Laplacian eigenvalues and optimality: IV. Further topics

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Groups and Graphs, Designs and Dynamics
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- Sylvester designs (an interesting class of examples);
- how to recognise the concurrence graph of a block design;
- variance-balanced designs;
- the relation of optimality parameters to other graph invariants such as the Tutte polynomial.

Block designs and concurrence graphs

We have seen that the values of the various parameters associated with optimality criteria of block designs depend only on the concurrence graph of the design: to find the optimal design we have to find the graph which maximizes the number of spanning trees, or minimizes the average resistance; or whatever.

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For block designs with block size 2, the design is the same as its concurrence graph (treatments are vertices and blocks are edges). But for larger block size, there are interesting questions.

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These designs have 36 points and 48 blocks of size 6. Two points are contained in either one or two blocks: the pairs lying in two blocks are the edges of the Sylvester graph, to be defined. So the concurrence matrix has 8 on the diagonal, and 1 or 2 off-diagonal, with 2 for edges of the Sylvester graph. Thus the concurrence matrix is $8I + (J - I + A)$, where A is the adjacency matrix of the Sylvester graph.

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Conjecture

Sylvester designs are A-, D- and E-optimal among all block designs with 36 *points and* 48 *blocks of size* 6*.*

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Now we define a graph on the vertex set $A \times B$ (the Cartesian product) by the rule that (a_1, b_1) is joined to (a_2, b_2) if and only if the transposition (a_1, a_2) on A corresponds to a product of three transpositions on B, one of which is (b_1, b_2). This is the Sylvester graph.

The outer automorphism of S_6

The group S_6 acts on a set A of six points. It also acts on the 15 2-subsets of A (edges of the complete graph, or duads in Sylvester's terminology), and on the $15 \cdot 6 \cdot 1/3! = 15$ partitions into three sets of two (1-factors, or Sylvester's synthemes). The set B of size 6 is the set of partitions of the duads into five synthemes (1-factorisations, or Sylvester's synthematic totals.

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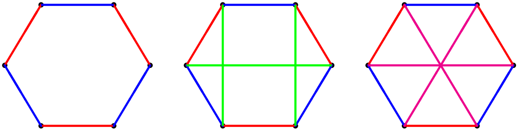

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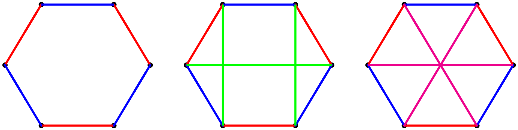

The first two synthemes in a total must form a 6-cycle. The remaining three must use the three long and six short diagonals. There are only two patterns for a syntheme of diagonals, shown in magenta and green. We cannot use the magenta since only short diagonals would remain. So the remaining three synthemes each consist of a long diagonal and two perpendicular short diagonals.

This shows that the synthematic total (partition of duads into synthemes) is unique up to isomorphism.

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Let B be the set of six synthematic totals. Then the group S_6 acts on B, and it is easy to see that this action is not isomorphic to the action on the set A of vertices; so there is an outer automorphism mapping the first to the second. Moreover, we can reverse the procedure, and find that the square of this automorphism is inner.

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It is remarkable that 6 is the only number n, finite or infinite, for which the symmetric group S_n has an outer automorphism.

The Sylvester graph

An alternative definition of the Sylvester graph: the vertex set is $A \times B$; the pairs (a_1, b_1) and (a_2, b_2) are joined if the duad $\{a_1, a_2\}$ belongs to the unique syntheme which the totals b_1 and b_2 have in common.

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The Sylvester graph is a distance-transitive graph on 36 vertices with valency 5. Its adjacency matrix has eigenvalues 5 (with multiplicity 1), 2 (multiplicity 16), -1 (multiplicity 10) and -3 (multiplicity 9). From these, the Laplacian eigenvalues of the concurrence matrix are easily computed: the non-trivial ones are 39, 42 and 44.

