Probabilistic Generation of Quantum Contextual Sets; Supplementary Material

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Abstract

Here we give supplementary material for the Appendices A-C.

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Appendix A. Algorithms and Programs behind Table 1

We used the program `mmpstrip` to strip edges from starting hypergraphs. We adjusted the increment parameter of `mmpstrip` so that, after each edge removal and post-processing step, we ended up with a sample of a desired size, say 1,000,000 hypergraphs. So after the full run of stripping a edges and post-processing, we ended up with 64 sample sets of up to 1,000,000 non-isomorphic KS hypergraphs each, with one sample set for each hypergraph size from 12 through 75 edges. For 12 edges and less, no KS sets have ever remained, probably because they don't exist.

The complete processing of the samples sets of this size, including finding all of the critical KS hypergraphs among them, took about 4 days on a single CPU. We ran 200 such jobs on a cluster, then combined the results. The random selection and the large sample space ensured that we would have, with high probability, completely different samples on successive program runs. Except near the extreme edge sizes of 75 and 12 where the sample space is essentially exhausted, we never found a duplicated hypergraph in our spot checking.

The overall iterative procedure we used is as follows. We started with the MMP hypergraph for the 60-75 KS set.

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1. We started with the 60-75 KS set and with `mmpstrip` obtained 75 new 60-74 sets—each with one less edge than the original 60-75. Then we repeated the procedure to obtain 2775 new 60-73 sets, etc. but not more than 1,000,000 hypergraphs to keep the run time reasonable. We used `mmpstrip`'s increment parameter i, which selects every ith edge on average, to achieve this limit. The increment parameter can be a non-integer to better control the output size. When it is greater than 1, the edges can be selected either with uniform spacing or randomly; the latter option was usually chosen.
2. A hypergraph is *connected* if there is a chain of zero or more edges connecting every pair of edges. Unconnected hypergraphs were removed with `mmpstrip`.
3. Duplicate hypergraphs result when one edge is removed at a time (rather than multiple edges combinatorially). These duplicates were removed.
4. Isomorphic hypergraphs were removed with `shortd`.
5. Colorable hypergraphs were filtered out with `states01` (described in [1]), leaving only non-colorable ones (i.e. KS sets).

Typically, we first ran these steps on a small sample of the hypergraphs (a hundred or so) so that the increment parameter for each `mmpstrip` call could be estimated, in order to end up with the same number of output hypergraphs as input hypergraphs after each edge removal step.

We examined the final set of MMP hypergraphs obtained after each iteration of the above process in order to determine which hypergraphs were critical, using an option of the `states01` program. Any critical sets found were collected for analysis.

The advantage of stripping one edge at a time then filtering at each stage is that many fewer MMP hypergraphs had to be examined, because at each step we consider only the non-isomorphic KS sets from the previous step. For example, from Fig. 3, there are $3.1 \cdot 10^{20}$ hypergraphs with 28 edges, of which only $1.6 \cdot 10^{13}$ are KS sets. The 23 critical sets were were found by examining a sample of only $6 \cdot 10^{7}$ KS sets rather than $1.2 \cdot 10^{15}$ starting MMP hypergraphs that would have otherwise been required, representing a speedup factor of about 20 million.

Appendix B. Samples of KS hypergraphs with even number of edges

Here we give samples of KS hypergraphs of each kind that we listed in Table 1 and did not give in Figures in Section 2..

Using our programs `longest` and `loopbig`, we can instantly determine the following structural features. Let us take the *45-26* hypergraph below. The program `longest` shows that its biggest loop is a 12-gon. The program `loopbig` gives 26 instances of its 12-gon representation, the first one of which is 2134,4YZE, EFGD,DfKN,NPQO,OeUd,dacb,bWL7,7586,6jMT,ThgV,ViR2. 9.A.B.C. H.I.G*8* J.K*L*M* R*S.Q*C. T*U*S.F* V*W*X.P* c*X.M*3* f*Z*R*7* g*e*I.3* i*j*Y*N* h*a*Y*H. a*B.6*2* e*Y*L*A. d*V*K*9. (The edges are the same as in *45-26* below, only in a different order. Also the vertices within an edge are mostly in a different order. Actually, all 26 instances are just different 12-gon arrangements of *45-26* below.) The edges 1234–ViR2 are *polygon edges* (see Sec. 2); vertices followed by "." are *free vertices*; edges containing *free vertices* are *free edges*; vertices followed by "*" are *polygon vertices*; edges containing only *polygon vertices* followed by "*"s are *span edges*; (in other words *span edges* are edges which are not *polygon edges* and which do not contain *free vertices*). Our script based on `Asymptote` draws 26 figures of *45-26* with 12-gons as shown in Fig. B.1.

