Some algorithms arising in the proof of the Kepler conjecture

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Abstract

By any account, the 1998 proof of the Kepler conjecture is complex. The thesis underlying this article is that the proof is complex because it is highly under-automated. Throughout that proof, manual procedures are used where automated ones would have been better suited. This paper gives a series of nonlinear optimization algorithms and shows how a systematic application of these algorithms would bring substantial simplifications to the original proof.

1 Introduction

In 1998 a proof of the Kepler conjecture was completed. By any account, that solution is complex (300 pages of text, 3GB stored data on the computer, computer calculations taking months, 40K lines of computer code, and so forth). The thesis underlying this article is that the 1998 proof is complex because it is highly under-automated. Throughout that proof, manual procedures are used where automated ones would have been better suited.

Ultimately, a properly automated proof of the Kepler conjecture might be short and elegant. The hope is that the Kepler conjecture might eventually become an instance of a general family of optimization problems for which general optimization techniques exist. Just as today linear programming problems of a moderate size can be solved without fanfare, we might hope that problems of a moderate size in this family might be routinely solved by general algorithms. The proof of the Kepler conjecture would then consist of demonstrating that the Kepler conjecture can be structured as a problem in this family, and then invoking the general algorithm to solve the problem.

As a step toward that objective, this article frames the primary algorithms of that proof in sufficient generality that they may be applied to much larger families of problems. The algorithms are arranged into four sections: Quantifier Elimination, Linear Assembly Problems, Automated Inequality Proving, Plane Graph Generation.

We do not claim any originality in the algorithms. In fact, the purpose is just the contrary: to exhibit the proof of the Kepler conjecture insofar as possible as an instance of standard optimization techniques. To keep things as general as possible, the algorithms we present here will make no mention of the particulars of the Kepler conjecture. A final section lists parts of the 1998 proof that can be structured according to these general algorithms.

2 Quantifier Elimination

We might try to structure the Kepler conjecture as a statement in the elementary theory of the real numbers. Tarski proved the decidability of this theory, through quantifier elimination. G. Collins and others have developed and implemented concrete algorithms to perform quantifier elimination. The Kepler conjecture, as formulated in \( \frac{1}{3} \), is not a statement in this theory, because the transcendental arctangent function enters into the statement.
However, it seems that the arctangent is not essential to the formulation of the Kepler conjecture, and that it enters only because no attempt was made to do without it. For example, it is plausible that it can be replaced with a close rational approximation, without doing violence to the proof. In fact, the computer calculations in that proof are already based on rational approximations with explicit error bounds, and on its rational derivative $1/(1 + x^2)$.

Assuming this can be done, quantifier elimination gives a procedure to solve the Kepler conjecture. Unfortunately, these algorithms are prohibitively slow (exponential, or doubly exponential in the number of variables).

Section 3 of this article proposes a different family of optimization problems for which algorithmic performance is satisfactory. These are called linear assembly problems.

Although quantifier elimination is too slow to be of practical value as a 1-step solution to the Kepler conjecture, it can be of great value in proving intermediate results. Recent algorithms are able to solve problems nearly at the level of difficulty of intermediate results in the Kepler conjecture [2], [13].

Instances of the following families of problems arise as intermediate steps in the Kepler conjecture. Each instance of the following families must provide an explicit set of parameters $r_k$ (or $d_{\text{min}}, d_{\text{max}}$), and the problem becomes to show that configurations of points in $\mathbb{R}^3$ with the given parameters do not exist. In theory, the problems are all amenable to solution by quantifier elimination.

**Problem 2.1.** Let $S$ be a simplex whose edges all have length at most given parameter values $r_i$. Show that there is no point in the interior of the simplex with distance at least $r$ from every vertex.

**Problem 2.2.** Show that there does not exist a triangle of circumradius at most $r_1$, and a segment of length at most $r_2$ such that the segment passes through the interior of the triangle and such that each endpoint of the segment has distance at least $r_3$ from each vertex of the triangle.

**Problem 2.3.** Show that there does not exist a configuration of 5 points $0, p_1, p_2, p_3, q$ with given minimum $d_{\text{min}}(p, q)$ and maximum $d_{\text{max}}(p, q)$ distances between each pair $(p, q)$ of points. The line through $(0, q)$ must link the triangle with vertices $p_i$.

**Problem 2.4.** Show that there does not exist a configuration of 6 points $0, p_1, \ldots, p_4, q$, with given minimum and maximum distances between each pair $(p, q)$ of points. The line $(0, q)$ must link the skew quadrilateral with vertices $q_i$ (ordered according to subscripts).

**Problem 2.5.** Show that there does not exist a configuration of 7 points $0, p_1, \ldots, p_4, q_1, q_2$ with given minimum $d_{\text{min}}(p, q)$ and maximum $d_{\text{max}}(p, q)$ distances between each pair $(p, q)$ of points. For $j = 1, 2$, the line $(0, q_j)$ must link the skew quadrilateral with vertices $q_i$ (ordered according to subscripts).