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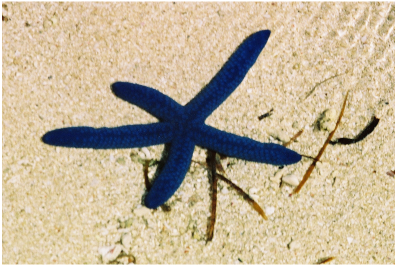
Its vertices can be regarded as the points of the 6×6 grid $A \times B$. A vertex and its five neighbours lie in distinct rows and columns. The graph contains no triangles or quadrangles. Any two vertices in different rows and columns lie at distance 1 or 2; if they are not adjacent, they have just one common neighbour.

Starfish



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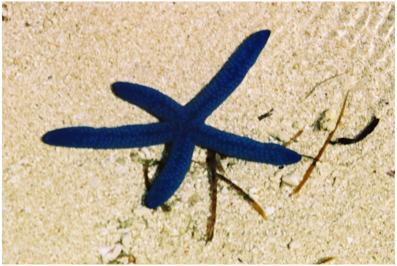

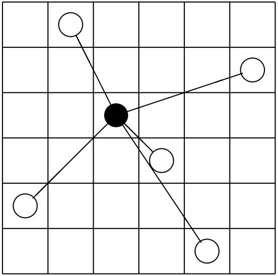

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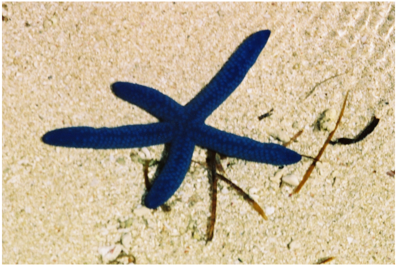

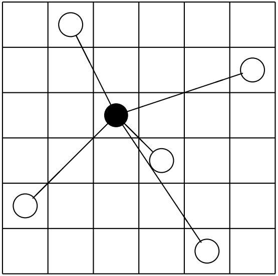

We define a starfish to consist of a vertex and its neighbours; a galaxy of starfish is the set of six starfish derived from the vertices in a column of the array.

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Good designs with lower replication can be obtained by using only some galaxies.

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This would probably be a very big computation!

Sparse versus dense

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Now sparse networks occur for the same reason as block designs with low replication, namely resource limitations. So these results are potentially of interest in network theory as well.

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The concurrence graph of such a design is the λ-fold complete graph in which any two vertices are joined by λ edges. Moreover, the design is binary.

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In the nineteenth century, Thomas Kirkman showed that this necessary condition is also sufficient for the existence of a Steiner triple system.

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Suppose that we have a BIBD with given k and λ. Given v, k, λ, the counting equations show that $r = \lambda(v-1)/(k-1)$ and $b = rv/k = \lambda v(v-1)/k(k-1)$. So a necessary condition is that $k-1$ divides $\lambda(v-1)$ and k divides $\lambda v(v-1)$.

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Theorem

If v is sufficiently large (in terms of k and λ), then the above necessary conditions are also sufficient for the existence of a BIBD.

Of course, this doesn't tell us either how large v has to be, or what to do if the necessary conditions are not satisfied!

Variance-balanced designs

A block design is variance-balanced if its concurrence matrix is a linear combination of I and the all-1 matrix J. Such a design, if binary, is a BIBD, and hence optimal on all criteria we have discussed; but here we do not assume that the design is binary. For short we write $\mathrm{VB}(v, k, \lambda)$ for a variance-balanced design with given values of these parameters, where λ is the common off-diagonal entry of the concurrence matrix.

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The non-binary design with $v = 5, k = 3$, and $b = 7$ given earlier, is variance-balanced with $\lambda = 2$:

1	1	1	1	2	2	2
1	3	3	4	3	3	4
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Treatments 1 and 2 concur twice in the first block; any other pair lie in two different blocks.

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The first design, with $\lambda = 5$, is a BIBD, and hence is optimal by Kiefer's Theorem. The second has $\lambda = 4$.

