The Pachner graph and the simplification of 3-sphere triangulations

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Abstract

It is important to have fast and effective methods for simplifying 3-manifold triangulations without losing any topological information. In theory this is difficult: we might need to make a triangulation super-exponentially more complex before we can make it smaller than its original size. Here we present experimental work suggesting that for 3-sphere triangulations the reality is far different: we never need to add more than two tetrahedra, and we never need more than a handful of local modifications. If true in general, these extremely surprising results would have significant implications for decision algorithms and the study of triangulations in 3-manifold topology.

The algorithms behind these experiments are interesting in their own right. Key techniques include the isomorph-free generation of all 3-manifold triangulations of a given size, polynomial-time computable signatures that identify triangulations uniquely up to isomorphism, and parallel algorithms for studying finite level sets in the infinite Pachner graph.

ACM classes F.2.2; G.2.1; G.2.2; D.1.3

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1 Introduction

Triangulations of 3-manifolds are ubiquitous in computational knot theory and low-dimensional topology. They are easily obtained and offer a natural setting for many important algorithms.

Computational topologists typically allow triangulations in which the constituent tetrahedra may be "bent" or "twisted", and where distinct edges or vertices of the same tetrahedron may even be joined together. Such triangulations (sometimes called *semi-simplicial* or *pseudotriangulations*) can describe rich topological structures using remarkably few tetrahedra. For example, the 3-dimensional sphere can be built from just one tetrahedron, and more complex spaces such as non-trivial surface bundles can be built from as few as six [15].

An important class of triangulations is the *one-vertex triangulations*, in which all vertices of all tetrahedra are joined together as a single point. These are simple to obtain [11, 14], and they are often easier to deal with both theoretically and computationally [6, 10, 14].

Keeping the number of tetrahedra small is crucial in computational topology, since many important algorithms are exponential (or even super-exponential) in the number of tetrahedra [5, 6]. To this end, topologists have developed a rich suite of local simplification moves that allow us to reduce the number of tetrahedra without losing any topological information [2, 16]. The most basic of these are the four *Pachner moves* (also known as *bistellar moves*). These include the 3-2 move (which reduces the number of tetrahedra but preserves the number of vertices), the 4-1 move (which reduces both numbers), and also their inverses, the 2-3 and 1-4 moves. It is known that any two triangulations of the same closed 3-manifold are related by a sequence of Pachner moves [21]. Moreover, if both are one-vertex triangulations then we can relate them using 2-3 and 3-2 moves alone [14].

However, little is known about how *difficult* it is to relate two triangulations by a sequence of Pachner moves. In a series of papers, Mijatović develops upper bounds on the number of moves required for various classes of 3-manifolds [17, 18, 19, 20]. All of these bounds are super-exponential in the number of tetrahedra, and some even involve exponential towers of exponential functions. For relating one-vertex triangulations using only 2-3 and 3-2 moves, no explicit bounds are known at all.

In this paper we focus on one-vertex triangulations of the 3-sphere. Here simplification is tightly linked to the important problem of 3-sphere recognition, where we are given an input triangulation \mathcal{T} and asked whether \mathcal{T} represents the 3-sphere. This problem plays an key role in other important topological algorithms, such as connected sum decomposition [11, 12] and unknot recognition [9], and it is now becoming important in computational 4-manifold topology. We can use Pachner moves for 3-sphere recognition in two ways:

- They give us a *direct* 3-sphere recognition algorithm: try all possible sequences of Pachner moves on \mathcal{T} up to Mijatović's upper bound, and return "true" if and only if we reach one of the well-known "canonical" 3-sphere triangulations with one or two tetrahedra.
- They also allow a *hybrid* recognition algorithm: begin with a fast and/or greedy procedure to simplify \mathcal{T} as far as possible within a limited number of moves. If we reach a canonical 3-sphere triangulation then return "true"; otherwise run a more traditional 3-sphere recognition algorithm on our new (and hopefully simpler) triangulation.

The direct algorithm lies well outside the realm of feasibility: Mijatović's bound is superexponential in the number of tetrahedra, and the running time is at least exponential in Mijatović's bound. Current implementations [3] use the hybrid method, which is extremely effective in practice. Experience suggests that when \mathcal{T} is the 3-sphere, the greedy simplification almost always gives a canonical triangulation. If simplification fails, we revert to the traditional algorithm of Rubinstein [22]; although this runs in exponential time, recent improvements by several authors have made it extremely effective for moderate-sized problems [6, 7, 11, 23].¹

Our aims in this paper are:

- to measure how easy or difficult it is *in practice* to relate two triangulations of the 3-sphere using Pachner moves, or to simplify a 3-sphere triangulation to use fewer tetrahedra;
- to understand why greedy simplification techniques work so well in practice, despite the prohibitive theoretical bounds of Mijatović;
- to investigate the possibility that Pachner moves could be used as the basis for a direct 3-sphere recognition algorithm that runs in sub-exponential or even polynomial time.

Fundamentally this is an experimental paper (though the theoretical underpinnings are interesting in their own right). Based on an exhaustive study of ~ 150 million triangulations (including ~ 31 million one-vertex triangulations of the 3-sphere), the answers appear to be:

¹See [7] for explicit measurements of running time.

- we can relate and simplify one-vertex triangulations of the 3-sphere using remarkably few Pachner moves;
- both procedures require us to add *at most two* extra tetrahedra, which explains why greedy simplification works so well;
- the number of moves required to simplify such a triangulation could also be bounded by a constant, which means polynomial-time 3-sphere recognition may indeed be possible.

These observations are extremely surprising, especially in light of Mijatović's bounds. If they can be proven in general—yielding a polynomial-time 3-sphere recognition algorithm—this would be a significant breakthrough in computational topology.