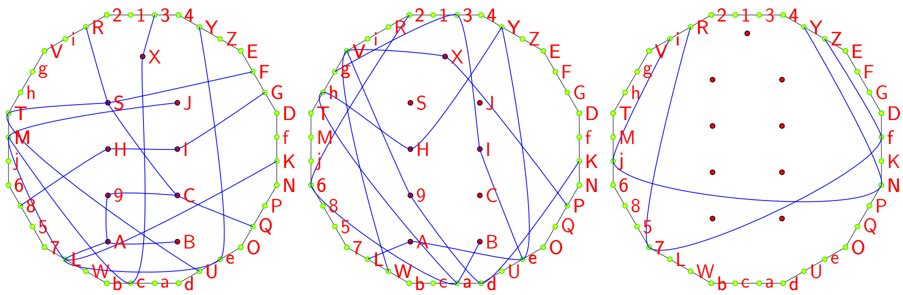

Figure B.1: A critical 45-26 KS set shown in three figures. The left and middle ones: maximal 16-gon + free edges. The right one: 16-gon + span edges.

Once the figures are drawn, the user can assign any ASCII symbol desired to any vertex. Also, by utilizing our program `vectorfind` she/he can ascribe vectors to vertices. 1,2,…,i,j $\to$ $\{\tau,0,\overline{1},\overline{\kappa}\}$, $\{0,1,0,0\}$, $\{\kappa,0,\tau,\overline{1}\}$, $\{1,0,\kappa,\tau\}$, $\{\kappa,\tau,1,0\}$, $\{\overline{1},0,\kappa,\tau\}$,$\{\overline{\tau},\kappa,0,\overline{1}\}$, $\{0,\overline{1},\tau,\overline{\kappa}\}$,$\{0,\tau,\kappa,1\}$, $\{1,\overline{1},1,1\}$,$\{\overline{\kappa},0,\tau,\overline{1}\}$, $\{\tau,\kappa,0,\overline{1}\}$,$\{\overline{1},1,1,\overline{1}\}$, $\{\overline{1},1,\overline{1},1\}$,$\{\overline{1},\overline{1},1,1\}$, $\{1,1,1,1\}$,$\{\overline{\kappa},\overline{1},0,\tau\}$, $\{\tau,\overline{1},\overline{\kappa},0\}$, $\{\kappa,\overline{\tau},\overline{1},0\}$, $\{0,\overline{1},\tau,\kappa\}$, $\{\overline{1},0,\overline{\kappa},\tau\}$, $\{\tau,\kappa,0,1\}$, $\{\tau,1,\kappa,0\}$,$\{\kappa,0,\overline{\tau},\overline{1}\}$, $\{0,\kappa,\overline{1},\tau\}$, $\{\overline{1},\tau,0,\overline{\kappa}\}$, $\{0,0,1,0\}$,$\{\kappa,1,0,\tau\}$,$\{0,\overline{1},\overline{\tau},\kappa\}$, $\{\tau,\overline{1},\kappa,0\}$,$\{1,0,0,0\}$,$\{0,1,\tau,\kappa\}$, $\{0,\tau,\overline{\kappa},\overline{1}\}$,$\{\overline{1},\kappa,\tau,0\}$, $\{\overline{1},\overline{\tau},0,\kappa\}$,$\{\tau,0,1,\kappa\}$, $\{\kappa,\tau,\overline{1},0\}$, $\{\overline{1},1,1,1\}$, $\{0,\overline{\kappa},\overline{1},\tau\}$,$\{1,\tau,0,\kappa\}$, $\{\kappa,\overline{1},0,\overline{\tau}\}$, $\{0,\kappa,\overline{1},\overline{\tau}\}$,$\{0,\overline{\tau},\kappa,\overline{1}\}$, $\{0,0,0,1\}$,$\{\overline{\kappa},\tau,\overline{1},0\}$, where $\tau=(\sqrt{5}+1)/2$ and $\kappa=1/\tau$; a bar over a number indicates its negative.