Although we hope that one day these problems will all be amenable to direct solution by quantifier elimination, in practice, we did not try to apply quantifier elimination directly without preprocessing them. The idea of preprocessing is that if a configuration exists, then the points can be moved in such a way to make various upper and lower bound constraints on distances bind. With a large number of binding constraints, the dimension of the configuration space becomes smaller and the problem easier to solve. In some cases, preprocessing reduces the configuration space to a single configuration, so that the existence of the configuration can be tested by choosing coordinates and calculating whether all the metric constraints are satisfied.

These five families of quantifier elimination problems have a similar feel to them. Let us give a preprocessing algorithm in general enough terms that it applies uniformly to all five problem families.

The primary preprocessing of the configurations is a deformation that we call pivoting. Fix any three of the points $p_1, p_2$, and $q$ of the configuration. We call a pivot through axis $(p_1, p_2)$ the continuous motion of $q$ in the perpendicular bisecting plane $B$ of $(p_1, p_2)$ at constant distance from $p_1$ and $p_2$. Thus, the pivot moves $q$ in a circular path in the plane $B$. 


Figure 1: A pivot is the circular motion of a point around a fixed axis.

Usually, the plane \( P = (p_1, p_2, q) \) through the three points is chosen to have the property that the entire configuration lies in a half-space through \( P \). If \( q \) moves away from the half-space containing \( P \), the distances from \( q \) to the other points of the configuration increase or remain the same. If \( q \) moves into the half-space, the distances decrease or remain the same.

More generally, we allow the plane \( P \) to separate the points of the configuration into two groups, such that the lower distance bounds from \( q \) to the first group do not bind, and such that the upper distance bounds from \( q \) to the second group do not bind.

To apply pivots, we must prescribe their directions, whether into the half-space or away from it. To do this, we give a model, which is a configuration that exists, of the form indicated in the problem family, but which is not required to satisfy the various constraints. Various edges in the model are marked with a strut (indicating a lower bound) or a cable (indicating an upper bound). If the model has a cable, then preprocessing pivots are applied to increase the corresponding distance in the configuration space, until the given upper bound is reached. Where the model has a strut, pivots are applied so as to decrease distances to the lower bound.

(Bob Connelly has pointed out that some of these problems can be viewed as tensegrity problems, but we do not see how to treat them all as tensegrities, so we do not pursue this point of view here. Globally rigid tensegrities are analogous to our models. However, our models are not claimed to be rigid.)

Example 2.6. In Problem 2.4, let the upper bounds on the edges of the simplex be \( \sqrt{8} \), and let \( r = 2 \). We take the model to be a regular tetrahedron with edges marked as cables. Mark the edges from the circumcenter to the vertices as struts. We apply pivots to the simplex to increase its edges to \( \sqrt{8} \). Move the interior point by a sequence of pivots so that it has distance exactly 2 to three of the four vertices of the simplex.

After these pivots are completed, the configuration is uniquely determined, and a calculation with explicit coordinates shows that the configuration does not exist, because the distance from the interior point to the fourth vertex of the simplex is too small.

In these problems, when we pivot in the correct direction, the distance constraints between points take care of themselves. However, some of the problems impose additional constraints. In Problem 2.1, the point is constrained to lie in the simplex. In the other problems, lines are required to be linked with various space polygons. A separate verification is required to see that pivots do not violate these additional constraints. These separate verifications are again quantifier elimination problems, of a smaller magnitude than the original problem.

For example, in Problem 2.1, we verify that the point cannot be an interior point of a face of the simplex. This insures that the point does not escape from the interior of the simplex during the sequence of pivots. The argument that there does not exist a point in a face, under the given metric constraints,
Figure 2: Some models for the sample quantifier elimination problems. Struts are doubled lines.

is similar to Example 2.6, but all the arguments are reduced to two dimensions, instead of three.

The preprocessing in most other cases is similar to Example 2.6, and can be reconstructed without difficulty from the models. The two exceptions are Problem 2.4 and Problem 2.5, which require substantial preprocessing and a lemma to insure that the pivots can be carried out. (I would much prefer to have arguments based on a pure quantifier elimination algorithm and bypass this lemma entirely, but the current quantifier elimination algorithms do not seem up to the task.)

