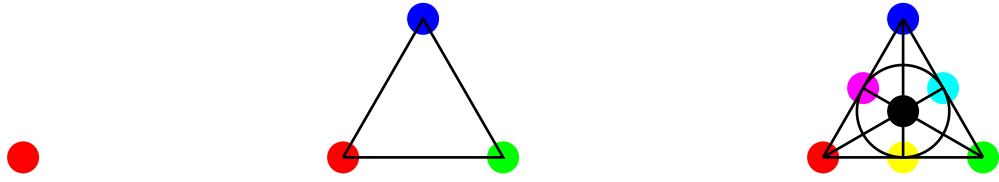


# Improved sampling of Steiner Triple Systems

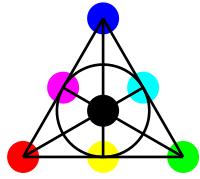
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Steiner Triple Systems are among the most-studied combinatorial designs, arising in applications as diverse as experimental design and the study of algebraic curves.

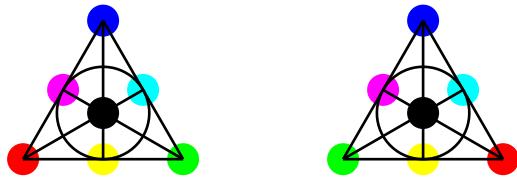
An  $\text{STS}(v)$  is a pair  $(V, \mathcal{B})$ , where  $V$  is a vertex set and  $\mathcal{B}$  is a collection of triples (3-sets) from  $V$ , with the condition that every unordered pair of vertices in  $V$  is contained in exactly one triple of  $\mathcal{B}$ .



TONCAS:  $v \equiv 1, 3 \pmod{6}$ .

**Sufficient** is not **enough** for  $v > 9$ , since not every STS( $v$ ) will be isomorphic to the recursive constructions used for sufficiency.

An *isomorphism* of an STS( $v$ ) is a permutation of the vertex set,  $\pi : V \mapsto V$ , that maps triple  $\{x, y, z\}$  to  $\{\pi x, \pi y, \pi z\}$ .

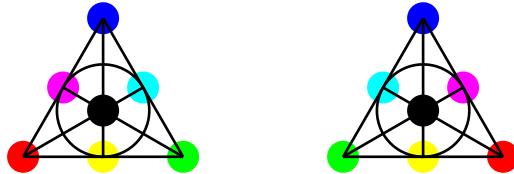


The number of pairwise nonisomorphic STS( $v$ ) (denoted  $N(v)$ ), quickly outstrips our ability to enumerate them:

- $N(v \in \{1, 3, 7, 9\}) = 1$
- $N(13) = 2$  — 1890s, paper and pencil.
- $N(15) = 80$  — 1917, paper and pencil exhaustive enumeration.
- $N(19) = 11,084,874,829$  — 2003, 2 CPU years, exhaustive enumeration.
- $N(v) \geq (e^{-5}v)^{v^2/6}$ . Exhaustive enumeration is doomed by abundance.

If we can't enumerate, the next best choice is reliable sampling. If we're sampling from the discrete uniform distribution over instances of  $\text{STS}(v)$ , then each isomorph occurs with equal probability. If isomorphism class  $C_i$  has automorphism group  $G_i$ , then the weight of  $C_i$  among all  $N$  isomorphism classes of the  $\text{STS}(v)$  is

$$\frac{v!/|G_i|}{\sum_j^N v!/|G_j|} = \frac{1}{|G_i| \sum_j^N 1/|G_j|}.$$



Hill-climbing algorithm finds  $C_i$  with a weight that is at least correlated to  $1/|G_i|$ , but still differs from the uniform distribution.

### **Unmodified hill-climbing**

while there are still some live vertices and fewer than  $1001b$  iterations:

1. randomly select a live vertex  $x$ .
2. randomly select neighbouring live vertices  $y$  and  $z$  with  $\{x, y\}$  and  $\{x, z\}$  not yet assigned to triples, and assign  $\{x, y, z\}$  to a new triple.
3. if  $\{y, z\}$  is already in a triple  $T$ , scrap  $T$ .