45-26 1234,5678,9ABC,DEFG,HIG8,JKLM,NOPQ,RSQC,TUSF,VWXP,YZE4,abcd,edUO, cXM3,fZR7,bWL7,geI3,fNKD,hgVT,ijYN,haYH,jTM6,aB62,iVR2,eYLA,dVK9.
46-28 1234,5678,9AB8,CDEF,GHIJ,KLMN,OPQR,STR4,UVNF,WXYZ,abZT,YQME,cdYB, efb7,gVSJ,hiPA,jfOI,idHD,aLIC,ieXN,jiS6,kgM5,khcG,kbU9,hL73,cON2,WSL9,gZOD.
47-28 1234,5674,89AB,CDEF,GHIJ,KLJ7,MNOB,PQR3,STUO,VWU6,XYI5,ZabL,cdYL,efbF, gaHA,hWG9,iTGE,jkZ2,lkNE,kdUR,lfXK,hXD1,XVQ8,jfPA,jcMC,ecSQ,khge,iaXM.
48-28 1234,5678,9ABC,DEC8,FGHI,JKLM,NOME,PQRB,STIA,UVWX,YXRL,Zab4,cdW3,efgT, hdbK,ijcJ,gVQH,kfJG,lhF7,jeb6,iUPD,faU9,YS72,mlZT,lQO3,kdYN,mUN6,iZYH.
49-28 1234,5678,9ABC,DEFG,HIJ8,KLG7,MNOP,QRSP,TUVJ,WLC4,XYZV,abS7,cdeb,fgUO, heZN,ijdI,kgaF,lcYM,jYRE,iXQG,fHGB,mfdW,mkTN,nhR3,nigA,lhFC,cTG3,mYA7.
49-30 1234,5678,9ABC,DEFG,HIJK,LMN8,OPQR,STUK,VWRC,XYZW,abcQ,deJ4,fghe,ijU3, kjQG,ZTNB,khA7,gYS8,lkV2,mcMF,mif6,lidE,nfXD,mPJB,gOI3,bX73,ndcC,lgaB,nkNI,lXMK.
51-30 1234,5678,9AB8,CDEF,GHIJ,KLMN,ONJ4,PQRS,TUB3,VWIA,XSOF,YZE7,aHD6,bcZX, defW,ghiM,cWR2,jkL9,liR5,mbUC,nkfb,onha,pgeX,pojG,mhdQ,oYP3,pmVK,nlTK,kgYH,ljd4.
52-30 1234,5678,9ABC,DEF4,GHIJ,KLMN,OPQ8,RSQJ,TUVI,WXYZ,abcJ,NHC3,defg,hijc, kgbB,lkZ7,mYMJ,njX4,fSNF,oWVA,piPA,qeVE,onml,qpna,ohdQ,pfYU,liLE,UQLB,qhN7,ngI8.