Lemma 2.7. Fix constants $\ell_i$, $k_i$, $\epsilon$, $h_i$, and $\ell$ subject to the constraints

$$\ell_i < \sqrt{8}, \quad k_i \in [2, 2.61], \quad \epsilon \geq 2, \quad h_i \in [2, \sqrt{8}], \quad \ell \in [2, \sqrt{8}]. \quad (1)$$

Pick the following parameters in Example 2.7:

$$\text{dmin}(p, q_j) = h_i, \quad \text{dmin}(q_1, q_2) = \epsilon, \quad \text{dmin}(\text{others}) = 2$$
$$\text{dmax}(0, p_i) = \ell_i, \quad \text{dmax}(0, q_j) = \ell, \quad \text{dmax}(p_i, p_{i+1}) = k_i$$

and let the other values of $\text{dmax}$ be $+\infty$. If a configuration of 7 points exists with these parameters, then
a configuration also exists with these parameters and the additional constraints that

\[ |p_i| = 2, \quad |p_i - p_{i+1}| = k_i, \quad |q_j| = \ell. \]

Furthermore, the same lemma and conclusion holds in the context of the 6-point configuration of Example 2.4, if we take \( q_1 = q_2 = q \) and \( \text{dmin}(q_1, q_2) = 0 \).

Proof. This is Lemma 4.3 of [7]. Some of the constants have been relaxed in a way that affects the proof in a very minor way. (Two modifications must be made to the proof. The assertion that the circumradius of a triangle of sides \( 2.1, 2.51, 2.51 \) is less than \( \sqrt{2} \) of the original must be replaced with the assertion that there exists an \( x > 2 \) such that the circumradius of the triangle of sides \( x, 2.61, 2.61 \) is less than \( \sqrt{2} \).

Also, an instance of Problem 2.1 is needed, with \( r = 2 \) and the length-bounds of the sides of the simplex \( 2.61, 2.61, \sqrt{8} \) at one vertex, and lengths at most \( \sqrt{8} \) at the edges opposite the edges of length at most \( 2.61 \).)

\[ \Box \]

3 Linear Assembly Problems

In this section we define a class of nonlinear optimization problems that we call linear assembly problems.

Assume given a topological space \( X \), and a finite collection of topological spaces, called local domains. For each local domain \( D \) there is a map \( \pi_D : X \to D \). There are functions \( u_i, i = 1, \ldots, N \), each defined on some local domain \( D_i = \text{dom}(u_i) \), and we let \( x_i \) denote the composite \( x_i = \pi_{D_i} \circ u_i \).

On each local domain \( D \), the functions \( u_i \) are related by a finite set of nonlinear relations

\[ \phi(u_i : \text{dom}(u_i) = D) \geq 0, \quad \phi \in \Phi_D. \quad (2) \]

We use vector notation \( x = (x_1, \ldots, x_N) \), with constant vectors \( c, b \), and matrix \( A \) given.

The problem is to maximize \( c \cdot x \) subject to the constraints

\[ Ax \leq b, \quad (3) \]

and to the nonlinear relations [3]. A problem of this form is called a linear assembly problem. (Intuitively, there are a number of nonlinear objects \( D \), that form the pieces of a jigsaw puzzle that fit together according to the linear conditions [3].)

Example 3.1. Assume a single local domain \( D \), and let \( \pi_D : X = D \) be the identity map. The function \( f = c \cdot x \) is nonlinear. The problem is to maximize \( f \) over \( D \) subject to the nonlinear relations \( \Phi_D \). This is a general constrained nonlinear optimization problem.

Example 3.2. Assume that each \( u_i \) has a distinct local domain \( D_i = \mathbb{R} \). Let \( X = \mathbb{R}^N \), let \( \pi_D \) be the projection onto the \( i \)th coordinate, and let \( x_i \) be the \( i \)th coordinate function on \( \mathbb{R}^n \). Assume that \( \Phi_D \) is empty for each \( D \). The problem becomes the general linear programming problem

\[ \max c \cdot x \]

such that \( Ax \leq b \).

These two examples give the nonlinear and linear extremes in linear assembly problems. The more interesting cases are the mixed cases which combine nonlinear and linear programming. Example 2.3 gives one such case.

Example 3.3. (2D Voronoi cell minimization). Take a packing of disks of radius 1 in the plane. Let \( \Lambda \) be the set of centers of the disks. Assume that the origin \( 0 \in \Lambda \) is one of the centers. The truncated
Voronoi cell at 0 is the set of all $x \in \mathbb{R}^2$ such that $|x| \leq t$, and $x$ is closer to the origin than to any other center in $\Lambda$. We assume $t \in (1, \sqrt{2})$.

Only the centers of distance at most $2t$ affect the shape and area of the truncated Voronoi cell. For each $n = 0, 1, 2, \ldots$, we have a topological space of all truncated Voronoi cells with $n$ nonzero disk centers $v_i$ at distance at most $2t$. Fix $n$, and let $X$ be the topological space.

