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 $b = vr/k$.

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 $L = rI - \Lambda/k$. 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 Λ 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 ≥ -2.)

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

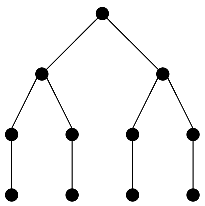
The case A_n

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 $j \to i$ 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 $v \to w$, 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).

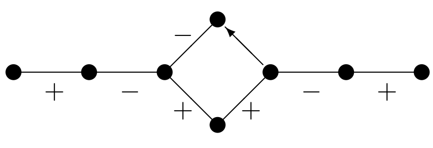


The case D_n

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.

Here is an example in E_8:

$$\begin{pmatrix} 0 & - & + & + & - & - & + & - \\ - & 0 & - & - & + & + & - & + \\ + & - & 0 & + & - & - & 0 & 0 \\ + & - & + & 0 & - & - & 0 & 0 \\ - & + & - & - & 0 & + & 0 & 0 \\ - & + & - & - & + & 0 & 0 & 0 \\ + & - & 0 & 0 & 0 & 0 & 0 & - \\ - & + & 0 & 0 & 0 & 0 & - & 0 \end{pmatrix}$$

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!