Optimal designs and root systems

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Block designs

A block design consists of a set of \( v \) points and a set of blocks, each block a \( k \)-set of points.

I will assume that it is a 1-design, that is, each point lies in \( r \) blocks. (More general versions of what follows hold without this assumption.) Then the number of blocks is \( b = \frac{vr}{k} \).

The incidence matrix \( N \) of the block design is the \( v \times b \) matrix with \((p, b)\) entry 1 if \( p \in B \), 0 otherwise. The matrix \( \Lambda = NN^\top \) is the concurrence matrix, with \((p, q)\) entry equal to the number of blocks containing \( p \) and \( q \). It is symmetric, with row and column sums \( rk \), and diagonal entries \( r \).

Optimality

The information matrix of the block design is \( L = rl - \Lambda/k \). It has a “trivial” eigenvalue 0, corresponding to the all-1 eigenvector.

The design is called

- **A-optimal** if it maximizes the harmonic mean of the non-trivial eigenvalues;
- **D-optimal** if it maximizes the geometric mean of the non-trivial eigenvalues;
- **E-optimal** if it maximizes the smallest non-trivial eigenvalue

over all block designs with the given \( v, k, r \).

A 2-design is optimal in all three senses. But what if no 2-design exists for the given \( v, k, r \)?

The question

For a 2-design, the concurrence matrix is \( \Lambda = (r - \lambda)I + \lambda J \), where \( J \) is the all-1 matrix. Ching-Shui Cheng suggested looking for designs where \( \Lambda \) is a small perturbation of this, say \( \Lambda = (r - t)I + tJ - A \), where \( A \) is a matrix with small entries (say 0, +1, −1). For E-optimality, we want \( A \) to have smallest eigenvalue as large as possible (say greater than \(-2\)).

So we want a square matrix \( A \) such that

- \( A \) has entries 0, +1, −1;
- \( A \) is symmetric with zero diagonal;
- \( A \) has constant row sums \( c \);
- \( A \) has smallest eigenvalue greater than \(-2\).

Call such a matrix admissible.

Root systems

If \( A \) is admissible, then \( 2I + A \) is positive definite, so is a matrix of inner products of a set of vectors in \( \mathbb{R}^n \).

These vectors form a subsystem of a root system of type \( A_n, D_n, E_6, E_7 \) or \( E_8 \) (as in the classification of simple Lie algebras by Cartan and Killing). Indeed, they form a basis for the root system.

(This idea was originally used by Cameron, Goethals, Seidel and Shult in 1979 for graphs with least eigenvalue \( \geq -2 \).)

So we try to determine the admissible matrices by looking for subsets of the root systems.
The case $A_n$

The vectors of $A_n$ are of the form $e_i - e_j$ for $1 \leq i, j \leq n + 1, i \neq j$, where $e_1, \ldots, e_{n+1}$ form a basis for $\mathbb{R}^{n+1}$.

So an admissible matrix of this type is represented by a tree with oriented edges. (We have an edge $j \rightarrow i$ if $e_i - e_j$ is in our subset.)

An oriented tree gives an admissible matrix if and only if
\[s(w) - s(v) = c + 2\]
for any edge $v \rightarrow w$, where $s(v)$ is the signed degree (number of edges in minus number out) and $c$ is the constant row sum.

Here is an example (edges directed upwards).

\[
\begin{pmatrix}
0 & - & + & + & - & - & + & - \\
- & 0 & - & + & + & - & + & - \\
+ & - & 0 & + & - & - & 0 & 0 \\
+ & - & + & 0 & - & - & 0 & 0 \\
- & + & - & - & 0 & + & 0 & 0 \\
- & + & - & - & + & 0 & 0 & 0 \\
+ & - & 0 & 0 & 0 & 0 & 0 & - \\
- & + & 0 & 0 & 0 & 0 & - & 0
\end{pmatrix}
\]

Conclusion

Having determined the matrices, we can use Leonard Soicher’s DESIGN software to look for block designs. Many examples exist.

An example in $E_6$ has point set $\{1, 2, 3, 4, 5, 6\}$ and blocks

\[
\{123, 125, 125, 134, 136, 136, 146, 156, 234, 245, 246, 246, 256, 345, 345, 356\}.
\]

The next step would be to go on and decide whether any $E$-optimal block designs are obtained in this way. This has not yet been done!

The case $D_n$

The vectors of $D_n$ are those of the form $\pm e_i \pm e_j$ for $1 \leq i < j \leq n$, where $e_1, \ldots, e_n$ form an orthonormal basis for $\mathbb{R}^n$.

This case is a bit more complicated. An admissible matrix is represented by a unicyclic graph, whose edges are either directed (if of form $e_i - e_j$) or undirected and signed (if of the form $\pm (e_i + e_j)$).

A similar condition for constant row sum can be formulated.

Here is an example:

The case $E_n$

There are three exceptional root systems not of the above form, in 6, 7 and 8 dimensions, called $E_6$, $E_7$ and $E_8$.

By a computer search, the numbers of admissible matrices which occur in these root systems are 2, 3, 12 respectively.