In Section 2 we outline preliminary concepts and introduce the *Pachner graph*, an infinite graph whose nodes represent triangulations and whose arcs represent Pachner moves. This graph is the framework on which we build the rest of the paper. We define *simplification paths* through the graph, as well as the key quantities of *length* and *excess height* that we seek to measure.

We follow in Section 3 with two key tools for studying the Pachner graph: an isomorph-free census of all closed 3-manifold triangulations with ≤ 9 tetrahedra (which gives us the nodes of the graph), and *isomorphism signatures* of triangulations that can be computed in polynomial time (which allow us to construct the arcs of the graph).

Section 4 describes parallel algorithms for bounding both the length and excess height of simplification paths, and presents the highly unexpected experimental results outlined above. We finish in Section 5 with a discussion of the implications and consequences of these results.

2 Triangulations and the Pachner graph

A 3-manifold triangulation of size n is a collection of n tetrahedra whose 4n faces are affinely identified (or "glued together") in 2n pairs so that the resulting topological space is a closed 3-manifold.² We are not interested in the shapes or sizes of tetrahedra (since these do not affect the topology), but merely the combinatorics of how the faces are glued together. Throughout this paper, all triangulations and 3-manifolds are assumed to be connected.

We do allow two faces of the same tetrahedron to be identified, and we also note that distinct edges or vertices of the same tetrahedron might become identified as a by-product of the face gluings. A set of tetrahedron vertices that are identified together is collectively referred to as a *vertex of the triangulation*; we define an *edge* or *face of the triangulation* in a similar fashion.

Figure 1 illustrates a 3-manifold triangulation of size n = 2. Here the back two faces of the first tetrahedron are identified with a twist, the front faces of the first tetrahedron are identified with the front faces of the second using more twists, and the back faces of the second tetrahedron are identified together by directly "folding" one onto the other. This is a *one-vertex triangulation* since all eight tetrahedron vertices become identified together. The triangulation has three distinct edges, indicated in the diagram by three distinct arrowheads.

Mijatović [17] describes a *canonical triangulation* of the 3-sphere of size n = 2, formed by a direct identification of the boundaries of two tetrahedra. In other words, given two tetrahedra

 $^{^{2}}$ It is sometimes useful to consider *bounded* triangulations where some faces are left unidentified, or *ideal* triangulations where the overall space only becomes a 3-manifold when we delete the vertices of each tetrahedron. Such triangulations do not concern us here.

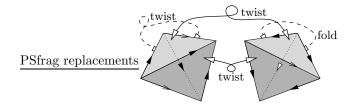


Figure 1: A 3-manifold triangulation of size n = 2

ABCD and A'B'C'D', we directly identify face ABC with A'B'C', ABD with A'B'D', and so on. The resulting triangulation has four faces, six edges, and four vertices.

The four *Pachner moves* describe local modifications to a triangulation. These include:

- the 2-3 move, where we replace two distinct tetrahedra joined along a common face with three distinct tetrahedra joined along a common edge;
- the 1-4 move, where we replace a single tetrahedron with four distinct tetrahedra meeting at a common internal vertex;
- the 3-2 and 4-1 moves, which are inverse to the 2-3 and 1-4 moves.

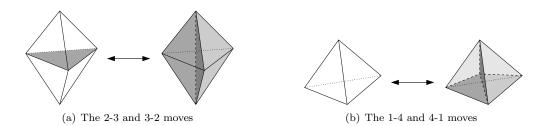


Figure 2: The four Pachner moves for a 3-manifold triangulation

These four moves are illustrated in Figure 2. Essentially, the 1-4 and 4-1 moves retriangulate the interior of a pyramid, and the 2-3 and 3-2 moves retriangulate the interior of a bipyramid. It is clear that Pachner moves do not change the topology of the triangulation (i.e., the underlying 3-manifold remains the same). Another important observation is that the 2-3 and 3-2 moves do not change the number of vertices in the triangulation.

Two triangulations are *isomorphic* if they are identical up to a relabelling of tetrahedra and a reordering of the four vertices of each tetrahedron (that is, isomorphic in the usual combinatorial sense). Up to isomorphism, there are finitely many distinct triangulations of any given size.

Pachner originally showed that any two triangulations of the same closed 3-manifold can be made isomorphic by performing a sequence of Pachner moves [21].³ Matveev later strengthened this result to show that any two *one-vertex* triangulations of the same closed 3-manifold with at least two tetrahedra can be made isomorphic through a sequence of 2-3 and/or 3-2 moves [14].

 $^{^{3}}$ As Mijatović notes, Pachner's original result was proven only for true simplicial complexes, but it is easily extended to the more flexible definition of a triangulation that we use here [17]. The key step is to remove irregularities by performing a second barycentric subdivision using Pachner moves.

The two-tetrahedron condition is required because it is impossible to perform a 2-3 or 3-2 move upon a one-tetrahedron triangulation (each move requires two or three distinct tetrahedra).

In this paper we introduce the *Pachner graph*, which describes *how* distinct triangulations of a closed 3-manifold can be related via Pachner moves. We define this graph in terms of *nodes* and *arcs*, to avoid confusion with the *vertices* and *edges* that appear in 3-manifold triangulations.

Definition (Pachner graph). Let M be any closed 3-manifold. The *Pachner graph* of M, denoted $\mathscr{P}(M)$, is an infinite graph constructed as follows. The nodes of $\mathscr{P}(M)$ correspond to isomorphism classes of triangulations of M. Two nodes of $\mathscr{P}(M)$ are joined by an arc if and only if there is some Pachner move that converts one class of triangulations into the other.