53-30 1234,5678,9ABC,DEFG,HIJK,LMNO,PQRS,TUVW,XYZW,abZS,cdVG,eRC4,fghY,ihK3, gdbJ,jkeI,lQOF,mki8,nopJ,qpjE,qhP7,roX7,nmUQ,rjcN,rfUB,pliT,paMB,mYNC,MIG7,lbC7.
51-32 1234,5678,9AB4,CDEF,GHFB,IJKL,MNOP,QRPL,STUH,VWXR,YZUQ,abcO,dZXE, eTK8,fgJA,hig3,jiN7,iSD9,khcY,lXMK,mnWA,opYI,ndc6,ljfC,mjZ2,lbS5,pV62,piaG,ogeb,keWG, onPC,kSP2.
52-32 1234,5674,89AB,CDE7,FGHB,IJKL,MLA3,NOP2,QRST,UVWX,YZaX,bcWT,dePK,fgSJ, hiaH,jkOG,lmW9,nmgN,oeVR,kife,pkZQ,pcE3,onHE,qjRM,qfbY,hbND,qp96,laR4,UJGD,qndU, dZB7,RNIB.
53-32 1234,5678,9A84,BCDE,FGHI,JKLM,NOPQ,RST3,UVW7,XYIA,Zabc,defM,ghYL,ijcT, kWQ2,ljfH,mhbV,nmiP,eSGE,oaUK,pgZR,qohO,plNK,ondI,ZXE2,rfUD,gdC6,qiD9,rpmk,qkJG, cNG5,mHC3.
54-32 1234,5678,9ABC,DEFG,HIJC,KLMN,OPQR,STUC,VWXY,URN4,Zabc,def3,ghcQ,ihMJ, jkB8,lifY,mkgT,nopA,qrlT,rpjP,ebX8,rhdG,qoeJ,maPF,naNI,sbLE,som7,oZYG,nWTE,rVN7, fQEB,YPLC.
55-32 1234,5678,9ABC,DEFC,GHIJ,KLMF,NOPQ,RSTU,VWXY,ZabE,cde8,fghe,ijeQ,klmU, mhbJ,nopB,qrpT,sjT4,todY,naMI,SHA3,tlP7,ngR7,rGF7,qZXO,tsZL,eWM3,fVLA,nmiV,dNF4, qkdA,mOC8.
53-34 1234,5674,89AB,CDEF,GHIJ,KLMN,OPQR,STUV,WVRB,XYUF,Zabc,decN,fgYJ,hijA, kjbE,lmQF,ePI3,aWMI,niXL,oZRH,phcT,pmH7,qkLB,pgKE,qhI6,rnmf,ncO2,mdSA,OJDA,roke, ogS6,lLJ4,raU4,nIE9.
54-34 (16) 1234,4567,789A,ABCD,DEFG,GHIJ,JKLM,MNOP,PQRS,STUV,VWXY,YZab,bcde, efgh,hijk,klm1,3EQb,5DWl,7JYk,8Ubl,CHXe,DKTa,EMfm,OTck,2nLZ,3To9,6FLq,7Nen,Bonm, IQWn,Ipdi,LRlp,Srsj,Ugrq. Shown in Fig. B.2.

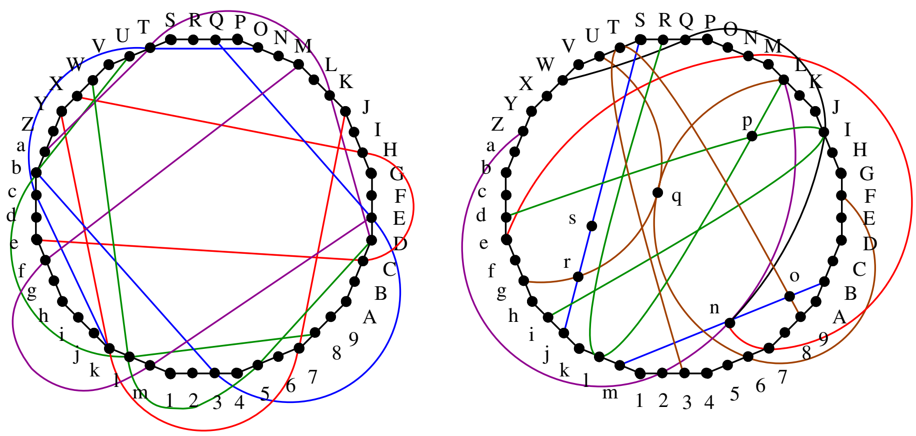

Figure B.2: A critical 54-34 KS set shown in two figures. (a) A maximal 16-gon + span edges; (b) 16-gon + free edges.

55-34 1234,5674,89AB,CDEF,GHIJ,KLJ7,MNOP,QRST,UVWT,XYZa,bcaW,dec6,fghI,ihPB, jkgS,kZVL,lmRO,noi3,pqYI,rNF3,qoeE,mbDA,sljc,rplU,sfXQ,kbH2,tsqN,ndYO,tU97,nfLA, reSJ,XUPH,siJD,kOE9.
56-34 1234,5674,89AB,CDEF,GHIJ,KLMN,OPQR,STUJ,VWXB,YURN,Zabc,defT,ghMF,ijQE, klmA,nLI9,opnc,pmhY,qjbH,oKD8,olX7,rsfa,iWS3,tsWM,utZP,urmJ,neO6,uqog,dHF3,skH6, qYV4,laIE,ieZY,fPD4.
57-34 1234,5674,89AB,CDEF,GHIJ,KLMN,OPQB,RSTU,VWXY,Zabc,defc,ghb7,ijkY,lmnU, ofT3,pqSA,rstR,qnXQ,uvmN,pkhN,ljgP,ieMA,tolJ,vdWI,aQJF,ueVP,ZPLE,sPI4,RNHD,voiZ, rnL3,bYDB,rpVF,dRQ7.