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Morgan and Srivastav have investigated these designs (which they call "completely symmetric").

VB designs with maximal trace

Morgan and Srivastav define two new parameters of a VB design, as follows:

$$r = \left\lfloor \frac{bk}{v} \right\rfloor, \qquad p = bk - vr,$$

so that $bk = vr + p$ and $0 \leq p \leq v - 1$. Thus, in a BIBD we have $p = 0$. Note that the use of r does not here imply that the design has constant replication!

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Morgan and Srivastav further say that a VB design has maximum trace if its parameters satisfy the equation $r(k-1) = (v-1)\lambda$.
In our examples above, $r = \lfloor 7 \cdot 6/7 \rfloor = 6$ and $p = 0$. Since $r(k-1)/(v-1) = 6 \cdot 5/6 = 5$, we see that the first design has maximal trace, but the second does not.

The reason for the term "maximal trace" is as follows. Since $bk < v(r+1)$, some treatment occurs at most r times on the bk plots. Each occurrence contributes at most $k-1$ edges to the concurrence graph, so the valency of this vertex is at most $r(k-1)$. But the concurrence graph of a VB design is regular, with valency $(v-1)\lambda$; so we have $(v-1)\lambda \leq r(k-1)$, and the trace of the concurrence matrix (which is $v(v-1)\lambda$) is at most $vr(k-1)$; equality for the trace implies that $(v-1)\lambda = r(k-1)$.

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In the examples, we have $r = 6$, $p = 0$, confirming that the first design has maximum trace but the second does not.

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Proof coming up …
It follows that our example of a non-binary design, with $v = 5$, $k = 3$ (which is variance-balanced and has one non-binary block) is E-optimal.

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$$b \leq \frac{\lambda v(v-1) + 2x}{k(k-1)}.$$

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The non-trivial Laplacian eigenvalues of the λ-fold complete graph are all equal to λv. So, if our design is not E-optimal, then a E-better design (with the same values of (v, b, k)) has least Laplacian eigenvalue greater than λv.

Let δ be the minimal degree of the concurrence graph of such a design. Then δ edges separate a single vertex from the rest of the graph.

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By the Cutset Lemma,

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so that $\delta > \lambda(v-1)$, or $\delta \geq \lambda(v-1) + 1$.
Hence the concurrence graph has at least $v(\lambda(v-1)+1)/2$ edges. Since each block of this design contributes at most $k(k-1)/2$ edges, we have

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Combining these two bounds for b, we see that $x \geq v/2$. So, if $x < v/2$, then no E-better design can exist.

Existence of VB designs of maximal trace

If we have two VB designs on the same set of v points with the same block size k, having parameters λ_1 and λ_2, then the multiset union of the block multisets is again VB, with parameter $\lambda_1 + \lambda_2$. The new design is not necessarily of maximum trace; but it is so if one of the VB designs we start with is a BIBD and the other is of maximum trace, or if the sum of their p parameters is less than v.

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For example, suppose that $k = 3$. A VB design of maximum trace satisfies $2r = (v-1)\lambda$, so that λ is even or v is odd. Moreover, $\lambda = 1$ is impossible (except for Steiner triple systems), since a non-binary block gives concurrence at least 2. Morgan and Srivastav proved that these necessary conditions are sufficient:

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Theorem

A $\mathrm{VB}(v, 3, \lambda)$ *design of maximum trace exists whenever* $\lambda(v-1)$ *is even and* $\lambda > 1$*.*

Proof

A BIBD with $k = 3$ and $\lambda = 6$ exists for all v. So it is enough to settle the existence question for λ in a complete set of non-zero residues mod 6. Now BIBDs exist in the following cases:

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- for $\lambda = 1$ or 5, if $v \equiv 1$ or 3 mod 6;
- for $\lambda = 2$ or 4, if $v \equiv 0$ or 1 mod 3;
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We construct VB designs for $\lambda = 2$ and $v \equiv 2$ mod 3; they have $p = 1$, so the union of two copies settles $\lambda = 4$. For $\lambda = 5$ or $\lambda = 7$, with v odd, there is a BIBD unless $v \equiv 5$ mod 6; in that case we can take a 2-design with $\lambda = 3$ and a VB design with $\lambda = 2$ or $\lambda = 4$.