The restricted Pachner graph of M, denoted $\mathscr{P}_1(M)$, is the subgraph of $\mathscr{P}(M)$ defined by only those nodes corresponding to one-vertex triangulations. The nodes of $\mathscr{P}(M)$ and $\mathscr{P}_1(M)$ are partitioned into finite levels $1, 2, 3, \ldots$, where each level n contains the nodes corresponding to n-tetrahedron triangulations.

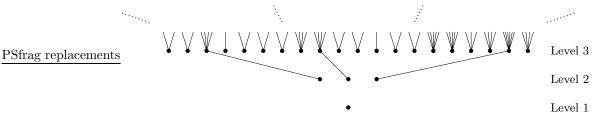


Figure 3: Levels 1–3 of the restricted Pachner graph of the 3-sphere

It is clear that the arcs are well-defined (since Pachner moves are preserved under isomorphism), and that arcs do not need to be directed (since each 2-3 or 1-4 move has a corresponding inverse 3-2 or 4-1 move). In the full Pachner graph $\mathscr{P}(M)$, each arc runs from some level i to a nearby level $i \pm 1$ or $i \pm 3$. In the restricted Pachner graph $\mathscr{P}_1(M)$, each arc must describe a 2-3 or 3-2 move, and must run from some level i to an adjacent level $i \pm 1$. Figure 3 shows the first few levels of the restricted Pachner graph of the 3-sphere.

We can now reformulate the results of Pachner and Matveev as follows:

Theorem 1 (Pachner, Matveev). The Pachner graph of any closed 3-manifold is connected. If we delete level 1, the restricted Pachner graph of any closed 3-manifold is also connected.

To simplify a triangulation we essentially follow a path through $\mathscr{P}(M)$ or $\mathscr{P}_1(M)$ from a higher level to a lower level, which motivates the following definition.

Definition (Simplification path). A simplification path is a directed path through either $\mathscr{P}(M)$ or $\mathscr{P}_1(M)$ from a node at some level i to a node at some lower level < i. The length of a simplification path is the number of arcs it contains. The excess height of a simplification path is the smallest $h \ge 0$ for which the entire path stays in or below level i + h.

Both the length and excess height measure how difficult it is to simplify a triangulation: the length measures the number of Pachner moves, and the excess height measures the number of extra tetrahedra required. For the 3-sphere, the only known bounds on these quantities are the following: **Theorem 2** (Mijatović [17]). Any triangulation of the 3-sphere can be converted into the canonical triangulation using less than $6 \cdot 10^6 n^2 2^{2 \cdot 10^4 n^2}$ Pachner moves.

Corollary 3. In the Pachner graph of the 3-sphere, from any node at level n > 2 there is a simplification path of length less than $6 \cdot 10^6 n^2 2^{2 \cdot 10^4 n^2}$ and excess height less than $3 \cdot 10^6 n^2 2^{2 \cdot 10^4 n^2}$.

In the *restricted* Pachner graph, no explicit bounds on these quantities are known at all.

3 Key tools

Experimental studies of the Pachner graph are difficult: the graph itself is infinite, and even the finite level sets grow super-exponentially in size. By working with isomorphism classes of triangulations, we keep the level sets considerably smaller than if we had used labelled triangulations instead. However, the trade-off is that both the nodes and the arcs of the graph are more difficult to construct.

In this section we outline two key algorithmic tools for studying the Pachner graph: a *census* of triangulations (which enumerates the nodes at each level), and polynomial-time computable isomorphism signatures (which allow us to construct the arcs).

3.1 A census of triangulations

To enumerate the nodes of Pachner graphs, we build a census of all 3-manifold triangulations of size $n \leq 9$, with each triangulation included precisely once up to isomorphism. Because we are particularly interested in one-vertex triangulations as well as triangulations of the 3-sphere, we extract such triangulations into separate censuses with the help of the highly optimised 3-sphere recognition algorithm described in [7]. The final counts are summarised in Table 1.

Number of	All closed 3	-manifolds	3-spheres only		
tetrahedra	No constraints	1-vertex only	No constraints	1-vertex only	
1	4	3	2	1	
2	17	12	6	3	
3	81	63	32	20	
4	577	433	198	128	
5	5184	3961	1903	1297	
6	57753	43584	19935	13660	
7	722765	538409	247644	169077	
8	9787509	7148483	3185275	2142197	
9	139103032	99450500	43461431	28691150	
Total	149676922	107185448	46916426	31017533	

Table 1: Counts for 3-manifold triangulations of various types in the census

The algorithms behind this census are sophisticated; see [4] for some of the techniques involved. The constraint that the triangulation must represent a 3-manifold is critical: if we just enumerate all pairwise identifications of faces up to isomorphism, there are at least

$$\frac{\left[(4n-1)\times(4n-3)\times\cdots\times3\times1\right]\cdot6^{2n}}{n!\cdot24^n} \simeq 2.35\times10^{16}$$

possibilities for n = 9. To enforce the 3-manifold constraint we use a modified union-find algorithm that tracks partially-constructed edge links and vertex links; see [4] for details.

Even with this constraint, we can prove that the census grows at a super-exponential rate:

Theorem 4. The number of distinct isomorphism classes of 3-manifold triangulations of size n grows at an asymptotic rate of $\exp(\Theta(n \log n))$.

The proof is detailed, and is given in the appendix.

For the largest case n = 9, the enumeration of all 3-manifold triangulations up to isomorphism required ~ 85 days of CPU time as measured on a single 1.7 GHz IBM Power5 processor (though in reality this was reduced to 2–3 days of wall time using 32 CPUs in parallel). The time required to extract all 3-sphere triangulations from this census was negligible in comparison.

