

First conjecture: a variation on Fejes Tóth's kissing problem estimate (1953). Let 14 nonoverlapping balls of diameter 1 be given with centers $P_i, i = 0, \dots, 13$. Let

$$a = 7/\sqrt{27} \approx 1.347$$

Is

$$\sum_{i=1}^{13} P_0 P_i \geq 12 + a \approx 13.347?$$

Let

$$L(h) = \begin{cases} \frac{h_0 - h}{h_0 - 1} & h \leq h_0 \\ 0 & h \geq h_0. \end{cases}$$

where $h_0 = 1.26$.

Theorem 1 (L_{12}). *Let P_0, \dots, P_N be the centers of N nonoverlapping balls. Set $h_i = P_0 P_i$. Then*

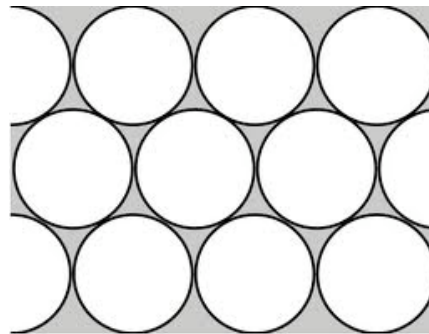
$$\sum_{i=1}^N L(h_i) \leq 12.$$

(If $N = 13$ and h_0 is increased to α , then it becomes Fejes Tóth's kissing number conjecture from 1953.)

Theorem 2 (Kepler (1611)). *The densest packing of congruent balls in \mathbb{R}^3 is attained (non-uniquely) by the face-centered cubic packing.*

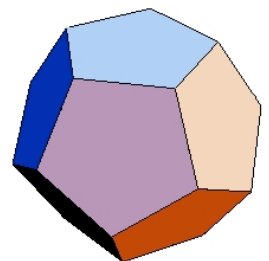
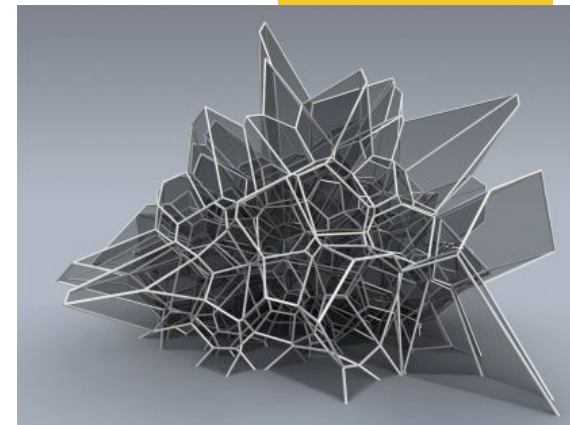
Theorem 3 (Fejes Tóth's full contact conjecture (1969)). *In 3-space a packing of equal balls such that each enclosed ball is touched by 12 others consists of hexagonal layers.*

(The corresponding problem in the plane is trivial. If each unit disk in the plane touches 6 others then it must be the regular hexagonal packing of disks.)



Theorem 4 (K. Bezdek's strong dodecahedral conjecture (2000)). *In every packing of congruent balls in \mathbb{R}^3 , the surface area of every Voronoi cell is at least that of the regular dodecahedron.*

(The strong dodecahedral conjecture implies the weak dodecahedral conjecture, which was proved by S. McLaughlin in 1998, and published last year.)



Theorem 5. *The L_{12} inequality (the variant of FT's kissing number estimate from 1953) implies all of the other conjectures:*

1. *L_{12} implies the Kepler conjecture.*
2. *L_{12} implies FT's full contact conjecture.*
3. *L_{12} implies the strong dodecahedral conjecture.*

L_{12} as a *graph classification theorem*. Let V be a packing in the annulus $[2, 2h_0]$ with $\text{card}(V) > 12$. Let E be the set of edges $\{\mathbf{u}, \mathbf{v}\} \subset V$ such that

$$0 < \|\mathbf{u} - \mathbf{v}\| \leq 2h_0.$$

and such that $\sum_{\mathbf{v} \in V} L(\|\mathbf{v}\|/2) > 12$. Then (V, E) does not exist.

Lemma 1. *Let V be a packing in \mathbb{R}^3 in which every ball touches twelve others. Then for all distinct $\mathbf{u}, \mathbf{v} \in V$, either $\|\mathbf{u} - \mathbf{v}\| = 2$ or $\|\mathbf{u} - \mathbf{v}\| \geq 2h_0$.*

Proof. Let $\mathbf{u}_1, \dots, \mathbf{u}_{12}$ be the twelve kissing points around \mathbf{u} . Assume that $\mathbf{v} \neq \mathbf{u}_i, \mathbf{u}$. By Inequality (L_{12}),

$$L(\|\mathbf{u} - \mathbf{v}\|/2) + 12 = L(\|\mathbf{u} - \mathbf{v}\|/2) + \sum_{i=1}^{12} L(\|\mathbf{u} - \mathbf{u}_i\|/2) \leq 12.$$

This implies that $L(\|\mathbf{u} - \mathbf{v}\|/2) \leq 0$, so $\|\mathbf{u} - \mathbf{v}\| \geq 2h_0$. \square

Definition 1. Let S^2 be the sphere of radius 2, centered at $\mathbf{0}$. Let \mathcal{V} be the set of packings $V \subset \mathbb{R}^3$ such that

1. $\text{card}(V) = 12$,
2. $V \subset S^2$.
3. $\|\mathbf{u} - \mathbf{v}\| \in \{0, 2\} \cup [2.52, 4]$ for all $\mathbf{u}, \mathbf{v} \in V$.