58-34 1234,5678,9ABC,DEF8,GHIJ,KLMN,OPQN,RSTU,VWXY,ZaMJ,bYU4,cdef,ghia,jkiQ, lmnT,onP8,phfL,qoeS,rROI,hbHC,srp3,qpmX,tuvo,wvdJ,wqb7,rkdK,jcWB,uscb,trlB,ukVT, lbZF,gVIF,vpjF,qgNB.

59-34 1234,5678,9ABC,DEFG,HIJK,LMNO,PQR8,STUV,WXYZ,abcZ,defg,higO,jklm,nopm, qric,slbR,tukQ,uV74,vuYN,srf3,paN3,wthC,jeKB,xwvj,qodX,xqUQ,jVMG,UJF3,nIC8,wWTH, cTE8,snWM,wdRF,oTOB.

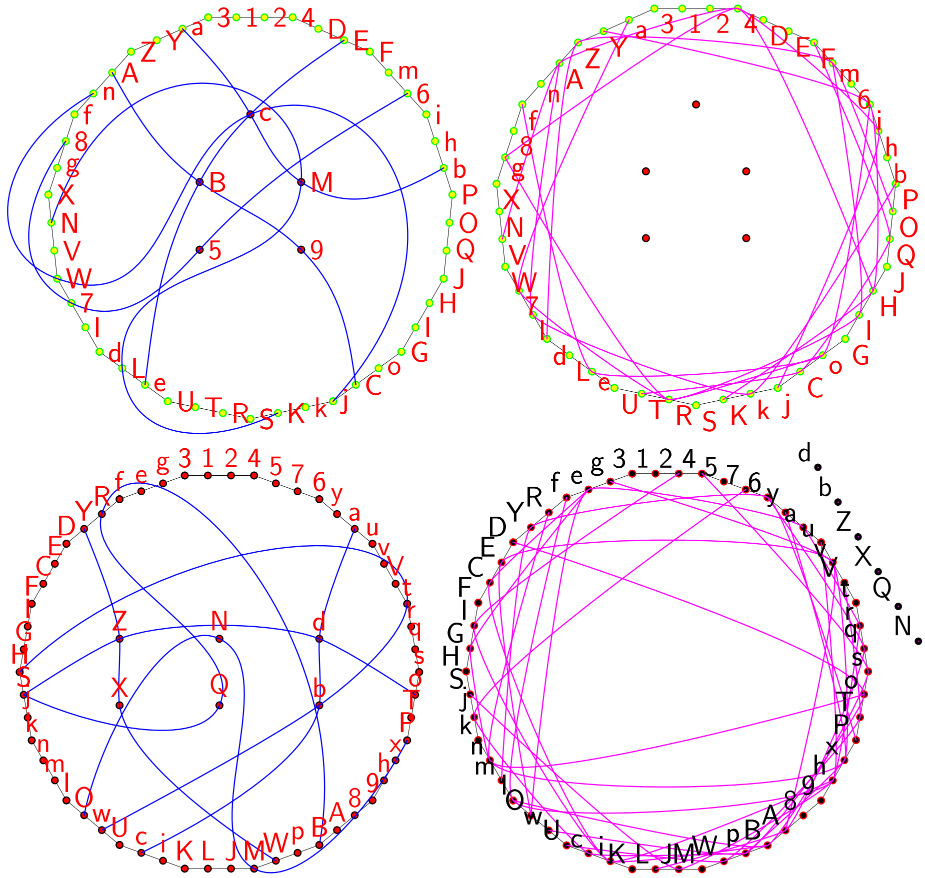

Figure B.3: Enlarged Fig. 2.

55-36 1234,5678,9AB4,CDEF,GHIJ,KLMF,NOP3,QRPM,STUJ,VWOB,XYZa,bcdA,efgh,ijkd, lmkU,haNJ,nocW,pREB,qrpj,mbZ2,ojJD,srM8,qgb7,tlaW,WTF7,qnQI,kYHE,sZIB,fXOD,iL62, tfl6,qSOL,leLA,neE8,rWH2,kfM4.