3.2 Isomorphism signatures

To construct arcs of the Pachner graph, we begin at a node—that is, a 3-manifold triangulation \mathcal{T} —and perform Pachner moves. Each Pachner move results in a new triangulation \mathcal{T}' , and our main difficulty is in deciding which node of the Pachner graph represents \mathcal{T}' .

A naïve approach might be to search through nodes at the appropriate level of the Pachner graph and test each corresponding triangulation for isomorphism with \mathcal{T}' . However, this approach is infeasible: although isomorphism testing is fast (as we prove below), the sheer number of nodes at level n of the graph is too large (see Theorem 4).

What we need is a property of the triangulation \mathcal{T}' that is easy to compute, and that uniquely defines the isomorphism class of \mathcal{T}' . This property could be used as the key in a data structure with fast insertion and fast lookup (such as a hash table or a red-black tree), and by computing this property we could quickly jump to the relevant node of the Pachner graph.

Here we define such a property, which we call the *isomorphism signature* of a triangulation. In Theorem 6 we show that isomorphism signatures do indeed uniquely define isomorphism classes, and in Theorem 7 we show that they are small to store and fast to compute.

A *labelling* of a triangulation of size n involves: (i) numbering its tetrahedra from 1 to n inclusive, and (ii) numbering the four vertices of each tetrahedron from 1 to 4 inclusive. We also label the four faces of each tetrahedron from 1 to 4 inclusive so that face i is opposite vertex i. A key ingredient of isomorphism signatures is *canonical labellings*, which we define as follows.

Definition (Canonical labelling). Given a labelling of a triangulation of size n, let $A_{t,f}$ denote the tetrahedron which is glued to face f of tetrahedron t (so that $A_{t,f} \in \{1, \ldots, n\}$ for all $t = 1, \ldots, n$ and $f = 1, \ldots, 4$). The labelling is *canonical* if, when we write out the sequence $A_{1,1}, A_{1,2}, A_{1,3}, A_{1,4}, A_{2,1}, \ldots, A_{n,4}$, the following properties hold:

- (i) For each $2 \le i < j$, tetrahedron *i* first appears before tetrahedron *j* first appears.
- (ii) For each $i \ge 2$, suppose tetrahedron *i* first appears as the entry $A_{t,f}$. Then the corresponding gluing uses the *identity map*: face *f* of tetrahedron *t* is glued to face *f* of tetrahedron *i* so that vertex *v* of tetrahedron *t* maps to vertex *v* of tetrahedron *i* for each $v \ne f$.

As an example, consider the triangulation of size n = 3 described by Table 2. This table lists the precise gluings of tetrahedron faces. For instance, the second cell in the bottom row indicates that face 2 of tetrahedron 3 is glued to tetrahedron 2, in such a way that vertices 1, 3, 4 of tetrahedron 3 map to vertices 4, 2, 3 of tetrahedron 2 respectively. This same gluing can be seen from the other direction by examining the first cell in the middle row.

	Face 1	Face 2	Face 3	Face 4	
	Vertices 234	Vertices 134	Vertices 124	Vertices 123	
Tet. 1	Tet. 1: 231	Tet. 2: 134	Tet. 3: 124	Tet. 1: 423	
Tet. 2	Tet. 3: 341	Tet. 1: 134	Tet. 2: 123	Tet. 2: 124	
Tet. 3	Tet. 3: 123	Tet. 2: 423	Tet. 1: 124	Tet. 3: 234	

Table 2: The tetrahedron face gluings for an example 3-tetrahedron triangulation

It is simple to see that the labelling for this triangulation is canonical. The sequence $A_{1,1}, \ldots, A_{n,4}$ is 1, 2, 3, 1, 3, 1, 2, 2, 3, 2, 1, 3 (reading tetrahedron numbers from left to right and then top to bottom in the table), and tetrahedron 2 first appears before tetrahedron 3 as required. Looking closer, the first appearance of tetrahedron 2 is in the second cell of the top row where vertices 1, 3, 4 map to 1, 3, 4, and the first appearance of tetrahedron 3 is in the following cell where vertices 1, 2, 4 map to 1, 2, 4. In both cases the gluings use the identity map.

Lemma 5. For any triangulation \mathcal{T} of size n, there are precisely 24n canonical labellings of \mathcal{T} , and these can be enumerated in $O(n^2 \log n)$ time.

Proof. In summary, we can choose any of the n tetrahedra to label as tetrahedron 1, and we can choose any of the 4! = 24 labellings of its four vertices. From here the remaining labels are forced, and can be deduced in $O(n \log n)$ time. The full proof is given in the appendix.

Definition (Isomorphism signature). For any triangulation \mathcal{T} of size n, enumerate all 24n canonical labellings of \mathcal{T} , and for each canonical labelling encode the full set of face gluings as a sequence of bits. We define the *isomorphism signature* to be the lexicographically smallest of these 24n bit sequences, and we denote this by $\sigma(\mathcal{T})$.

To encode the full set of face gluings for a canonical labelling, we could simply convert a table of gluing data (such as Table 2) into a sequence of bits. For practical implementations we use a more compact representation, which will be described in the full version of this paper.

Theorem 6. Given two 3-manifold triangulations \mathcal{T} and \mathcal{T}' , we have $\sigma(\mathcal{T}) = \sigma(\mathcal{T}')$ if and only if \mathcal{T} and \mathcal{T}' are isomorphic.

Proof. It is clear that $\sigma(\mathcal{T}) = \sigma(\mathcal{T}')$ implies that \mathcal{T} and \mathcal{T}' are isomorphic, since both signatures encode the same gluing data. Conversely, if \mathcal{T} and \mathcal{T}' are isomorphic then their 24*n* canonical labellings are the same (though they might be enumerated in a different order). In particular, the lexicographically smallest canonical labellings will be identical; that is, $\sigma(\mathcal{T}) = \sigma(\mathcal{T}')$.