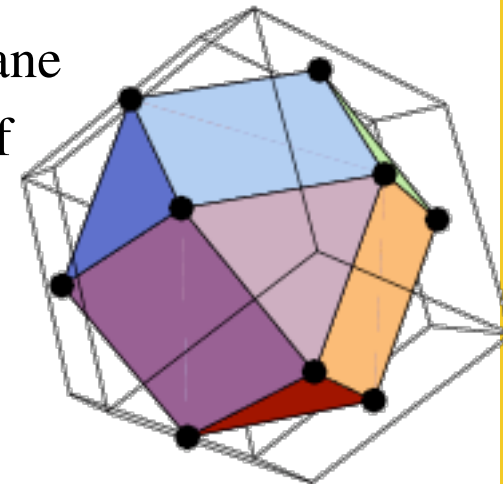
For each $V \in \mathcal{V}$, let E_{ctc} be the contact graph on vertex set V ; that is, the set of $\{\mathbf{u}, \mathbf{v}\} \subset V$ such that $\|\mathbf{u} - \mathbf{v}\| = 2$.

Fejes Tóth's contact conjecture follows from L_{12} and

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Theorem 6 (contact graph classification theorem). *Let $V \in \mathcal{V}$. Then (V, E_{ctc}) is the contact graph of the kissing configuration of the face-centered cubic or hexagonal-close packing.*

(These two kissing configurations can fill space only when arranged in hexagonal layers: the HCP has a preferred plane of symmetry; as soon as one HCP piece occurs, a plane of HCPs is forced.)



Two classification theorems:

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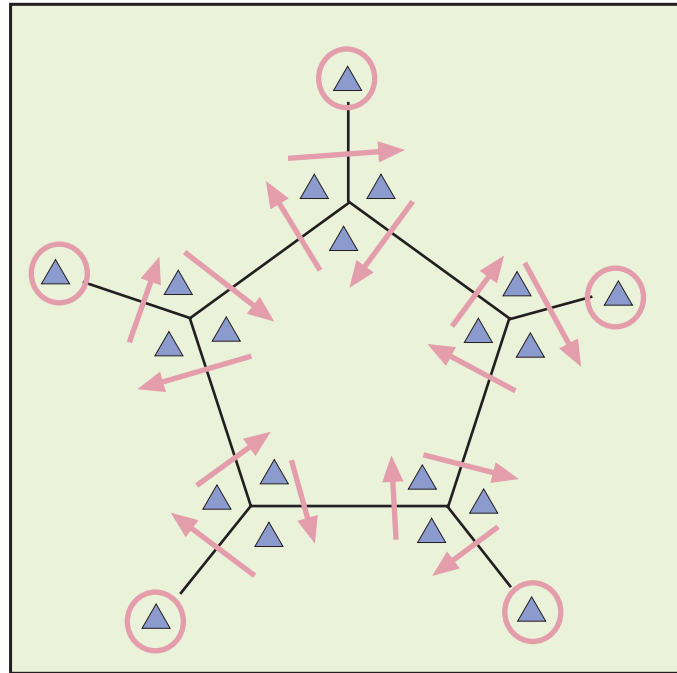
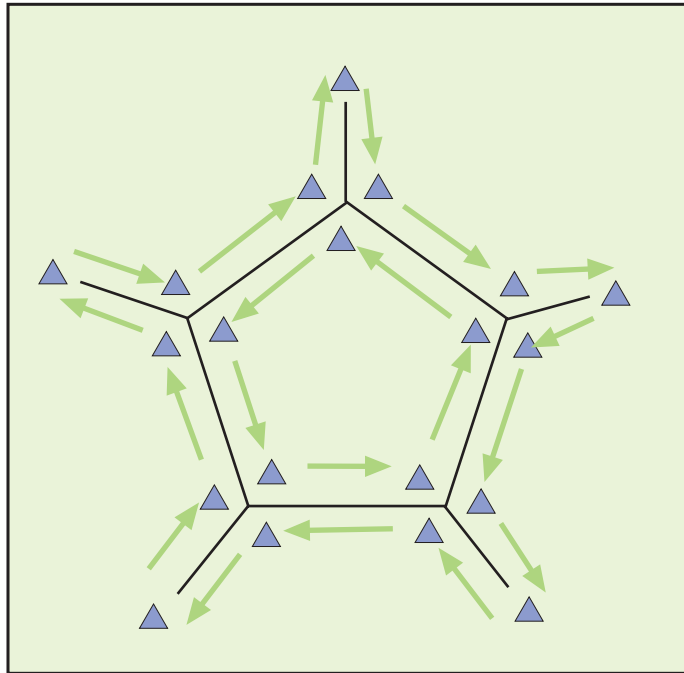
In summary, to prove Fejes Tóth's contact conjecture, it is enough to prove two graph classification theorems:

- L_{12} : no graphs with 13 or more vertices satisfy the L_{12} inequality.
- Only the HCP and FCC contact graphs have 12 vertices and no edges in the range $(2, 2h_0)$.