56-36 1234,5674,89AB,CDEF,GHIJ,KLMF,NOPQ,RST3,UVWX,YZaX,bcdW,efgB,hVE7,ijgQ, kTPM,lmnd,oQJD,pqrs,faC2,tsnl,kjcA,tZOA,uib6,mYS9,uonf,rliR,sUQL,qXPH,poZ4,rG97, mkeU,hRIB,qmh2,mOK6,ocRK,bPC9.

57-36 1234,5674,89A3,BCDE,FGHI,JKLM,NOPQ,RSTU,VWXY,ZaYQ,bcdl,efE2,ghM3,ijkf, lhda,mecP,nOL7,oXU6,pqbA,kNHD,rsqZ,pnfT,cWSK,ZJGE,tunl,vsVO,ljUG,vgTD,umiR,oiOI, rmh6,iWCA,vtA6,usH4,mYD9,qIKD.

58-36 1234,5674,89AB,CDEF,GHI3,JKLM,NOPQ,RSTM,UVB7,WXYI,ZaYT,bcaQ,dcSF,efgh, ijkR,lmhP,ngXL,nmZH,opWV,qplK,rpaA,sJE4,trkG,tnD9,usoZ,vfbl,qjf6,wXO6,wtse,vtld, kbVC,uhUM,wpiF,ujdN,kh84,pnN4.

59-36 1234,5674,89AB,CDEF,GHB7,IJKL,MNOP,QRPF,STUV,WXYA,ZabL,cdef,ghij,kfbY, kVR6,lKH3,mjO9,nopX,qrlU,siXT,tule,vwpS,odRK,xusJ,xwc6,thYG,daOE,wrm2,iND4,uZSA, xqF9,rnfN,vtNL,rgEA,phPJ,XLF2.
60-36 1234,5678,9AB8,CDEF,GHIJ,KLMN,OPQJ,RSTU,VWXN,YZab,cdeB,fgX7,hgeM,ijQF, kljd,mnoN,phbI,qrif,saEB,tolH,uvn4,srUL,wMD3,xmkf,wroZ,vcbT,ywjS,hWSP,ukYL,kVTJ, yvHE,uqP8,xUH8,tfbD,poQB,fSB4.
57-38 1234,5674,89AB,CDE7,FGHI,JKLM,NOPB,QRS3,TUVW,XYZa,bcde,fgPM,heWE,ijVS, klRI,mnol,podH,qrU6,sraP,toOL,ukaK,tgZG,cKD3,vspQ,vueO,vTJ7,vqgA,pkjh,nibP,jfcY, rmjG,nY94,viXI,tiE2,tkT9,qYHE,mQEB,cUIB.
58-38 1234,5674,89AB,CDEB,FGHI,JKL7,MNOP,QRST,UVWX,YZaA,bcLE,defg,hia3,jkXP, lmZK,ngWT,opnI,qrkH,rpSB,sfRO,tjRK,sYVL,umUG,vcPF,wm96,qeUD,okid,udbQ,wdYN,vpf2, wnhc,qnMK,utra,viW9,sliD,wtD2,QPD7,usn4.
59-38 1234,5674,89A3,BCD7,EFGH,IJKL,MNOL,PQRS,TUVW,XYZW,abZ2,cdeb,fgK6,hijA, aVSH,klJ9,mnoG,pID8,qrYC,stO1,oeRO,ujgF,vuol,wutU,xkid,wnZJ,mjcX,rfdQ,rhaN,xwPC, vcNE,qpkR,wpfM,vpV5,rmT8,tmkB,sWPF,vsiK.
60-38 1234,5674,89A7,BCDE,FGHI,JKLM,NOPE,QRST,UVWT,XYZa,bcde,fghA,eWMI,ijkl, mnlV,opha,qrgU,spnD,tdL3,trSP,cZRK,uveO,qkYI,jRHD,wrZ9,xiQ4,vtXV,mJC7,ywN6,yxtf, pibN,ysKG,wjhd,romG,upT2,xumY,yqC2,viGA.
59-40 1234,5678,9ABC,DEF8,GHI4,JKLM,NOPI,QRSC,TUVW,XYZH,abMB,cWPC,debZ,fgh7, ijkF,lmnk,opje,qnaV,rsmU,tjU3,lhYS,uSE2,sqdA,kgXR,upfO,vTQN,qfL3,wnNK,vuJG,wfbF, xicK,tgcE,vqoX,xura,xlTA,vcb6,spcY,rgeN,leG8,XUK8.

