Verified Enumeration of Plane Graphs Modulo Isomorphism

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1. Background

2. Generic enumeration

3. Application

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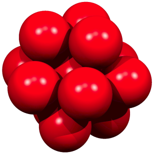
Kepler Conjecture (1611)

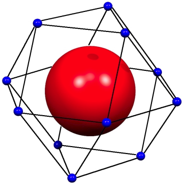
Theorem (Hales 1998). No packing of 3-dimensional balls of the same radius has density greater than the *face-centered cubic packing*.

Proof ideas

- Reduce infinite problem to (small!) finite one:



- Represent cluster as graph:



Sketch of Hales's proof

Proof by contradiction.

Assume there is a counterexample D.

Associate a plane graph (*contravening graph*) with D.

Theorem 0. Every contravening graph is *tame*.

Theorem 1. Every tame plane graph is isomorphic to a graph in the *Archive*.

Theorem 2. No graph in the Archive is contravening.

QED

Hales's proof of Theorem 1

- Java program to enumerate all tame plane graphs.
- Run program and check that each enumerated graph is isomorphic to one in the Archive.

But is the program correct?

The Flyspeck project

Check *all* of the proof with *interactive theorem provers*

Tom Hales & Co	Pitt & Vietnam	HOL light
John Harrison	Intel	HOL light
Steven Obua	TUM	Isabelle/HOL
Gertrud Bauer, T.N.	TUM	Isabelle/HOL

A first contribution

N., Bauer, Schultz verified Theorem 1 (IJCAR 2006):

- HOL is a functional programming language.
- Express executable enumeration of tame plane graphs in HOL (instead of Java).
- Verify that enumeration is complete.
- Execute enumeration and check against Archive.

Hales was right

Executing HOL

Execution by equational logic:

$$\mathit{last}[1,2,3] = \mathit{last}[2,3] = \mathit{last}[3] = 3$$

Too inefficient for Flyspeck.

Execution by compilation (to ML):

$$\mathit{last}[1,2,3] \overset{\mathrm{ML}}{\leadsto} 3$$

$100 \times$ less time and space.

Statistics for 2006 proof

Size of proof:	17 000 lines
Execution time:	1 hour
Number of graphs generated:	23 000 000
Number of tame graphs found:	35 000
Number of tame graphs mod iso:	3 000
Average size of graphs in Archive:	13 nodes, 18 faces

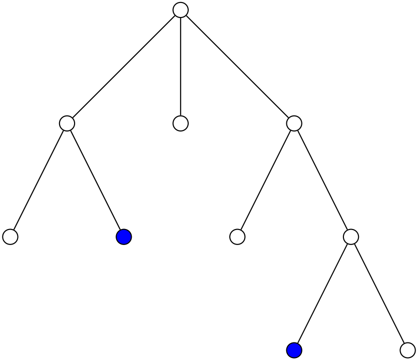
An improved proof

Christian Marchal. *Study of the Kepler's conjecture: The problem of the closest packing.*
Mathematische Zeitschrift. Published online 2009.

$\rightsquigarrow$

- simplifies geometric consideration
- simpler notion of tameness
- new archive of 19 000 tame graphs (mod iso)
- adapted Isabelle/HOL enumeration of tame graphs runs out of space

An enumeration tree



tame

The formalization

Given:

$succs : graph \to (graph)list$
$tame : graph \to bool$

A naive depth-first search:

$enum : (graph)list \to (graph)list \to (graph)list$

$enum\ []\ tgs \ = \ tgs$
$enum\ (g \cdot gs)\ tgs \ =$
$enum\ (succs\ g\ @\ gs)\ (\text{if } tame\ g \text{ then } g \cdot tgs \text{ else } tgs)$

Problems and solutions

Problems:

- Termination
- Removal of isomorphic tame graphs

Generic solutions:

- While combinator for partial functions
- Collections over a preorder (subsumption relation)

Termination

HOL:

- A logic of total functions
- Can also define partial functions by totalizing them

Function *enum*:

- Do not want to prove its termination — difficult
- It should suffice that its actual execution terminates
- Currently not directly definable in Isabelle
  (or elsewhere)

A while combinator

With a few tricks definable

$\mathit{while} : (\alpha \to \mathit{bool}) \to (\alpha \to \alpha) \to \alpha \to (\alpha)\mathit{option}$

where datatype $(\alpha)\mathit{option} = \mathit{None} \mid \mathit{Some}\ \alpha$

Lemmas:

$\mathit{while}\ b\ c\ s\ =\ (\text{if } b\ s \text{ then } \mathit{while}\ b\ c\ (c\ s) \text{ else } \mathit{Some}\ s)$

$$\frac{\mathit{while}\ b\ c\ s = \mathit{Some}\ t \quad P\ s \quad \forall s.\ P\ s \wedge b\ s \longrightarrow P(c\ s)}{P\ t}$$

A worklist function

$worklist\ succs\ f\ []\ s\ =\ Some\ s$

$worklist\ succs\ f\ (x \cdot ws)\ s\ =$
$worklist\ succs\ f\ (succs\ x\ @\ ws)\ (f\ x\ s)$

Easily definable from *while*.