The proofs of these two classification results differ in detail, but the high-level structure is the same in both cases.

- Represent graphs purely combinatorially as hypermaps.
- A computer program classifies hypermaps (satisfying given properties) up to isomorphism.
- Linear programs eliminate the extraneous cases; those that exist combinatorially but that do not admit a geometric realization.
- The inequalities used in the linear program are proved by computer.

Hypermap



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A hypermap (D, e, n, f) is a finite set D together with three permutations e, n, f on D such that $enf = I$.

- Hypermaps replace geometric aspects of planar graphs with purely combinatorial notions.
- All basic notions of planar graphs (planarity, connectedness, biconnectedness, degrees, of vertices, edges, Euler characteristic, etc.) can be translated to hypermaps.
- Hypermaps are more natural for computer algorithms and proof formalization.
- (Gonthier's formalization of the 4CT is based on hypermaps.)

Graph (hypermap) Generation:

- The formalization of the computer program that classifies planar graphs was the first success of the Flyspeck project (G. Bauer and T. Nipkow)
- Nipkow visited Pittsburgh in August 2010 to update the formal proof so that it gives L_{12} graph classification.
- In doing so, he uncovered a bug in my original code (that went unexercised in the original proof). The bug was an uninitialized structure that gets used in symmetry reductions.
- L_{12} classification: there are about 25K such graphs.
- Contact graph classification: 8 graphs.

L12 preprocessing:

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211 **Lemma 8.16** [FCDJDOT] *Assume that there exists a counterexample to In-*
212 *equality 8.1. Then there also exists a counterexample V to the inequality with*
213 *the following properties:*

- 214 1. $V \subset \mathcal{B}$ is a packing.
215 2. $\mathcal{L}(V) > 12$, and no finite packing in \mathcal{B} attains a value larger than $\mathcal{L}(V)$.
216 3. The cardinality of V is thirteen, fourteen, or fifteen.
217 4. Every node \mathbf{v} is surrounded in the standard fan (V, E_{std}) .
218 5. Every node \mathbf{v} that is not surrounded in the contact fan (V, E_{ctc}) satisfies
219 $|\mathbf{v}| = 2$.

Notation:

$$\mathcal{L}(V) = \sum_{\mathbf{v} \in V} L(\|\mathbf{v}\|/2).$$

\mathcal{B} = closed annulus $[2, 2h_0]$.

fan = (projective) graph.

surrounded = at least 3 edges, angles $< \pi$.

246 Set

$$h(x) = |\text{node}(x)|/2.$$

Define the weight function

$$\tau(V, E, F) = \sum_{x \in F} \text{azim}(x) \left(1 + \frac{\text{sol}_0}{\pi} (1 - L(h(x))) \right) + (\pi + \text{sol}_0) (2 - k(F))$$

$\text{sol}_0 = 0.55 \dots = \text{area of spherical triangle } \pi/3$

254 **Lemma 8.19** (target) [HRXEFD] *Let V be a contravening packing. Then*

$$\sum_F \tau(V, E_{std}, F) < 4\pi - 20 \text{sol}_0 .$$

444 **Definition 7.43** (standard, superior, diagonal) [KRACSCQ] Let (V, E) be a fan.

445 We write $|\epsilon|$ for $|\mathbf{v} - \mathbf{w}|$, when $\epsilon = \{\mathbf{v}, \mathbf{w}\} \subset V$. We say that ϵ is *standard* if

$$2 \leq |\epsilon| \leq 2h_0.$$

446 We say that ϵ is *superior* if

$$2h_0 \leq |\epsilon| \leq \sqrt{8}.$$

447 If $\mathbf{v}, \mathbf{w} \in V$ are distinct, and $\epsilon = \mathbf{v}, \mathbf{w}$ is not an edge in E , then we call ϵ a

448 *diagonal* of the fan.

Main L12 estimate

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Theorem 7.44 (main estimate) [JEJTVGB] *Let (V, E, F) be a nonreflexive local fan (Definition 7.2). We make the following additional assumptions on (V, E, F) :*

1. (PACKING) V is a packing. That is, for every $\mathbf{v}, \mathbf{w} \in V$, if $|\mathbf{v} - \mathbf{w}| < 2$, then $\mathbf{v} = \mathbf{w}$.
2. (ANNULUS) $V \subset \mathcal{B}$.
3. (DIAGONAL) For all distinct elements $\mathbf{v}, \mathbf{w} \in V$, if $\{\mathbf{v}, \mathbf{w}\} \notin E$, then

$$|\mathbf{v} - \mathbf{w}| \geq 2h_0.$$

4. (CARD) Let $k = \text{card}(E) = \text{card}(F)$. Then $3 \leq k \leq 6$.

