, n\}$ of S is represented by a triplet of vertices in $X(S)$ – a "cherry" – formed by a green vertex u_i adjacent to two red vertices $v_i^{(1)}$ and $v_i^{(2)}$. $V = \{u_1, \ldots, u_n\} \cup \{v_1^{(1)}, v_1^{(2)}, \ldots, v_n^{(1)}, v_n^{(2)}\}$. The edge set in addition contains edges based on the elements S_{ij}.
$E = \{\{u_i, v_i^{(k)}\}\} \cup \{\{v_i^{(k)}, v_j^{(k)}\} \colon S_{ij} = 1\} \cup \{\{v_i^{(k)}, v_j^{(3-k)}\} \colon S_{ij} = -1\}$.

Example for $n = 2$

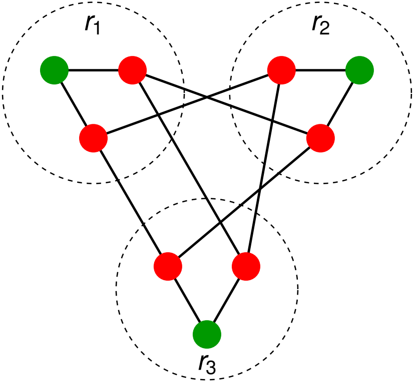
The Seidel matrix $S = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ is represented by the hexagon with a pair of antipodal green vertices.

Example of graph representation

$$S = \begin{bmatrix} 0 & -1 & 1 \\ -1 & 0 & -1 \\ 1 & -1 & 0 \end{bmatrix} \rightsquigarrow$$

The rows r_1, r_2, and r_3 correspond to the encircled "cherries".

$X(S)$



- S is represented by $X(S)$, a 2-colored graph on 9 vertices.
- Equivalence is now reduced to deciding graph isomorphism.
- $X(S)$ should be designed carefully.

Generation of Seidel matrices

Assume that $\mathcal{X}_n$ is a complete set of representatives of Seidel matrices of order n. For example, $\mathcal{X}_1 = \{\left[\begin{array}{c} 0 \end{array}\right]\}$. Starting from $\mathcal{X}_n$, we generate $\mathcal{X}_{n+1}$ by the method of canonical augmentation (McKay, 1998):

- **For** every $S \in \mathcal{X}_n$. Set up a container $\mathcal{C} \leftarrow \emptyset$.
- **For** every possible row $v \in \{\pm 1\}^n$, append v to S forming its last row and column ($S \rightsquigarrow \widehat{S}$, the dependence on v is not shown).
- Discard $\widehat{S}$ if S is not its canonical parent.
- Add $\widehat{S}$ to $\mathcal{C}$ if this equiv. class has not yet been found. **End for.**
- Output $\mathcal{C}$. **End for.**

(Some irrelevant, minor details are being skipped here, such as why anything like this would work, and how one should choose a canonical parent in the first place...)

The main point is that the equivalence class $\widehat{S}$ can be obtained from multiple starting point matrices, say from $S_0 := S, S_1, \ldots, S_k \in \mathcal{X}_n$ such that $\widehat{S_0} \sim \widehat{S_1} \sim \cdots \sim \widehat{S_k}$. We avoid duplicates by declaring a canonical parent, say S_j, to the equivalence class of $\widehat{S}$. Then $\widehat{S}_i$ is kept only if $i = j$.

Interlacing eigenvalues

Q: How do we get *large* Seidel matrices (corresponding to large set of equiangular lines)?
We have yet to use the spectrum of S.

Theorem[Interlacing:Basic version]

Assume that S is a Seidel matrix, and $\lambda \in \Lambda(S)$ of multiplicity $m \geq 2$. Let T be any principal submatrix of S. Then $\lambda \in \Lambda(T)$ of multiplicity at least $m-1$. Moreover, if λ is the smallest eigenvalue of S, then it is the smallest eigenvalue of T.

If m is "large", then we can use this result iteratively to conclude that a "small" principal submatrix of S has a prescribed eigenvalue. This structural information can be exploited during the matrix generation.