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Suppose first that $v \equiv 2 \bmod 6$. There exist Steiner triple systems of orders $v \pm 1$. Take two such systems, on the point sets $\{1,\ldots,v+1\}$ and $\{1,\ldots,v-1\}$ respectively; let the sets of blocks be $\mathcal{B}_1$ and $\mathcal{B}_2$. Without loss of generality, suppose that the third point of the block B of $\mathcal{B}_1$ containing v and $v+1$ is $v-1$.

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Now we take the point set of the new design to be $\{1,\ldots,v\}$. For the blocks, we first remove the block B from $\mathcal{B}_1$; then we replace each occurrence of $v+1$ in any other block with v; the resulting blocks together with $[v-1,v-1,v]$ make up the design.

We have to check that $\{v-1, v\}$ lies only in $[v-1, v-1, v]$, while every other pair $\{i, j\}$ lies in two blocks. For the first, note that the only other candidate, namely B, has been removed. For the second, there are two cases:

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- $j = v, i \neq v-1$: in $\mathcal{B}_1$, there is one block containing i and v, and one containing i and $v+1$ (in which $v+1$ is replaced by v). No block of $\mathcal{B}_2$ can occur.

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- $j = v$, $i \neq v-1$: in $\mathcal{B}_1$, there is one block containing i and v, and one containing i and $v+1$ (in which $v+1$ is replaced by v). No block of $\mathcal{B}_2$ can occur.
- $v \notin \{i, j\}$: one block of $\mathcal{B}_1$ and one of $\mathcal{B}_2$ contain $\{i, j\}$, and these two points are unchanged in these blocks.

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Since there are many non-isomorphic Steiner triple systems, this construction gives rise to many VB designs with $k=3$.

Example

Consider the case $v = 5$, $k = 3$, $\lambda = 2$. Each block contributes either a triangle or a double edge to the concurrence graph, depending on whether or not it is binary. There are four cases:

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The values of (r, p) in the four cases are $(4, 1)$, $(4, 4)$, $(5, 2)$ and $(6, 0)$. So the first two have maximum trace; the others don't.

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If the design is binary, then each block contributes a complete graph of size k; so we have to decide whether G is the edge-disjoint union of complete graphs of size k. This is the question which is answered by Wilson's theorem in the case of the λ-fold complete graph. In general, it is necessary that every vertex has valency divisible by $k - 1$, and the total number of edges is divisible by $k(k - 1)/2$.

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What happens in general?

Weighted cliques

Let $w_1, w_2, \ldots, w_m$ be positive integers, where $m > 1$. A weighted clique with weights $w_1, \ldots, w_m$ is a graph on m vertices, in which the ith and jth vertices are joined by $w_i w_j$ edges. Its weight is the sum of the weights w_i.

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Theorem

The graph G is the concurrence graph of a block design with block size k if and only if it is an edge-disjoint union of weighted cliques each with weight k.

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This generalizes the "graph decomposition" interpretation of BIBDs. As we saw, the weighted cliques of weight 3 are a triangle and a double edge.

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- The Fano plane arises from a decomposition of the 21 edges of K_7 into seven triangles. It is unique up to isomorphism, but there are 30 different ways to make the decomposition (corresponding to the fact that the automorphism group of the Fano plane has index 30 in the symmetric group S_7).
- In our variance-balanced design with $v = 5$, $k = 3$ and $b = 7$, we took the block $[1, 1, 2]$. However, the block $[1, 2, 2]$ would have been just as good, and would have given us the same concurrence graph.

Other graph parameters

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Other evaluations of the Tutte polynomial give lots more information about the graph: number of proper colourings with a given number of colours, number of acyclic or totally cyclic orientations, etc.