In this context, we have the following conclusions.

1. Assume $k \geq 4$. If every edge of E is standard, then

$$\tau(V, E, F) \geq d(k), \text{ where } d(k) = \begin{cases} 0.206, & \text{if } k = 4, \\ 0.4819, & \text{if } k = 5, \\ 0.712, & \text{if } k = 6. \end{cases}$$

2. Assume $k = 5$. Assume that every edge of E is standard. Assume that every diagonal ε of the fan satisfies $|\varepsilon| \geq \sqrt{8}$. Then

$$\tau(V, E, F) \geq 0.616.$$

3. Assume $k = 5$. Assume there exists some superior edge in E and that the other four are standard. Then

$$\tau(V, E, F) \geq 0.616.$$

4. Finally, assume that $k = 4$. Assume that there exists some superior edge in E and that the other three are standard. Then

$$\tau(V, E, F) \geq 0.477.$$

There are two related inequalities that we will prove separately. For that reason, we state them as a separate lemma.

Lemma 7.45 [HGDRXAN] *Under the same hypotheses on (V, E, F) ,*

1. Assume $k = 3$. Then

$$\tau(V, E, F) \geq 0.$$

2. Assume $k = 4$. Assume that every edge of E is standard. Assume that both diagonals ε of the fan satisfy $|\varepsilon| \geq 3$. Then

$$\tau(V, E, F) \geq 0.467.$$

64 **Definition 8.4** (b) [00VCYPI] [$b \leftrightarrow b_tame$] Define $b : \mathbb{N}^2 \rightarrow \mathbb{R}$ by
 65 $b(p, q) = \text{tgt}$, except for the values in the following table:

	$q = 0$	1	2	3	4
$p = 0$	tgt	tgt	tgt	0.618	0.97
1	tgt	tgt	0.656	0.618	tgt
2	tgt	0.797	0.412	1.2851	tgt
3	tgt	0.311	0.817	tgt	tgt
4	0.347	0.366	tgt	tgt	tgt
5	0.04	1.136	tgt	tgt	tgt
6	0.686	tgt	tgt	tgt	tgt
7	1.450	tgt	tgt	tgt	tgt

66

67 **Definition 8.5** (d) [BTDOPP] [$d \leftrightarrow d_tame$] Define $d : \mathbb{N} \rightarrow \mathbb{R}$ by

$$d(k) = \begin{cases} 0 & k \leq 3, \\ 0.206 & k = 4, \\ 0.4819 & k = 5, \\ 0.7578 & k = 6, \\ \text{tgt} = 1.541 & \text{otherwise.} \end{cases}$$

68

69 **Definition 8.6** (weight assignment) [DUSOAYQ] [admissible \Leftrightarrow admissible_weight]
 70 [total_weight \Leftrightarrow total_weight] A *weight assignment* of a hypermap H
 71 is a real-valued function τ on the set of faces of H . A weight assignment τ is
 72 *admissible* if the following properties hold:

73 1. (BOUND A) [0.63 \Leftrightarrow a_tame] [\Leftrightarrow adm_3] Let v be any node of type
 74 $(5, 0, 1)$ and let A be the set of triangles meeting that node. Then

$$\sum_{F \in A} \tau(F) \geq 0.63.$$

75 2. (BOUND B) [\Leftrightarrow adm_2] If a node v has type $(p, q, 0)$, then

$$\sum_{F: v \cap F \neq \emptyset} \tau(F) \geq b(p, q).$$

76 3. (BOUND D) [\Leftrightarrow adm_1] If the face F has cardinality k , then $\tau(F) \geq d(k)$.

77 The sum $\sum_F \tau(F)$ (over all faces) is called the *total weight*.

79 **Definition 8.7** (tame) [YOHGLNA] [tame \leftrightarrow tame_hypermap] A hyper-
80 map is *tame* if it satisfies the following conditions:

- 81 1. (PLANAR) [\leftrightarrow tame_1] The hypermap is plain and planar.
- 82 2. (SIMPLE) [\leftrightarrow tame_2] The hypermap is connected and simple. In partic-
83 ular, each intersection of a face with a node contains at most one dart.
- 84 3. (NONDEGENERATE) [\leftrightarrow tame_3] The edge map e has no fixed points.
- 85 4. (NO LOOPS) [\leftrightarrow tame_4] The two darts of each edge lie in different nodes.
- 86 5. (NO DOUBLE JOINS) [\leftrightarrow tame_5a] At most one edge meets any two (not
87 necessarily distinct) nodes.
- 88 6. (FACE COUNT) [\leftrightarrow tame_8] The hypermap has at least three faces.
- 89 7. (FACE SIZE) [\leftrightarrow tame_9a] The cardinality of each face is at least three and
90 at most six.
- 91 8. (NODE COUNT) [\leftrightarrow tame_10] There are thirteen, fourteen, or fifteen nodes.
- 92 9. (NODE SIZE) [\leftrightarrow tame_11a] The cardinality of every node is at least three
93 and at most seven.
- 94 10. (NODE TYPES) [\leftrightarrow tame_12o] If a node has type (p, q, r) with $p + q + r \geq 6$
95 and $r \geq 1$, then $(p, q, r) = (5, 0, 1)$.
- 96 11. (WEIGHTS) [\leftrightarrow tame_13a] There exists an admissible weight assignment
97 of total weight less than the target, $\text{tgt} = 1.541$.