Lemma

Let S be a Seidel matrix of order n, and let $\lambda \in \Lambda(S)$ of multiplicity $m \geq 1$. Then $m = n - \mathrm{rank}(S - \lambda I)$. Moreover if $\lambda \notin \Lambda(S)$ then $\mathrm{rank}(S - \lambda I) = n$.

Exploiting interlacing: a test case

Example[$n = 28$ lines in $\mathbb{R}^7$ with common angle $\alpha = 1/3$]

Consider a Seidel matrix S corresponding to $n = 28$ equiangular lines in $\mathbb{R}^7$ (the common angle is $1/3$). S is of order 28 with $\lambda_{\min}(S) = -3$ of multiplicity exactly $m = 21$. So any 27×27 principal minor of S should have λ as an eigenvalue of multiplicity at least $20, \ldots,$ any 8×8 principal minor of S should have $\lambda = -3$ as (the smallest) an eigenvalue!

The number of Seidel matrices (up to equivalence) with $\lambda_{\min} = -3$ of multiplicity at least $n - 7$:

n	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29
#	23	37	54	70	90	101	103	101	90	70	54	37	23	16	10	5	3	2	1	1	1	0

- Recall that $|\mathcal{X}_8| = 243$, and $|\mathcal{X}_{13}| \approx 1.2 \times 10^{10}$.
- Note that there are 2^n ways to augment an $n \times n$ Seidel matrix with a new row/column (actually, enough to check half of these). For $n = 28$ this is about 268×10^6, a manageable number of cases.

Exploiting interlacing: towards catching a BIG fish

Theorem[Östergård and Sz., 2015]

The maximum number of equiangular lines in $\mathbb{R}^{12}$ with common angle $\alpha = 1/5$ is 20. There are exactly 32 distinct configurations.

Proof: along the same lines as previous example.

- Assume that there exist 21 equiangular lines in $\mathbb{R}^{12}$.
- Then it is represented by a 21×21 Seidel matrix with smallest eigenvalue -5 of multiplicity exactly 9.
- Then any 13×13 principal minor T has $\lambda_{\min}(T) = -5$.
- There are at most 26.030.960 such Seidel matrices.
- Augment these with a new row/column and increase the multiplicity of -5.
- There are no 21×21 examples.

The number of Seidel matrices with $\lambda = -5 \in \Lambda(S)$ of multiplicity at least $n - 12$:

n	13	14	15	16	17	18	19	20	21
#	26030960	8897086	2931650	851892	155223	16385	852	32	0

28 or 29 lines in $\mathbb{R}^{14}$?

Annoying, but not so important problem:

Problem

Are there $n = 29$ equiangular lines in $\mathbb{R}^{14}$ (with $\alpha = 1/5$)?

The framework developed previously could be – in principle – applied for this long standing open problem. There is a tiny caveat, however.

First steps of a (potential) proof:

- Assume that there exist 29 equiangular lines in $\mathbb{R}^{14}$.
- Then it is represented by a 29×29 Seidel matrix with smallest eigenvalue -5 of multiplicity exactly 15.
- Then any 15×15 principal minor T has $\lambda_{\min}(T) = -5$.
- We estimate, that there are about 3×10^{10} such Seidel matrices...

Remark: one may circumvent the problem of 15×15 matrices by considering 14 linearly independent equiangular vectors in $\mathbb{R}^{14}$. This corresponds to 14×14 Seidel matrices *without* the eigenvalue -5. Experiments show that there are about the same number of such matrices as above (ie. in the range of 10^{10}).

We should do 1000 times better (theory+implementation+CPUs time)

The extended binary Golay code

Theorem: $N(18) \geq 54$.

$$G := \begin{bmatrix} I_6 & O & 0 & j \\ O & I_6 & j^T & C \end{bmatrix}, \quad \text{where } C = \mathrm{Circ}(0,1,0,0,0,1,1,1,0,1,1).$$

is the generator matrix of the extended binary Golay code.