Appendix C. Details for Sample Space Statistics

The plots of Fig. 3 provide an overview of the subsets of 60-75. Because they were determined by statistical inference from small samples of this space, most of the numbers are approximate. As a practical matter, some of the sample sets, or portions of them, were obtained with the more efficient semi-random method mentioned in the footnote in Sec. 2, which has an effect.[1] Overall, the numbers should be trusted only to within an order of magnitude or so. The plots are intended to provide a rough guideline for planning future work, such as an exhaustive search of certain ranges, and for that purpose it should be adequate.

Several techniques, which we describe below, were used to obtain the values for the plots. The total number of MMP hypergraphs is simply $\binom{75}{b} = \frac{75!}{b!(75-b)!}$, where b is the number of edges given at the abscissa.

The `mmpstrip` program was used to identify and remove unconnected hypergraphs. We do not include the resulting numbers of MMP hypergraphs in Fig. 3 but briefly describe them as follows. For 1 through 4 edges, the number of unconnected MMP hypergraphs are exactly 0, 2175, 59725, and 1101450. For 67–75 edges there are exactly 0. For the rest, we used samples of 10^6 MMP

[1] To test this effect, we used non-isomorphic MMPs with 67 edges, where the actual count is known from an exhaustive search. Using semi-random sampling, a value of $1.4 \cdot 10^6$ was estimated, compared to the actual count of $1.2 \cdot 10^6$. This is apparently due to some kind of systematic bias that occurred when samples were taken uniformly from the set of input KS sets, leading to the overcount. Using true random sampling, the estimate was very close to the actual $1.2 \cdot 10^6$, as we describe below.

hypergraphs for each number of edges. For 47–66 edges, no unconnected hypergraphs were observed. For 5–46 edges, the number of unconnected hypergraphs (estimated from the ones observed in the sample) decreases to zero as a percentage the total number of MMP hypergraphs, from $1.56 \cdot 10^7$ (out of $1.73 \cdot 10^7$ total) for 5 edges to $1 \cdot 10^{15}$ (out of $5.1 \cdot 10^{20}$ total) for 46 edges.

To calculate the the number of non-isomorphic MMP hypergraphs, unconnected hypergraphs were discarded and the rest passed through the `shortd` program, which filters isomorphic hypergraphs, keeping only one canonical representative from each isomorphism class. For small and large numbers of edges, exhaustive generation of all MMPs yielded exact values. For 1–4 edges there are 1, 1, 2, and 5 (connected) isomorphism classes; for 67–75 edges, there are 1183189, 141314, 15014, 1463, 154, 19, 4, 1, and 1. For the other edge sizes, the number of isomorphism classes was estimated from a sample. Finding this estimate is called the "coupon collector's problem," [2] and the maximum likelihood estimator is the smallest integer $j \geq c$ such that

$$\frac{j+1}{j+1-c}\left(\frac{j}{j+1}\right)^n < 1, \tag{C.1}$$

where n is the number of samples (with replacement) and c is the observed number of isomorphism classes in the sample. For example, we observed $c = 516604$ isomorphism classes in a random sample of $n = 545961$ 13-edge hypergraphs. The criteria of Eq. (C.1) yields $j = 4893025 \approx 4.9 \cdot 10^6$, which is the point shown for 13 edges in the non-isomorphic MMP hypergraphs plot of Fig. 3. We mention that in our implementation, we expressed Eq. (C.1) as $\log(j+1) - \log(j+1-c) + n(\log j - \log(j+1)) < 0$ and determined j with a binary search method. Because the computation involves the subtraction of almost-equal terms, high-precision floating-point operations are necessary. For the calculations of Fig. 3, Eq. (C.1) gave incorrect answers with less than 35 significant digits, and we used 100 significant digits for robustness.

As a rough check of the statistical model used by the coupon collector's problem, 10 random samples of 50000 67-edge MMP hypergraphs yielded from 48900 to 48975 isomorphism classes, corresponding to predictions of 1119613 to 1202764 total classes by Eq. (C.1). This compares to the actual number of 1183189 classes obtained by exhaustive generation of MMP hypergraphs.