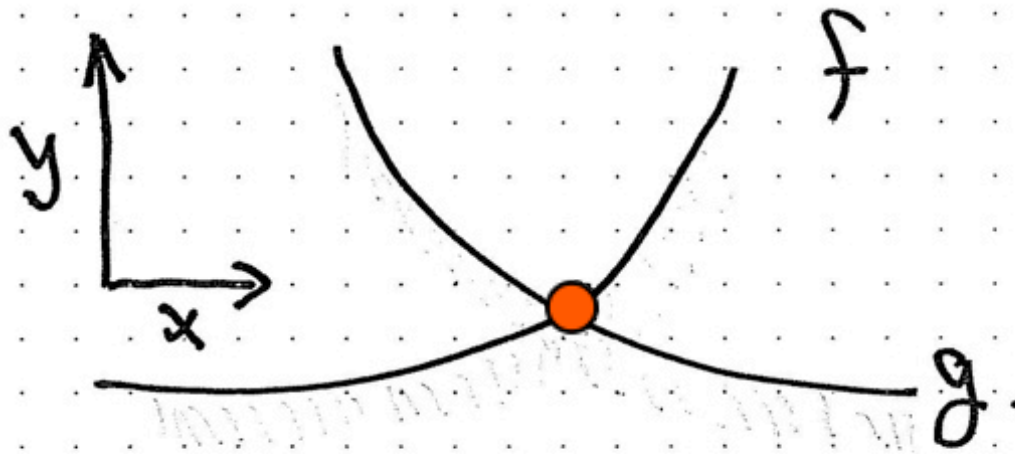
Theorem 7. *Every (preprocessed) counterexample (V, E_{std}) has a tame hypermap.*

393 **Theorem 8.37** [WTEMDTA] *Every tame hypermap is isomorphic to a hyper-*
394 *map in the list [22] or is isomorphic to the opposite of a hypermap in the list.*
395

This classification completes the first part of the proof of L_{12} .
The second part of the proof of L_{12} uses linear programs to
eliminate all $25K$ hypermaps.

Nonlinear optimization

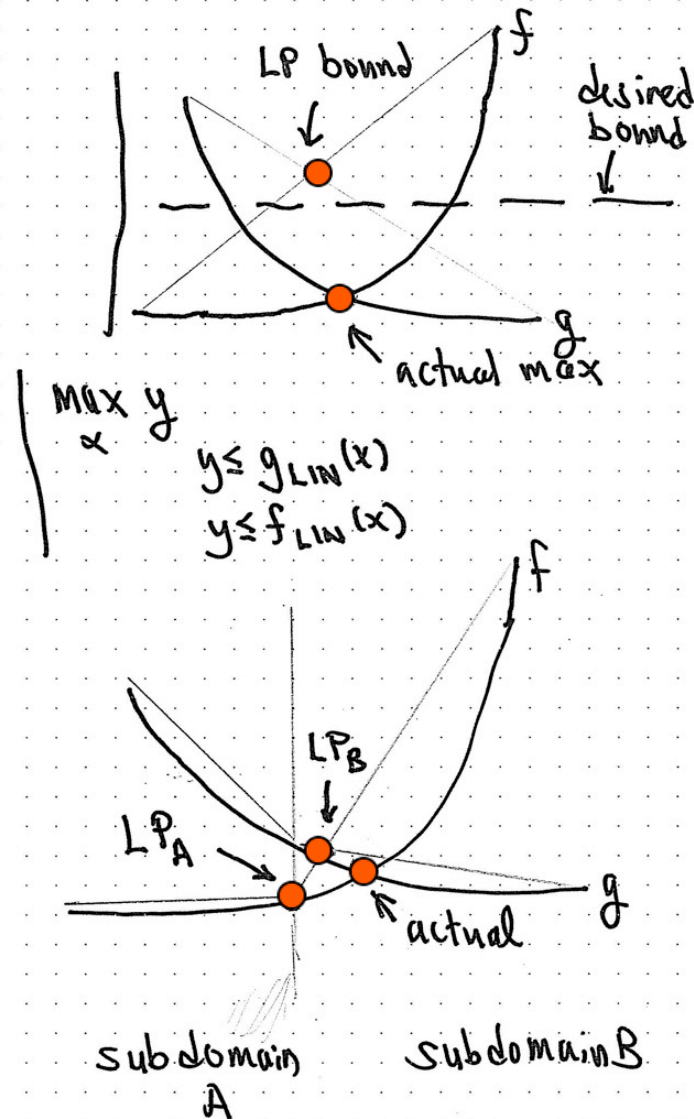
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$$\begin{array}{l} \max_x y \\ \text{s.t. } y \leq g(x) \text{ and} \\ y \leq f(x) \end{array}$$