Theorem 7. Given a 3-manifold triangulation \mathcal{T} of size n, the isomorphism signature $\sigma(\mathcal{T})$ has $O(n \log n)$ size and can be generated in $O(n^2 \log n)$ time.

Proof. To encode a full set of face gluings, at worst we require a table of gluing data such as Table 2, with 4n cells each containing four integers. Because some of these integers require $O(\log n)$ bits (the tetrahedron labels), it follows that the total size of $\sigma(\mathcal{T})$ is $O(n \log n)$.

The algorithm to generate $\sigma(\mathcal{T})$ is spelled out explicitly in its definition. The 24*n* canonical labellings of \mathcal{T} can be enumerated in $O(n^2 \log n)$ time (Lemma 5). Because a full set of face gluings has size $O(n \log n)$, we can encode the 24*n* bit sequences and select the lexicographically smallest in $O(n^2 \log n)$ time, giving a time complexity of $O(n^2 \log n)$ overall.

This space complexity of $O(n \log n)$ is the best we can hope for, since Theorem 4 shows that the number of distinct isomorphism signatures for size n triangulations grows like $\exp(\Theta(n \log n))$.

It follows from Theorems 6 and 7 that isomorphism signatures are ideal tools for constructing arcs in the Pachner graph, as explained at the beginning of this section. Moreover, the relevant definitions and results are easily extended to bounded and ideal triangulations (which are beyond the scope of this paper). We finish with a simple but important consequence of our results:

Corollary 8. Given two 3-manifold triangulations \mathcal{T} and \mathcal{T}' each of size n, we can test whether \mathcal{T} and \mathcal{T}' are isomorphic in $O(n^2 \log n)$ time.

4 Analysing the Pachner graph

As discussed in the introduction, our focus is on one-vertex triangulations of the 3-sphere. We therefore direct our attention to $\mathscr{P}_1(S^3)$, the restricted Pachner graph of the 3-sphere.

In this section we develop algorithms to bound the shortest length and smallest excess height of any simplification path from a given node at level n of $\mathscr{P}_1(S^3)$. By running these algorithms over the full census of 31 017 533 one-vertex triangulations of the 3-sphere (as described in Section 3.1), we obtain a computer proof of the following results:

Theorem 9. From any node at level n of the graph $\mathscr{P}_1(S^3)$ where $3 \leq n \leq 9$, there is a simplification path of length ≤ 13 , and there is a simplification path of excess height ≤ 2 .

The bound $3 \le n$ is required because there are no simplification paths in $\mathscr{P}_1(S^3)$ starting at level 2 or below (see Figure 3). For n > 9 a computer proof becomes computationally infeasible.

The results of Theorem 9 are astonishing, especially in light of Mijatović's super-exponential bounds. Furthermore, whilst it can be shown that the excess height bound of ≤ 2 is tight, the length estimate of ≤ 13 is extremely rough: the precise figures could be much smaller still. These results have important implications, which we discuss later in Section 5.

In this section we describe the algorithms behind Theorem 9, and we present the experimental results in more detail. Our algorithms are constrained by the following factors:

- Their time and space complexities must be close to linear in the number of nodes that they examine, due to the sheer size of the census.
- They cannot loop through all nodes in $\mathscr{P}_1(S^3)$, since the graph is infinite. They cannot even loop through all nodes at level $n \ge 10$, since there are too many to enumerate.
- They cannot follow arbitrary breadth-first or depth-first searches through $\mathscr{P}_1(S^3)$, since the graph is infinite and can branch heavily in the upward direction.⁴

Because of these limiting factors, we cannot run through the census and directly measure the shortest length or smallest excess height of any simplification path from each node. Instead we develop fast, localised algorithms that allow us to bound these quantities from above. To our delight, these bounds turn out to be extremely effective in practice. The details are as follows.

⁴In general, a node at level n can have up to 2n distinct neighbours at level (n + 1).

4.1 Bounding excess heights

In this section we compute bounds H_n so that, from every node at level n of the graph $\mathscr{P}_1(S^3)$, there is some simplification path of excess height $\leq H_n$. As in Theorem 9, we compute these bounds for each n in the range $3 \leq n \leq 9$.

Algorithm 10 (Algorithm for computing H_n). This algorithm runs by progressively building a subgraph $G \subset \mathscr{P}_1(S^3)$. At all times we keep track of the number of distinct components of G (which we denote by c) and the maximum level of any node in G (which we denote by ℓ).

- 1. Initialise G to all of level n of $\mathscr{P}_1(S^3)$. This means that G has no arcs, the number of components c is just the number of nodes at level n, and the maximum level is $\ell = n$.
- 2. While c > 1, expand the graph as follows:
 - (a) Construct all arcs from nodes in G at level ℓ to (possibly new) nodes in $\mathscr{P}_1(S^3)$ at level $\ell + 1$. Insert these arcs and their endpoints into G.
 - (b) Update the number of components c, and increment ℓ by one.
- 3. Once we have c = 1, output the final bound $H_n = \ell n$ and terminate.

In step 2(a) we construct arcs by performing 2-3 moves. We only construct arcs from nodes *already* in G, which means we only work with a small portion of level ℓ for each $\ell > n$. In step 2(b) we use union-find to update the number of components in small time complexity.

It is clear that Algorithm 10 is correct for any $n \ge 3$: once we have c = 1 the subgraph G is connected, which means there is a path from any node at level n to any other node at level n. By Theorem 1 at least one such node allows a 3-2 move, and so any node at level n has a simplification path of excess height $\le \ell$.