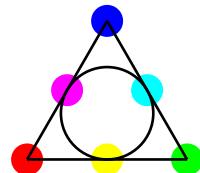
We

- show that there is a poor fit between sampling by hill-climbing and the uniform distribution,
- identify some sources of this discrepancy,
- fix hill-climbing (a little), producing variants that are a less-bad fit with the uniform distribution

For orders where the uniform distribution is known ( $\text{STS}(v \in \{13, 15, 19\})$ ), the Pearson  $\chi$ -squared test gives strong evidence that the hill-climbing sample is not from the uniform distribution

$$X^2 = \sum_j^N \frac{(o_i - e_i)^2}{e_i},$$

. . . provided  $N, e_i \geq 5$ . Since  $e_i$  (the expected number of occurrences of  $C_i$ ) may be very small we need categories that are bigger than isomorphism classes, but not too big: Pasch count categories. Pasch count is an isomorphism invariant.



For STS(15), all isomorphism classes except Class #1 have a reasonable expected value in a sample of size 1 million, so combine Class #1 and Class #2:

Properties of STS(15)s												
Class #	Pasches	mitres	Fanos	$ G_i $	probability	Class #	Pasches	mitres	Fanos	$ G_i $	probability	
1	105	0	15	20160	1.076028e-06	41	12	19	0	1	2.169272e-02	
2	73	0	7	192	1.129829e-04	42	8	23	0	2	1.084636e-02	
3	57	0	3	96	2.259658e-04	43	10	21	0	6	3.615453e-03	
4	49	4	3	8	2.711590e-03	44	8	21	0	2	1.084636e-02	
5	49	8	3	32	6.778975e-04	45	9	21	0	1	2.169272e-02	
6	37	12	3	24	9.038634e-04	46	7	22	0	1	2.169272e-02	
7	33	24	3	288	7.532195e-05	47	10	20	0	1	2.169272e-02	
8	37	8	1	4	5.423180e-03	48	8	21	0	1	2.169272e-02	
9	31	10	1	2	1.084636e-02	49	7	22	0	1	2.169272e-02	
10	31	12	1	2	1.084636e-02	50	6	25	0	1	2.169272e-02	
11	23	16	1	2	1.084636e-02	51	9	21	0	1	2.169272e-02	
12	32	9	1	3	7.230907e-03	52	9	20	0	1	2.169272e-02	
13	33	10	1	8	2.711590e-03	53	10	20	0	1	2.169272e-02	
14	37	6	1	12	1.807727e-03	54	11	20	0	1	2.169272e-02	
15	25	16	1	4	5.423180e-03	55	9	21	0	1	2.169272e-02	
16	49	0	1	168	1.291233e-04	56	8	21	0	1	2.169272e-02	
17	25	18	1	24	9.038634e-04	57	5	24	0	1	2.169272e-02	
18	25	14	1	4	5.423180e-03	58	8	22	0	1	2.169272e-02	
19	17	24	1	12	1.807727e-03	59	13	18	0	3	7.230907e-03	
20	20	15	1	3	7.230907e-03	60	7	24	0	1	2.169272e-02	
21	20	15	1	3	7.230907e-03	61	14	21	1	21	1.032987e-03	
22	17	18	1	3	7.230907e-03	62	7	21	0	3	7.230907e-03	
23	18	16	0	1	2.169272e-02	63	7	24	0	3	7.230907e-03	
24	19	15	0	1	2.169272e-02	64	10	21	0	3	7.230907e-03	
25	20	15	0	1	2.169272e-02	65	7	22	0	1	2.169272e-02	
26	23	13	0	1	2.169272e-02	66	6	23	0	1	2.169272e-02	
27	14	19	0	1	2.169272e-02	67	5	24	0	1	2.169272e-02	
28	15	18	0	1	2.169272e-02	68	6	22	0	1	2.169272e-02	
29	19	15	0	3	7.230907e-03	69	5	24	0	1	2.169272e-02	
30	14	19	0	2	1.084636e-02	70	9	21	0	1	2.169272e-02	
31	18	18	0	4	5.423180e-03	71	5	23	0	1	2.169272e-02	
32	13	19	0	1	2.169272e-02	72	5	24	0	1	2.169272e-02	
33	12	19	0	1	2.169272e-02	73	6	26	0	4	5.423180e-03	
34	12	19	0	1	2.169272e-02	74	8	22	0	4	5.423180e-03	
35	13	18	0	3	7.230907e-03	75	7	24	0	3	7.230907e-03	
36	10	20	0	4	5.423180e-03	76	10	20	0	5	4.338544e-03	
37	6	24	0	12	1.807727e-03	77	2	24	0	3	7.230907e-03	
38	9	22	0	1	2.169272e-02	78	6	26	0	4	5.423180e-03	
39	12	19	0	1	2.169272e-02	79	6	30	0	36	6.025756e-04	
40	13	18	0	1	2.169272e-02	80	0	30	0	60	3.615453e-04	