Linear relaxation and subdivision

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Benchmarks

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#	Inconsistent	Time
1	Yes	15.4
2	Yes	21.9
3	Yes	17.6
4	Yes	39.8
5	Yes	19.4
6	Yes	23.1
7	Yes	26.9
8	Yes	24.3
9	Yes	41.5
10	Yes	40.7
11	Yes	37.7
12	Yes	30.4
13	Yes	30.9
14	Yes	47.3
15	Yes	53.5
16	Yes	66.8
17	Yes	56.1
18	?	47.3
19	Yes	15.9
20	Yes	12.7
21	Yes	20.0
22	Yes	20.8
23	Yes	22.9
24	Yes	23.6
25	Yes	24.3
26	Yes	21.8

source: Obua's thesis

Run times

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Finally, the 'Time' column tells us how many minutes the examination of the tame graph lasted. We used the SML mode of the HOL Computing Library. Each tame graph has been examined by its own Isabelle process. Each Isabelle process ran on a dedicated processor of a cluster of 32 four processor 2.4GHz Opteron 850 machines with 8 GB RAM per machine. The quickest process needed 8.4 minutes, the slowest 67. The examination of *all* tame graphs took about 7.5 hours of cluster runtime. This corresponds to about 40 days on a single processor machine.

We were able to prove the inconsistency of 2565 of the graph systems, and failed on 206. This yields a success rate of about 92.5%.

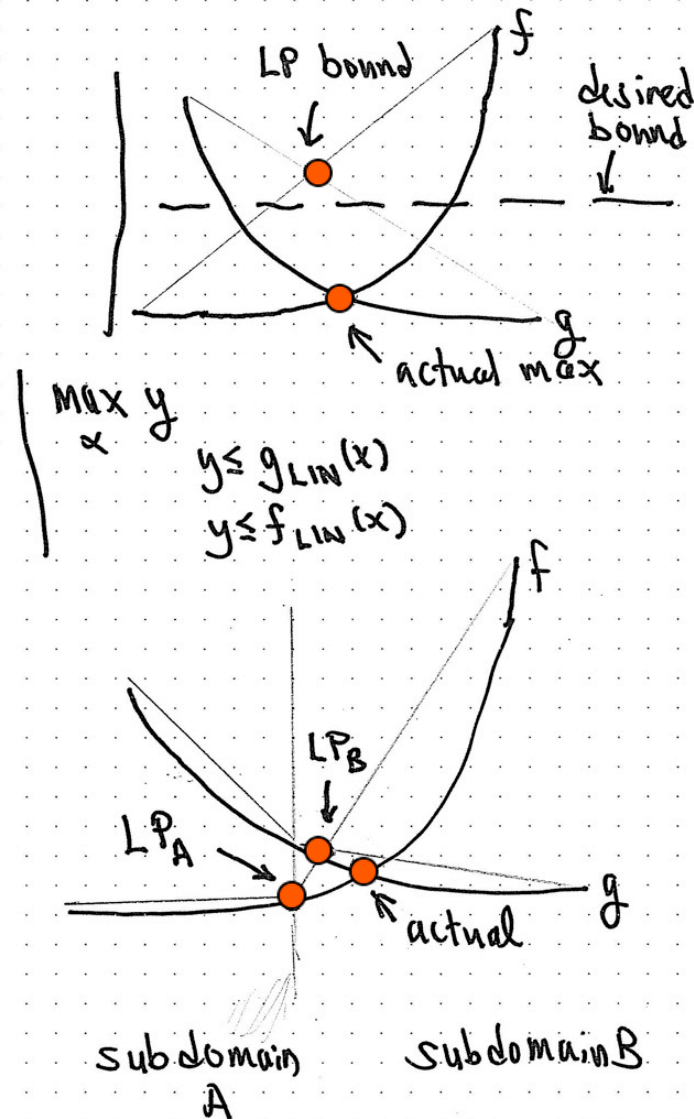
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The current approach

- The linear programming is done in GLPK.
- There is an AMPL model that is independent of the hypermap. (It is the same model for all 25,000 hypermaps.)
- There is a OCAML generated AMPL data file for each linear program.

Nonlinear inequalities as infeasibility problems

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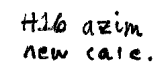
Subdivision