However, it is not clear that Algorithm 10 terminates: it might be that *every* simplification path from some node at level n passes through nodes that we never construct at higher levels $\ell > n$. Happily it does terminate for all $3 \le n \le 9$, giving an output of $H_2 = 2$ each time. Table 3 shows how the number of components c changes throughout the algorithm in each case.

Input level n	3	4	5	6	7	8	9
Value of c when $\ell = n$	20	128	1297	13660	169077	2142197	28691150
Value of c when $\ell = n + 1$	8	50	196	1074	7784	64528	557428
Value of c when $\ell = n + 2$	1	1	1	1	1	1	1
Final bound H_n	2	2	2	2	2	2	2

Table 3: Results obtained when running Algorithm 10 for $3 \le n \le 9$

It is straightforward to show that the space and time complexities of Algorithm 10 are linear and log-linear respectively in the number of nodes in G (other small polynomial factors in n and ℓ also appear). Nevertheless, the memory requirements for n = 8 were found to be extremely large in practice (~29 GB), and for n = 9 they were too large for the algorithm to run (estimated at 400–500 GB). In the case of n = 9 a *two-phase* approach was necessary:

1. Use Algorithm 10 for the transition from level n to level n + 1, and terminate if $H_n = 1$.

- 2. From each node v at level n + 1, try all possible *combinations* of a 2-3 move followed by a 3-2 move. Let w be the endpoint of such a combination (so w is also a node at level n + 1). If $w \in G$ then merge the components and decrement c if necessary. Otherwise do nothing (since w would never have been constructed in the original algorithm).
- 3. If c = 1 after this procedure then output $H_n = 2$; otherwise terminate with no result.

It is important to note that, if this two-phase approach *does* output a result, it will always be the same result as Algorithm 10. Essentially Step 2 simulates the transition from level n + 1to n+2 in the original algorithm, with the advantage of a much smaller memory footprint (since it does not store any nodes at level n+2), but with the disadvantage that it cannot move on to level n+3 if required (and so it cannot output any result if $H_n > 2$).

Of course by the time we reach n = 9 there are reasons to suspect that $H_n = 2$ (following the pattern for $3 \le n \le 8$), and so this two-phase method seems a reasonable (and ultimately successful) approach. For n = 9 the memory consumption was ~ 50 GB, which was (just) within the capabilities of the host machine.

4.2 Bounding path lengths

Our next task is to compute bounds L_n so that, from every node at level n of $\mathscr{P}_1(S^3)$, there is some simplification path of length $\leq L_n$. Once again we compute L_n for $3 \leq n \leq 9$.

Because it is infeasible to perform arbitrary breadth-first searches through $\mathscr{P}_1(S^3)$, we only consider paths that can be expressed as a series of *jumps*, where each jump involves a pair of 2-3 moves followed by a pair of 3-2 moves. This keeps the search space and memory usage small: we always stay within levels n, n+1 and n+2, and we never need to explicitly store any nodes above level n. On the other hand, it means that our bounds L_n are very rough—there could be much shorter simplification paths that we do not detect.

Algorithm 11 (Algorithm for computing L_n). First identify the set I of all nodes at level n of $\mathscr{P}_1(S^3)$ that have an arc running down to level n-1. Then conduct a breadth-first search across level n, beginning with the nodes in I and using jumps as the steps in this breadth-first search. If j is the maximum number of jumps required to reach any node in level n from the initial set I, then output the final bound $L_n = 4j + 1$.

To identify the initial set I we simply attempt to perform 3-2 moves. When we process each node v, we must enumerate all jumps out from v; that is, all combinations of two 2-3 moves followed by two 3-2 moves. The number of such combinations is $O(n^4)$ in general.

This time we can guarantee both correctness and termination if $3 \le n \le 9$. Because $n \ge 3$ the initial set I is non-empty (Theorem 1), and from our height experiments in Section 4.1 we know that our search will eventually reach all of level n. It follows that every node at level n of $\mathscr{P}_1(S^3)$ has a path of length $\le 4j$ to some $v \in I$, and therefore a simplification path of length $\le 4j + 1$. Table 4 shows how the search progresses for each n.

This time the space and time complexities are linear and log-linear respectively in the number of nodes at level n (again with further polynomial factors in n). This is considerably smaller than the number of nodes processed in Algorithm 10, and so for Algorithm 11 memory is not a problem: the case n = 9 runs in under 4 GB.

Input level n	3	4	5	6	7	8	9
Size of I	3	46	504	6975	91283	1300709	18361866
Nodes remaining	17	82	793	6685	77794	841488	10329284
Nodes remaining after 1 jump	3	1	19	75	496	4222	31250
Nodes remaining after 2 jumps	0	0	1	1	0	6	12
Nodes remaining after 3 jumps	0	0	0	0	0	0	0
Final bound L_n	9	9	13	13	9	13	13

Table 4: Results obtained when running Algorithm 11 for $3 \le n \le 9$

4.3 Parallelisation and performance

For n = 9, both Algorithms 10 and 11 have lengthy running times: Algorithm 10 requires a very large number of nodes to be processed at levels 9, 10 and 11 of the Pachner graph, and Algorithm 11 spends significant time enumerating the $O(n^4)$ available jumps from each node.

We can parallelise both algorithms by processing nodes simultaneously (in step 2 of Algorithm 10, and during each stage of the breadth-first search in Algorithm 11). We must be careful however to serialise any updates to the graph.

The experiments described here used an 8-core 2.93 GHz Intel Xeon X5570 CPU with 72 GB of RAM (using all cores in parallel). With the serialisation bottlenecks, Algorithms 10 and 11 achieved roughly 90.5% and 98.5% CPU utilisation for the largest case n = 9, and ran for approximately 6 and 15 days respectively. All code was written using the topological software package *Regina* [1, 3].