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Other evaluations of the Tutte polynomial give lots more information about the graph: number of proper colourings with a given number of colours, number of acyclic or totally cyclic orientations, etc.

We will define the Tutte polynomial and consider how it is related to some of the invariants we have met.

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It is well-known that the number of proper colourings of G is the evaluation at q of a monic polynomial of degree $n = |V(G)|$, known as the chromatic polynomial of G.

This is usually proved by "deletion-contraction". It suits my purpose here to give a different proof, using "inclusion-exclusion".

Let S be the the set of all (proper or not) vertex-colourings of G with q colours. For any edge e, let T_e be the set of colourings for which e is improper (has both ends of the same colour); and for $A \subseteq E(G)$ let

$$T_A = \bigcap_{e \in A} T_e,$$

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Let $k(A)$ be the number of connected components of the graph $(V(G), A)$. A colouring in $T(A)$ has the property that all the vertices in a connected component of this graph have the same colour. So $|T_A| = q^{k(A)}$. Then there are $q^{k(A)}$ colourings in which all the edges in A are bad.

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So by PIE, the number of proper colourings is

$$\sum_{A \subseteq E(G)} (-1)^{|A|} q^{k(A)} = P_G(q),$$

where P_G is the chromatic polynomial of G.

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Rank has another interpretation. Recall the (signed) vertex-edge incidence matrix Q of G, as defined in Lecture 2. Then $r(A)$ is the rank (in the sense of linear algebra) of the submatrix formed by the columns indexed by edges in A. The proof is an exercise.

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In particular, if $G = (V, E)$ is connected, then $r(E) = n - 1$.

The Tutte polynomial

The Tutte polynomial of the graph $G = (V, E)$ is the polynomial

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Many important graph parameters are obtained by plugging in special values for x and y, possibly multiplying by a simple factor.
In particular, putting $x = y = 2$, every term is 1, so that $T_G(2,2) = 2^{|E|}$.

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Putting $x = 1$, the only non-zero terms are those which have the exponent of $(x - 1)$ equal to 0, that is, $r(A) = r(E)$, so that the graph (V, A) is connected. Similarly, putting $y = 1$, the only non-zero terms are those with $|A| = r(A)$, in other words, the set A contains no cycles.

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Hence

- $T_G(1, 2)$ is the number of connected spanning subgraphs of G;

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Putting $x = 1$, the only non-zero terms are those which have the exponent of $(x - 1)$ equal to 0, that is, $r(A) = r(E)$, so that the graph (V, A) is connected. Similarly, putting $y = 1$, the only non-zero terms are those with $|A| = r(A)$, in other words, the set A contains no cycles.
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However, other optimality parameters don't appear to be specialisations of the Tutte polynomial.

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In one direction, all trees on n vertices have Tutte polynomial x^{n-1}; but we have seen that they can be very different on A- or E-optimality, and hence on Laplacian spectra.
In the other direction, the two strongly regular graphs with the same parameters on 16 vertices have the same Laplacian spectra, but have different Tutte polynomials: see below.

Chromatic polynomial revisited

The formula for the Tutte polynomial looks very similar to the formula we deduced for the chromatic polynomial. Indeed, a little persistence shows that, for a connected graph G,

$$P_G(q) = (-1)^{n-1} q T_G(0, -q+1),$$

so the numbers of colourings are values of T_G at integer points on the negative real axis.

Two strongly regular graphs

Consider the following pair (G_1, G_2) of graphs: on the left, the 4×4 square lattice graph (in which vertices in the same row or column are joined), and on the right, the Shrikhande graph (which is shown drawn on a torus: nearest neighbours are joined, and opposite edges are identified).