- $\mathcal{C}$ is the 759-element subset of the 2^{12} codewords of weight 8
- Let e_i be the standard basis in $\mathbb{R}^{24}$, and let $e_\Sigma := \sum_{i=1}^{24} e_i$.
- Let $f(x) := (4x - 4e_1 - e_\Sigma)/\sqrt{80}$
- Let c_1, c_2, m be explicit "magic" vectors from $\mathbb{R}^{24}$. Then

$\mathcal{L}_{22} := \{f(d) \colon d \in \mathcal{C}, \langle f(d), 4e_1 + e_\Sigma \rangle = \langle f(d), e_1 - e_2 \rangle = 0\}$ forms 176 lines in $\mathbb{R}^{22}$,

$\mathcal{L}_{21} := \mathcal{L}_{22} \cap \{f(d) \colon d \in \mathcal{C}, \langle f(d), e_1 - e_3 \rangle = 0\}$ forms 126 lines in $\mathbb{R}^{21}$,

$\mathcal{L}_{20} := \mathcal{L}_{21} \cap \{f(d) \colon d \in \mathcal{C}, \langle f(d), c_1 \rangle = 0\}$ forms 90 lines in $\mathbb{R}^{20}$,

$\mathcal{L}_{19} := \mathcal{L}_{20} \cap \{f(d) \colon d \in \mathcal{C}, \langle f(d), c_2 \rangle = 0\}$ forms 72 lines in $\mathbb{R}^{19}$,

$\mathcal{L}_{18} := \mathcal{L}_{19} \cap \{f(d) \colon d \in \mathcal{C}, \langle f(d), m \rangle = 0\}$ forms 54 lines in $\mathbb{R}^{18}$.

Problem 1

The number of Seidel matrices (up to equivalence) with $\lambda_{\min} = -3$ of multiplicity at least $n - 7$:

n	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29
#	23	37	54	70	90	101	103	101	90	70	54	37	23	16	10	5	3	2	1	1	1	0

Problem 1

Why is it so, that the number of objects on $n \geq 8$ vertices is the same as on $28 - k$?

- Is it true that all of these sub-configurations are actually inside the configuration of 28 lines?
- Is it true than that a submatrix and its "cofactor" are in 1:1 correspondence?
- What about 276 lines in $\mathbb{R}^{23}$? Do we witness the same phenomenon?

Problem 2

Problem 2

What is the number of optimal configurations in dimensions $1 \leq d \leq 23$?

- For $d = 23$ the 276-line configuration is unique.
- What about its subconfigurations, e.g. $d = 21, 22$?
- Enumerate the 48-line configurations in $\mathbb{R}^{17}$.

Problem 3

Returning once again to the question of 28 or 29 in $\mathbb{R}^{14}$.

Problem 3

Assume that there exists $n = 29$ equiangular lines in $\mathbb{R}^{14}$. Give an upper bound on its largest eigenvalue!

- Trivial: $\lambda_{\max} \geq \sqrt{437/14} > 5.58$
- Is it true that $\lambda_{\max} < 7$? This would help to get rid of junk at early stages.

In principle, results of the following flavor can be obtained **computationally**. Let $u \geq 0$ be fixed.

Theorem

There are no 29 equiangular lines in $\mathbb{R}^{14}$ with $\lambda_{\max} \leq u$.

This is true for $u = 3$ (you get stuck with the Hadamard matrices of order 16 and spectrum $\{[-5]^6, [3]^{10}\}$.) For $u = 5$ you get stuck at order 26 (conference graphs), for $u = 7$ you (maybe?) get stuck at $n = 28$.

Problem 4

Asked by B. Sudakov and coauthors:

Problem 4

Are there $O(d^4)$ bi-angular lines in dimension d?

For equiangular lines $O(d^2)$ lines can be constructed in dimension d, and this is the best possible.

Theorem[I.bd. with Greaves and others]

$$32/1089d^2 \leq n(d) \leq d(d+1)/2$$

Dr. E. King mentioned relative difference sets in Atlanta, with 3 or 4 (?) distinct inner products. Is it useful for attacking this problem? How about 4-class association schemes ($n = 17$, index type-4 circulant schemes)?

Problem 5

Problem 5

Is the 54-line configuration the largest possible in $\mathbb{R}^{18}$?

Probably not.

- There is some room for improvement up to 60 lines.
- Having noninteger eigenvalues is also somewhat suspicious.

$$\Lambda(S) = \{[-5]^{36}, [7]^{6}, [11]^{8}, [13]^{2}, [12-\sqrt{37}]^{1}, [12+\sqrt{37}]^{1}\}$$

Thank you

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