Simple instance: $f\ x\ s = \text{if } tame\ x \text{ then } x \cdot s \text{ else } s$

Must avoid collecting isomorphic graphs!

Ignore x if $x \preceq y$ for some y already encountered

for some preorder $\preceq$

Collections over a preorder

An abstract data type:

$$
\begin{array}{ll}
\preceq: & e \rightarrow e \rightarrow \mathit{bool} \\[1ex]
\mathit{empty}: & s \\
\mathit{insert\text{-}mod}: & e \rightarrow s \rightarrow s \\
\mathit{set\text{-}of}: & s \rightarrow (e)\mathit{set}
\end{array}
$$

$$
\mathit{set\text{-}of}(\mathit{insert\text{-}mod}\ x\ s) = \{x\} \cup (\mathit{set\text{-}of}\ \ s) \vee \\
(\exists y \in \mathit{set\text{-}of}\ \ s.\ x \preceq y) \wedge \mathit{insert\text{-}mod}\ x\ s = s
$$

Enumeration modulo $\preceq$

$enum\ succs\ P\ =$
$worklist\ succs\ (\lambda x\ s.\ \text{if}\ P\ x\ \text{then}\ insert\text{-}mod\ x\ s\ \text{else}\ s)$

Implementing collections over $\preceq$

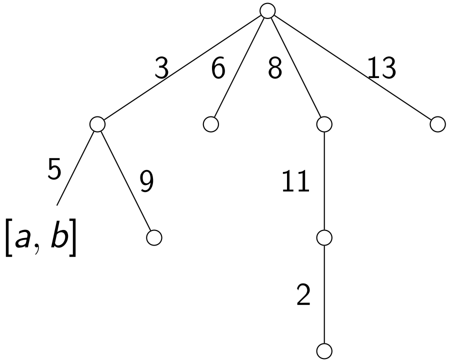
By hash-maps to lists of elements:

$$\begin{array}{ll} \mathit{key} : & e \rightarrow k \\ \mathit{lookup} : & m \rightarrow k \rightarrow (e)\mathit{list} \\ \mathit{update} : & m \rightarrow k \rightarrow (e)\mathit{list} \rightarrow m \end{array}$$

$$\begin{array}{l} \mathit{insert\text{-}mod}\ x\ m\ = \\ \text{let}\ \ k = \mathit{key}\ x; \\ \quad\ \ \mathit{ys} = \mathit{lookup}\ m\ k \\ \text{in}\ \ \text{if}\ \ \exists y \in \mathit{set}\ \mathit{ys}.\ x \preceq y\ \ \text{then}\ \ m \\ \quad\ \ \text{else}\ \ \mathit{update}\ m\ k\ (x \cdot \mathit{ys}) \end{array}$$

Implementing hash-maps

By tries ($\Longrightarrow$ key must be a list)



$$[3, 5] \mapsto [a, b], \ldots$$

Realisation in Isabelle

- Specify ADT as “locale” (= parameterised theory)
- Implement ADT by theory interpretation

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To apply the generic enumeration theory to tame plane graphs we need

- a graph isomorphism test ($\preceq$)
- a hash function for graphs

Plane graph isomorphism test

Three alternatives:

- Implement and verify efficient linear-time algorithm
  — hard
- Implement unverified test and verify result-checker
  — the clever cop out
- Implement and verify reasonable algorithm
  — not too hard, and lets you sleep better

Hash function

$$key : graph \rightarrow (nat)list$$

$$key\ g \;=\; sort(map\ degree\ (nodes\ g))$$

Results

Execution time:	10 hours
Number of graphs generated:	2×10^9
Number of tame graphs found:	350 000
Number of tame graphs mod iso:	19 000
Avg number of graphs per trie node:	3

Found 2 graphs that were missing from Hales's Archive!

Two days later Hales emailed me:

> *I found the bug in my code! It was in the code that uses symmetry to reduce the search space. This is a bug that goes all the way back to the 1998 proof. It is just a happy coincidence that there were no missed cases in the 1998 proof. This is a good example of the importance of formal proof in computer-assisted proofs.*