For STS(19) the overwhelming majority of isomorphism classes have very small expected tallies. Even when combined according to Pasch count, Pasch counts 0–2 and 40–84 are best combined to give reasonable expected values in a sample size of 1 million.

STS(19)s, by Pasch count					
Pasches	probability	Pasches	Probability	Pasches	Probability
0	2.303578e-07	1	3.224900e-06	2	2.378104e-05
3	1.186311e-04	4	4.473271e-04	5	1.361802e-03
6	3.471446e-03	7	7.607619e-03	8	1.461858e-02
9	2.497890e-02	10	3.843540e-02	11	5.379188e-02
12	6.909960e-02	13	8.214046e-02	14	9.099054e-02
15	9.453033e-02	16	9.266067e-02	17	8.612790e-02
18	7.628393e-02	19	6.464733e-02	20	5.262322e-02
21	4.129568e-02	22	3.133304e-02	23	2.305749e-02
24	1.650321e-02	25	1.151236e-02	26	7.848494e-03
27	5.236980e-03	28	3.428645e-03	29	2.206207e-03
30	1.397215e-03	31	8.716567e-04	32	5.370220e-04
33	3.267913e-04	34	1.972839e-04	35	1.173950e-04
36	6.969809e-05	37	4.076921e-05	38	2.395607e-05
39	1.370282e-05	40	8.167795e-06	41	4.592727e-06
42	2.757953e-06	43	1.525754e-06	44	1.008302e-06
45	5.386811e-07	46	3.811454e-07	47	1.928318e-07
48	1.623295e-07	49	6.487869e-08	50	7.300544e-08
51	3.207097e-08	52	3.524349e-08	53	7.036669e-09
54	1.741125e-08	55	6.179639e-09	56	1.021670e-08
57	1.757497e-09	58	6.720921e-09	59	4.811398e-10
60	1.712181e-09	62	2.706411e-09	64	1.390795e-10
66	5.713535e-10	70	3.157480e-10	78	3.007124e-11
84	1.670624e-12				

# Where does the bias come from?

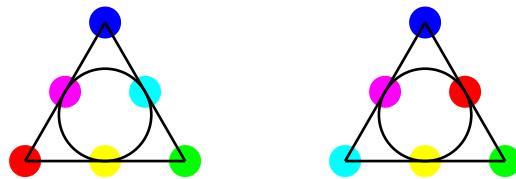
## **Unmodified hill-climbing**

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- sampling from live vertices versus sampling from live edges
- short swap cycles
- Pasch trades are discouraged

An  $\text{STS}(v)$ 's closest neighbours — those  $\text{STS}(v)$ s that have the largest intersection with  $\mathcal{B}$  — are a Pasch trade away:



To move between the two means that triples  $ryg$ ,  $rvb$ ,  $tyv$ , and  $tgb$  are replaced by  $tyg$ ,  $tvb$ ,  $ryv$ , and  $rgb$ . This requires at least six tightly-sequenced invocations of step 3 of hill-climbing

By correcting for each source of bias, using edge selection, tabu lists, and adding a Pasch trade, we generate samples with a less-bad fit. Here's the result for STS(19), adding a Pasch trade with probability 0.8:

one million STS(19)s per sample, <b>Pasch trade hill-climbing</b> , $p = 0.8$						
Rank	unmodified $X^2$	modified $X^2$	unmodified Pasches	modified Pasches	unmodified Mitres	modified Mitres
1	5.224137e+03	1.111816e+02	15654730	15970532	32715233	32579335
2	5.248441e+03	1.115942e+02	15655797	15971288	32717224	32580615
3	5.269851e+03	1.211230e+02	15657136	15972653	32717899	32582746
4	5.307556e+03	1.233207e+02	15659858	15972933	32722229	32585659
5	5.312683e+03	1.277789e+02	15660796	15973203	32722548	32585750
6	5.318761e+03	1.330783e+02	15661151	15974179	32723531	32586301
7	5.321584e+03	1.343794e+02	15662650	15975064	32723855	32587621
8	5.331643e+03	1.363757e+02	15662755	15975917	32724172	32590856
9	5.337050e+03	1.379567e+02	15662841	15976294	32725094	32591682
10	5.357167e+03	1.406806e+02	15663347	15978086	32725101	32591838
11	5.358333e+03	1.408173e+02	15663397	15978203	32726963	32594063
12	5.362857e+03	1.411166e+02	15664706	15980031	32728126	32594172
13	5.373310e+03	1.413105e+02	15665047	15980500	32728933	32594181
14	5.397101e+03	1.484691e+02	15665238	15980983	32729124	32594721
15	5.425309e+03	1.504426e+02	15665350	15981303	32729163	32596034
16	5.432722e+03	1.515335e+02	15665816	15981419	32729592	32596117
17	5.437995e+03	1.530015e+02	15665929	15982483	32729653	32596144
18	5.452984e+03	1.540823e+02	15666364	15982626	32730676	32597551
19	5.465653e+03	1.579629e+02	15666565	15983936	32730793	32598232
20	5.505072e+03	1.584489e+02	15666748	15984786	32731334	32598359
21	5.527179e+03	1.699103e+02	15666781	15985800	32731735	32599384
22	5.546573e+03	1.748498e+02	15667114	15986403	32732307	32601725
23	5.642612e+03	1.834109e+02	15667878	15986539	32733265	32605211
24	5.706865e+03	1.861724e+02	15669223	15987137	32733352	32605422
25	5.741408e+03	1.995209e+02	15669381	15987453	32734521	32613553

The modifications were inexpensive, it costs  $O(v^3)$  to find all the tradeable Pasches, compared to empirically ( $v^2 \log v$ ) performance of hill-climbing.

Running time (seconds/system) for $\text{STS}(v)$			
<b>Unmodified hill-climbing versus Pasch trade hill-climbing with <math>p = 0.8</math></b>			
$v$	unmodified	modified	modified/unmodified
19	1.100000e-03	9.000000e-04	8.181818e-01
39	5.400000e-03	4.200000e-03	7.777778e-01
79	2.520000e-02	2.010000e-02	7.976190e-01
159	1.114000e-01	1.016000e-01	9.120287e-01
319	5.934000e-01	4.758000e-01	8.018200e-01
639	3.263200e+00	3.919300e+00	1.201060e+00
1279	1.686510e+01	4.020750e+01	2.384065e+00

Now what?

- We need a way to evaluate sampling when the uniform distribution is unknown ( $v > 19$  for the next while)
- We need to remove all bias
- Perhaps other design problems that use hill-climbing can benefit