5 Discussion

As we have already noted, the bounds obtained in Section 4 are astonishingly small. Although we only consider $n \leq 9$, this is not a small sample: the census includes ~ 150 million triangulations including ~ 31 million one-vertex 3-spheres; moreover, nine tetrahedra are enough to build complex and interesting topological structures [4, 13]. Our results lead us to the following conjectures:

Conjecture 1. From any node at any level $n \ge 3$ of the graph $\mathscr{P}_1(S^3)$ there is a simplification path of excess height ≤ 2 .

If true, this result (combined with Theorem 4) would reduce Mijatović's bound in Theorem 2 from $\exp(O(n^2))$ to $\exp(O(n \log n))$ for one-vertex triangulations of the 3-sphere. Furthermore, it would help explain why 3-sphere triangulations are so easy to simplify in practice.

There are reasons to believe that a proof might be possible. As a starting point, a simple Euler characteristic argument shows that every closed 3-manifold triangulation has an edge of degree ≤ 5 ; using at most two "nearby" 2-3 moves, this edge can be made degree three (the setting for a possible 3-2 simplification). The details will appear in the full version of this paper.

Conjecture 2. From any node at any level $n \ge 3$ of the graph $\mathscr{P}_1(S^3)$ there is a simplification path of length ≤ 13 .

This is a bolder conjecture, since the length experiments are less consistent in their results. However, the fact remains that every 3-sphere triangulation of size $n \leq 9$ can be simplified after just three jumps, and this number does not rise between n = 5 and n = 9. If true, this second conjecture would yield an immediate polynomial-time 3-sphere recognition algorithm: for any triangulation of size $n \ge 3$ we can enumerate all $O(n^{4\times 3})$ combinations of three jumps, and test each resulting triangulation for a 3-2 move down to n-1 tetrahedra. By repeating this process n-2 times, we will achieve either a recognisable 2-tetrahedron triangulation of the 3-sphere, or else a proof that our input is not a 3-sphere triangulation.

Even if Conjecture 2 is false and the length bounds do grow with n, this growth rate appears to be extremely slow. A growth rate of $L_n \in O(\log n)$ or even $O(\sqrt{n})$ would still yield the first known sub-exponential 3-sphere recognition algorithm (using the same procedure as above), which would be a significant theoretical breakthrough in algorithmic 3-manifold topology.

Looking forward, it is natural to ask whether this behaviour extends beyond the 3-sphere to triangulations of arbitrary 3-manifolds. Initial experiments suggest "partially": the Pachner graphs of other 3-manifolds also appear to be remarkably well-connected, though not enough to support results as strong as Conjectures 1 and 2 above. We explore these issues further in the full version of this paper.

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Appendix: Additional proofs

Here we offer full proofs for Theorem 4 and Lemma 5, which were omitted from the main text to simplify the exposition.

Theorem 4. The number of distinct isomorphism classes of 3-manifold triangulations of size n grows at an asymptotic rate of $\exp(\Theta(n \log n))$.

Proof. An upper bound of $\exp(O(n \log n))$ is easy to obtain. If we count all possible gluings of tetrahedron faces, without regard for isomorphism classes or other constraints (such as the need for the triangulation to represent a closed 3-manifold), we obtain an upper bound of

 $[(4n-1) \times (4n-3) \times \dots \times 3 \times 1] \cdot 6^{2n} < (4n)^{2n} \cdot 6^{2n} \in \exp(O(n \log n)).$

Proving a lower bound of $\exp(\Omega(n \log n))$ is more difficult—the main complication is that most pairwise identifications of tetrahedron faces do not yield a 3-manifold at all [8]. We work around this by first counting 2-manifold triangulations (which are much easier to obtain), and then giving a construction that "fattens" these into 3-manifold triangulations without introducing any unwanted isomorphisms. To create a 2-manifold triangulation of size 2m (the size must always be even), we identify the 6m edges of 2m distinct triangles in pairs. Any such identification will always yield a closed 2-manifold (that is, nothing can "go wrong", in contrast to the three-dimensional case).

There is, however, the issue of connectedness to deal with (recall from the beginning of Section 2 that all triangulations in this paper are assumed to be connected). To ensure that a labelled 2-manifold triangulation is connected, we insist that for each $k = 2, 3, \ldots, 2m$, the first edge of the triangle labelled k is identified with some edge from one of the triangles labelled $1, 2, \ldots, k - 1$. Of course many connected labelled 2-manifold triangulations do not have this property, but since we are proving a lower bound this does not matter.

We can now place a lower bound on the number of labelled 2-manifold triangulations. First we choose which edges to pair with the first edges from triangles $2, 3, \ldots, 2m$; from the property above we have $3 \times 4 \times \ldots \times 2m \times (2m+1) = \frac{1}{2}(2m+1)!$ choices. We then pair off the remaining 2m+2 edges, with $(2m+1) \times (2m-1) \times \ldots \times 3 \times 1 = (2m+1)!/2^m m!$ possibilities overall. Finally we note that each of the 3m pairs of edges can be identified using one of two possible orientations. The total number of labelled 2-manifold triangulations is therefore at least

$$\frac{(2m+1)!}{2} \cdot \frac{(2m+1)!}{2^m m!} \cdot 2^{3m} = \frac{(2m+1)! \cdot (2m+1)! \cdot 2^{2m}}{2 \cdot m!}$$

Each isomorphism class can contain at most $(2m)! \cdot 6^{2m}$ labelled triangulations, and so the number of distinct *isomorphism classes* of 2-manifold triangulations is bounded below by

$$\frac{(2m+1)! \cdot (2m+1)! \cdot 2^{2m}}{2 \cdot m! \cdot (2m)! \cdot 6^{2m}} = \frac{(2m+1) \cdot (2m+1)!}{2 \cdot m! \cdot 3^{2m}}$$

> $(2m+1) \times 2m \times \dots \times (m+2) \times (m+1) \times \left(\frac{1}{9}\right)^m$
> $(m+1)^{m+1} \cdot \left(\frac{1}{9}\right)^m$
 $\in \exp(\Omega(m \log m)).$

We fatten each 2-manifold triangulation into a 3-manifold triangulation as follows. Let F denote the closed 2-manifold described by the original triangulation.