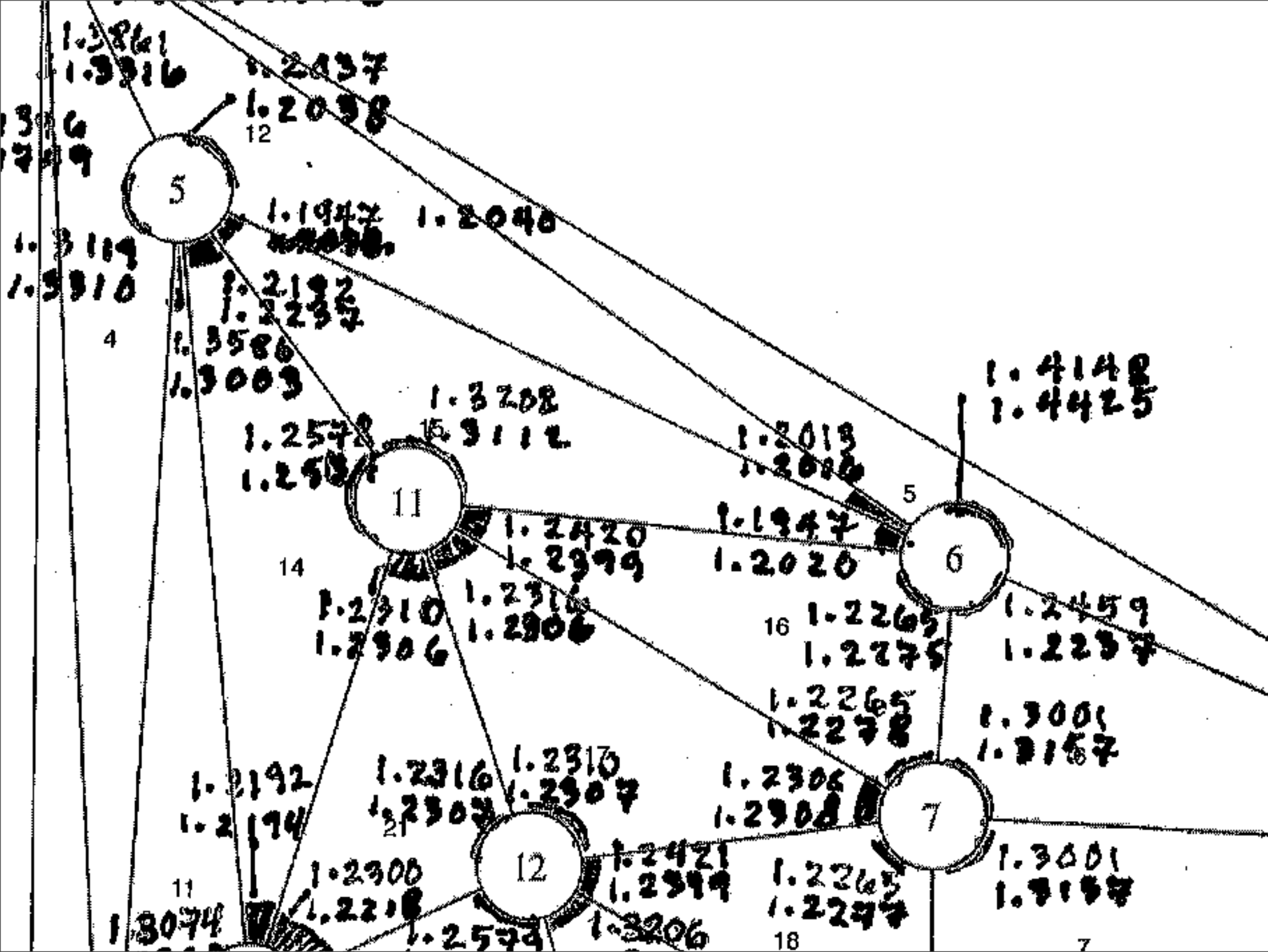
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Subdivision

- Subdivision of a problem that is already linear causes a needless blowup in the number of cases.
- An intelligent scheme for subdivision of the problem should be based on the location of the nonlinearities.

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Nonlinear analysis

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Our approach is to compute all of the dihedral angles (based on optimal edge lengths returned by the linear program) and compare them to the linearized dihedral angles.

The angles are ranked by the size of the error.

Each angle is attached a weight, according to the number of subdivisions that have already occurred at that angle.

The angle with the largest weight error is used for subdivision.

Generating new inequalities

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Adding new inequalities

- Several programs are used (all automated).
- A mathematica procedure based on heuristics is used to generate a candidate inequality.
- The inequality is shipped to cfsqp for testing by nonlinear optimization methods.
- A formal specification is automatically generated in HOL Light.
- The AMPL model is automatically updated with the new inequality. (The inequality is added to all linear programs.)

- This work was all *informal*, but done with formalization in mind.
- At this point A. Solovyev took over the project and began to formalize the linear programming.
- He implemented linear program checking inside HOL Light.
- He optimized real arithmetic calculations inside HOL Light.
- He can now make a formal verification of a large-scale linear program in about 3 seconds. (Read/write operations rather than real arithmetic dominate the times.)
- Compare Obua's benchmarks of about 20 minutes per LP, even when performing real arithmetic outside the proof assistant.

The contact graph classification:

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When $V \in \mathcal{V}$, each U_F is bounded by a finite number $k(U_F) \in \mathbb{N}$ of cones. Write

$$\tau(V, E_{ctc}, F) = \text{sol}(U_F) + (2 - k(U_F)) \text{sol}_0,$$

where sol_0 is the solid angle of an equilateral spherical triangle on the unit sphere of side $\pi/3$.