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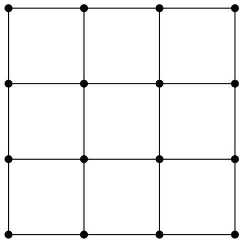

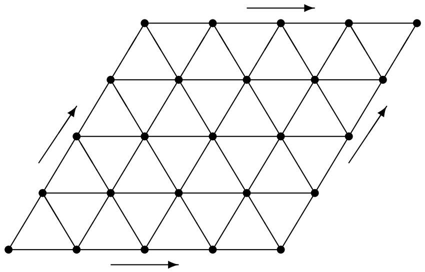

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There are two essentially different Latin squares of order 4: they are the Cayley tables of the Klein group V_4 and the cyclic group C_4. The corresponding graphs are the lattice graph $L_2(4)$ and the Shrikhande graph respectively.

Colouring the graphs

A colouring of the square lattice with four colours is nothing but a Latin square of order 4 (see below). There are 576 Latin squares, and hence $P_{G_1}(4) = 576$.

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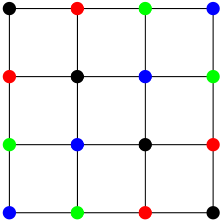

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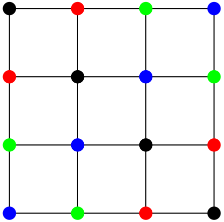

Each colour gives the positions of a symbol in a Latin square.

Orientations

An orientation of the edges of a graph G is acyclic if there are no directed cycles; it is totally cyclic if every edge is contained in a directed cycle.
Richard Stanley showed that the number $a(G)$ of acyclic orientations of G is

$$a(G) = |P_G(-1)| = |T_G(0, 2)|.$$

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It is also known that the number of totally cyclic orientations is $c(G) = |T_G(2, 0)|$.
Now recall that the number of spanning trees is $t(G) = T_G(1, 1)$.

The Merino–Welsh conjecture

These three numbers are connected by a remarkable conjecture of Merino and Welsh:

Conjecture

If G has no loops or bridges, then $t(G) \leq \max\{a(G), c(G)\}$.

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That is, either the number of acyclic orientations or the number of totally cyclic orientations dominates the number of spanning trees.
The best result so far is by Carsten Thomassen, who showed that this is true for sufficiently sparse graphs (where the number of acyclic orientations wins) and for sufficiently dense graphs (where the number of totally cyclic orientations wins).

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- *If G has at most* $16n/15$ *edges, then* $t(G) \leq a(G)$.

The first result applies if the average valency is at least 8; the second if it is at most $32/15 = 2.133\ldots$.

Jackson's Theorem

A related theorem of Bill Jackson is intriguing:

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Of course, replacing 3 by 2 would give a strengthening of the Merino–Welsh conjecture!

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If so, what happens for average replication below r_0? There may be further "phase changes".

Open problem: dense simple graphs

For dense simple graphs (those obtained by removing just a few edges from the complete graph), independent studies by Aylin Cakiroglu and Robert Schumacher suggest that, both for optimality and for maximizing the number of acyclic orientations, the best graphs resemble Turán graphs: that is, the edges removed should be as close as possible to a disjoint union of complete graphs of the same size.

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If we remove complete graphs of the same size, we get a group-divisible design.

Problem

Prove the above assertion.

Open problem: adding complete graphs

Aylin Cakiroglu and J. P. Morgan have investigated the following problem. Choose an optimality parameter. For a non-negative integer s, and given v, order the simple graphs on v vertices with a fixed number of edges (or the regular simple graphs of prescribed valency) by the rule that $G_1 <_s G_2$ if the union of G_2 with s copies of K_v beats the union of G_1 with s copies of K_v.

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One can also make the problem "continuous" by expressing the parameter in terms of s and then allowing s to take real values.

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More generally, there are theorems about decomposing the edge set of a graph into complete graphs of given sizes; find theorems about decomposing the edge set of a graph into weighted k-cliques, with perhaps some restrictions on the cliques (e.g. as few as possible where the weights are not all 1).

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Problem

What is the relation, if any, between optimality of different truncations or residuals of the same higher-rank geometry?

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