To estimate the KSs in Fig. 3, KS sets were identified using the `states01` program. For small numbers of edges (≤ 12), we never observed a KS set. For large numbers of edges (≥ 63), we never observed a non-KS set, so for them the two plots coincide. For those in between, we took a random sample of non-isomorphic hypergraphs for each edge size and plotted the fraction of observed KS sets times the estimated non-isomorphic MMP hypergraphs.

We show the number of isomorphically unique critical hypergraphs we observed, as identified by the `-c` ("critical") option of the `states01` program, in the "observed odd criticals" and "observed even critical" plots of Fig. 3. We include these to show the actual currently known (not estimated) number of critical sets. It is not, however, intended to convey the distribution of critical hypergraphs vs. edge size; for that purpose, the estimated maximum number of critical sets in Fig. 3 should be used.[2]

In the range of 12 through 62 edges, the "estimated max crit." plot shows the upper 95% confidence limit derived from Bernoulli trial probabilities, based on the model of sampling with replacement from a search space where the *a priori* probability is unknown. [3] If K is the total number of KSs (from the "estimated KSs" plot), n is the sample size (with replacement) of random KS sets, and m is the observed number of critical sets, then the lower 95% confidence level is [3, Eq. (1)]

$$K \cdot I^{-1}_{\frac{1}{2}(1-0.95)}(m+1, n-m+1) \tag{C.2}$$

and the upper 95% confidence level is [3, Eq. (3)]

$$K \cdot I^{-1}_{\frac{1}{2}(1+0.95)}(m+1, n-m+1) \tag{C.3}$$

where I^{-1} is the inverse regularized incomplete beta function. For example, for the 35-edge case, $K = 9.0 \cdot 10^{15}$, $n = 52800000$, and $m = 580$. Thus for upper 95% confidence level we have $K \cdot I^{-1}_{\frac{1}{2}(1+0.95)}(m+1, n-m+1) = K \cdot I^{-1}_{0.975}(581, 52799421) \approx K \cdot 0.0000119163 \approx 1.1 \cdot 10^{11}$. This is the value in the "estimated max crit." plot for 35 edges.

The "estimated min crit." plot shows either the the lower 95% confidence limit from Eq. (C.2) or zero (in which case we omit the "estimated min crit." point from the plot since it is outside the logarithmic scale). A value of zero is used whenever no critical sets were observed. Of course this is the most conservative value possible, but there are two other motivations. First, the trend of the "estimated max crit." curve starts to fall rapidly at 41 edges, and a smooth extrapolation would suggest that it plummets, perhaps to zero, very soon after that point. Second, when no critical sets were observed for a given edge size, the probability distribution of the Bernoulli trial estimation is not "Gaussian-like" but is highly skewed, with a mode (maximum likelihood) of zero critical sets, even though Eq. (C.2) may predict a small positive number.

We emphasize that in the cases where no critical sets were observed, "estimated max crit." merely represents a statistical upper bound based on the number of random samples we took, meaning it is improbable that the actual number of critical sets would *exceed* that number. For sizes greater than 41 edges where no critical sets have been observed, there may be an overriding theoretical reason (that is currently unknown) that would lead to the actual

[2] The "observed odd [even] criticals" in Fig. 3 are not directly related to the distribution of critical sets vs. edge size because we used varying sample sizes. For example, the 879 critical sets with 34 edges were observed in $1.1 \cdot 10^8$ KS samples whereas the 580 critical sets with 35 edges were observed in only $5.28 \cdot 10^7$ KS samples. Since the number of observed critical sets grows with the number of samples, it is likely that the actual number of critical sets with 35 edges—that would be obtained with an exhaustive search—is larger, not smaller, than the number with 34 edges.

number of critical sets being zero. In that case, “estimated max crit.” would get smaller and smaller, approaching zero, as we increased the number of samples. But for any given number of samples, the statistical upper bound is the best unbiased estimate we can make without either a proof that the number of critical sets is zero or an exhaustive set of samples (which would amount to that proof). Thus the estimated range on Fig. 3 is as objectively conservative as possible, even though there is subjective evidence, based on extrapolation at 41 edges, that the actual number of critical sets becomes identically zero very soon after that point (and that would be our conjecture).

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