- 1. Replace each triangle with a prism and glue the vertical faces of adjacent prisms together, as illustrated in Figure 4(a). This represents a *bounded* 3-manifold, which is the product space $F \times I$.
- 2. Cap each prism at both ends with a triangular pillow, as illustrated in Figure 4(b). The two faces of each pillow are glued to the top and bottom of the corresponding prism, effectively converting each prism into a solid torus. This produces the *closed* 3-manifold $F \times S^1$, and the complete construction is illustrated in Figure 4(c).
- 3. Triangulate each pillow using two tetrahedra, which are joined along three internal faces surrounding an internal vertex. Triangulate each prism using 14 tetrahedra, which again all meet at an internal vertex. Both triangulations are illustrated in Figure 4(d).

If the original 2-manifold triangulation uses 2m triangles, the resulting 3-manifold triangulation uses n = 32m tetrahedra. Moreover, if two 3-manifold triangulations obtained using this construction are isomorphic, the original 2-manifold triangulations must also be isomorphic. The reason for this is as follows:

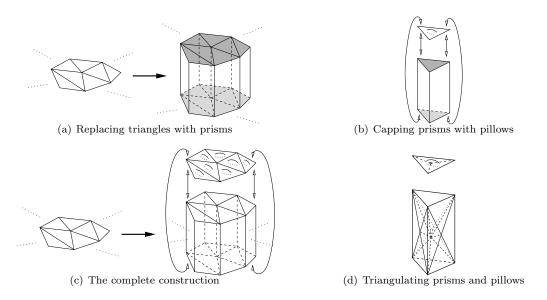


Figure 4: Fattening a 2-manifold triangulation into a 3-manifold triangulation

- Any isomorphism between two such 3-manifold triangulations must map triangular pillows to triangular pillows. This is because the internal vertex of each triangular pillow meets only two tetrahedra, and no other vertices under our construction have this property.
- By "flattening" the triangular pillows into 2-dimensional triangles, we thereby obtain an isomorphism between the underlying 2-manifold triangulations.

It follows that, for n = 32m, we obtain a family of $\exp(\Omega(m \log m)) = \exp(\Omega(n \log n))$ pairwise non-isomorphic 3-manifold triangulations.

This result is easily extended to $n \neq 0 \mod 32$. Let V_n denote the number of distinct isomorphism classes of 3-manifold triangulations of size n.

- Each triangulation of size n has at least n-1 distinct 2-3 moves available (since any face joining two distinct tetrahedra defines a 2-3 move, and there are at least n-1 such faces).
- On the other hand, each triangulation of size n + 1 has at most 6(n + 1) distinct 3-2 moves available (since each 3-2 move is defined by an edge that meets three distinct tetrahedra, and the triangulation has at most 6(n + 1) edges in total).

It follows that $V_{n+1} \ge V_n \cdot \frac{n-1}{6(n+1)} \ge V_n/18$ for any n > 1. This gives $V_{32m+k} \ge V_{32m}/18^{31}$ for sufficiently large m and all $0 \le k < 32$, and so we obtain $V_n \in \exp(\Omega(n \log n))$ with no restrictions on n.

Remark. Of course, we expect that $V_{n+1} \gg V_n$ (and indeed we see this in the census). The bounds that we use to show $V_{n+1} \ge V_n/18$ in the proof above are very loose, but they are sufficient for the asymptotic result that we seek.

Lemma 5. For any triangulation \mathcal{T} of size n, there are precisely 24n canonical labellings of \mathcal{T} , and these can be enumerated in $O(n^2 \log n)$ time.

Proof. For n = 1 the result is trivial, since all 24 = 4! possible labellings are canonical. For n > 1 we observe that, if we choose (i) any one of the *n* tetrahedra to label as tetrahedron 1, and (ii) any one of the 24 possible labellings of its four vertices, then there is one and only one way to extend these choices to a canonical labelling of \mathcal{T} .

To see this, we can walk through the list of faces $F_{1,1}, F_{1,2}, F_{1,3}, F_{1,4}, F_{2,1}, \ldots, F_{n,4}$, where $F_{t,i}$ represents face *i* of tetrahedron *t*. The first face amongst $F_{1,1}, \ldots, F_{1,4}$ that is joined to an unlabelled tetrahedron must in fact be joined to tetrahedron 2 using the identity map; this allows us to deduce tetrahedron 2 as well as the labels of its four vertices.

We inductively extend the labelling in this manner: once we have labelled tetrahedra $1, \ldots, k$ and their corresponding vertices, the first face amongst $F_{1,1}, \ldots, F_{k,4}$ that is joined to an unlabelled tetrahedron must give us tetrahedron k+1 and the labels for its four vertices (again using the identity map). The resulting labelling is canonical, and all of the labels can be deduced in $O(n \log n)$ time using a single pass through the list $F_{1,1}, \ldots, F_{n,4}$. The log *n* factor is required for manipulating tetrahedron labels, each of which requires $O(\log n)$ bits.

It follows that there are precisely 24n canonical labellings of \mathcal{T} , and that these can be enumerated in $O(n^2 \log n)$ time using 24n iterations of the procedure described above.