Using Lexell theorem, we obtain lower bounds on the function $\tau(V, E_{ctc}, F)$ as a function of $k(F)$. This is used to constrain the combinatorial possibilities of the graph. A computer search is made of all planar graphs satisfying the combinatorial properties obtained from the study of τ . As it turns out, there are only eight possibilities. Two of the eight possibilities are the HCP and FCC. Five of the six are subsequently eliminated with linear programming inequalities.

181 **Theorem 9.19** (main estimate) [VGJDQJV] *Let V be a packing in $S^2(2)$, E a*
 182 *set of edges, and F a face of $\text{hyp}(V, E)$ such that (V, E, F) is a local fan (but not*
 183 *necessarily nonreflexive). Assume that F has at least three darts Assume that*
 184 *every edge in E has length at most 3. Let S be a subset of E such that the length*
 185 *of every edge in S is at least 2.52. Let $U = U_F$ be the topological component*
 186 *of $Y(V, E)$ corresponding to F . Assume that if $\{\mathbf{u}, \mathbf{v}\} \subset V$ with $C^0\{\mathbf{u}, \mathbf{v}\} \subset U$,*
 187 *then $|\mathbf{u} - \mathbf{v}| \geq 2.52$. Let $r = \text{card}(E \setminus S)$ and $s = \text{card}(S)$. Then*

$$\tau(V, E, F) \geq \min(d(r, s), \text{tgt}),$$

188 where

$$d(r, s) = \begin{cases} 0.103(2 - s) + 0.2759(r + 2s - 4), & r + 2s > 3 \\ 0, & r + 2s \leq 3. \end{cases}$$

303 **Lemma 9.31** (biconnected) [BTZPFMU] *Let $V \in \mathcal{V}$. Then $\text{hyp}(V, E_{ctc})$ is*
304 *biconnected.*

340 **Definition 9.33** (d) [VUJQZCG] Define $d : \mathbb{N} \rightarrow \mathbb{R}$ by

$$d(k) = \begin{cases} 0, & k \leq 3, \\ 0.206 + 0.2759(k - 4), & k = 4, \dots, 8, \\ \text{tgt}, & k > 8. \end{cases}$$

341 The function d is related to the two-variable function in Lemma 9.19: $d(k) =$
342 $d(k, 0)$, when $4 \leq k \leq 8$.

343 **Definition 9.34** (weight assignment) [GLIQSFM] Recall that a *weight assign-*
344 *ment* on a hypermap H is a function τ on the set of faces of H taking values in
345 the set of nonnegative real numbers. A weight assignment τ is a *contact weight*
346 assignment if the following two properties hold:

- 347 1. If the face F has cardinality k , then $\tau(F) \geq d(k)$.
348 2. If a node \mathbf{v} has type $(p, q, 0)$, then

$$\sum_{F: \mathbf{v} \cap F \neq \emptyset} \tau(F) \geq b(p, q).$$

349 The sum $\sum_F \tau(F)$ is called the *total weight* of τ .

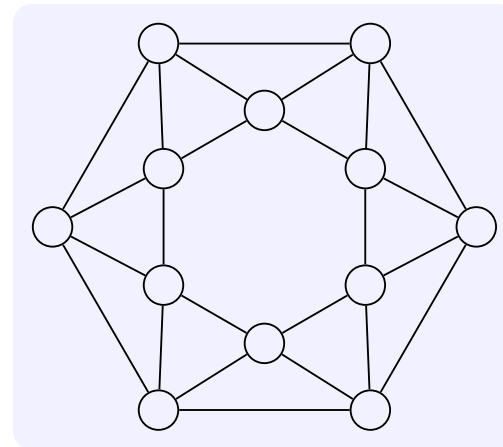
350 **Definition 9.35** (tame contact) [XJPQTIV] A hypermap has *tame contact* if
351 it satisfies the following conditions:

- 352 1. (PLANAR) The hypermap is plain and planar.
353 2. (BICONNECTED) The hypermap is biconnected. In particular, each face meets
354 each node in at most one dart.
355 3. (NONDEGENERATE) The edge map e has no fixed points.
356 4. (NO LOOPS) The two darts of each edge lie in different nodes.
357 5. (NO DOUBLE JOIN) At most one edge meets any two given nodes.
358 6. (FACE COUNT) The hypermap has at least two faces.
359 7. (FACE SIZE) The cardinality of each face is at least three and at most eight.
360 8. (NODE COUNT) The hypermap has twelve nodes.
361 9. (NODE SIZE) The cardinality of every node is at least two and at most four.
362 10. (WEIGHTS) There exists a contact weight assignment of total weight less than
363 tgt.

422 There are some linear programming constraints that are immediately avail-
423 able to us:

- 424 1. The angles around each node sum to 2π .
- 425 2. Each angle of a triangle is α_3 .
- 426 3. Each angle of each rhombus lies between α_4 and β_4 .
- 427 4. The opposite angles of each rhombus are equal.

428 By a linear programming *computer calculation*⁸ [22], these systems of con-
429 straints are infeasible in the remaining five cases. \square





Thank You!

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