Let $D = D_i$, $i = 1, \ldots, n$, be the sectors lying between consecutive segments $(0, v_i)$. Each sector is characterized by its angle $\alpha$ and the lengths $y_a$ and $y_b$ of the two segments $(0, v_i), (0, v_j)$ between which the sector lies. The part $A$ in $D$ of the area of the truncated Voronoi cell is a function of the variables $\alpha, y_a, y_b$. A nonlinear implicit equation $\phi = 0$ relates $A, \alpha, y_a, y_b$ on $D$. The variables $u_i$ of the linear assembly problem for the local domain $D$ are $A, y_a, y_b, \alpha$.

We have a linear assembly problem. The function $c \cdot x$ is the area of the truncated Voronoi cell, viewed as a sum of variables $A$, for each sector $D$ (or rather, their pullbacks to $X$ under the natural projections $X \to D$).

The assembly constraints are all linear. One linear relation imposes that the angles of the $n$ different sectors must sum to $2\pi$. Other linear relations impose that the variable $y_a$ on $D$ equals the variable $y_b$ on $D'$ if the two variables represent the length of the same segment $(0, v_i)$ in $X$.

### 3.1 Solving linear assembly problems

In this section we describe how various linear assembly problems are solved in the proof of the Kepler conjecture in terms sufficiently general to apply to other linear assembly problems as well.

Let us introduce some general notation. Let $x_D = (x_i : \text{dom}(u_i) = D)$ be the vector of variables with local domain $D$. Write $c \cdot x$ in the form $\sum_D c_D \cdot x_D$ and the assembly conditions as

$$Ax = \sum_D A_D x_D,$$

according to the local domain of the variable.
3.1.1 Linear relaxation

The first general technique is linear relaxation. We replace the nonlinear relations \( \phi(x_D) \geq 0, \phi \in \Phi_D \) with a collection of linear inequalities that are true whenever the constraints \( \Phi_D \) are satisfied: \( A'Dx_D \leq b_D \).

A linear program is obtained by replacing the nonlinear constraints \( \Phi_D \) with the linear constraints. Its solution dominates the nonlinear optimization problem. In this way, the nonlinear maximization problem can be bounded from above.

Let us review some constructions that insure rigor in linear programming solutions. We assume general familiarity with the basic theory and terminology of linear programming. It is well-known that the primal has a feasible solution if the dual is bounded. We will formulate our linear programs in such a way that both the primal and the dual problems are feasible and bounded.

We use vector notation to formulate a primal problem as

\[
\max c \cdot x
\]

such that \( Ax \leq b \), where \( x \) is a column vector of free variables (no positivity constraints), \( A \) is a matrix, \( c \) is a row vector, and \( b \) is a column vector.

We can insure that this primal problem is bounded by bounding each of the variables \( x_i \). (This is easily achieved considering the geometric origins of our problem, which provides interpretations of variables as particular dihedral angles, edge lengths, and volumes.) We assume that these bounds form part of the constraints \( Ax \leq b \).

The linear programs we consider have the property that if the maximum is less than a constant \( K \), the solution does not interest us. (For instance, in the dodecahedral conjecture, Voronoi cell volumes are of interest only if the volume is less than the volume of the regular dodecahedron.) This observation allows us to replace the primal problem with one having an additional variable \( t \):

\[
\max c \cdot x + K t
\]

such that \( Ax + bt \leq b \), and \( 0 \leq t \leq 1 \). This modified primal is bounded for the same reasons that the original primal is. It has the feasible solution \( x = 0 \) and \( t = 1 \).

**Lemma 3.4.** If the maximum \( M \) of the original primal is greater than \( K \), then the optimal solution of the modified primal has \( t = 0 \), and hence its maximum is also \( M \).

*Proof.* Assume that \( (x_0, t_0) \) gives an optimal solution to the modified problem for some \( 1 > t_0 > 0 \), with \( c \cdot x_0 + Kt_0 > M \). Then \( (x_1, t_1) = (x_0/(1-t_0), 0) \) is also a feasible solution and it beats the optimal solution

\[
c \cdot x_1 + Kt_1 > c \cdot x_0 + Kt_0.
\]

This contradiction proves \( t_0 = 0 \). \( \square \)

The output from linear programs that are solved by numerical methods can be transformed into a rigorous bound as follows. Based on the preceding remarks, we assume that these linear programs are feasible and bounded. The dual is then also feasible and bounded. We assume that the numerical solutions are carried out with sufficient accuracy to insure bounded feasible approximations to the true optima.

To explain the rigorous verification, we separate the equality constraints from the inequality constraints, and rewrite the problem as

\[
\max c \cdot x
\]

such that \( A'x = b' \), \( Ax \leq b \), with \( x \) free. The dual problem yields a solution to

\[
\min yb' + zb,
\]
such that \( yA' + zA = c \), with \( z \geq 0 \) and \( y \) free. Let \((y_0,z_0)\) be a numerically obtained approximation to the dual solution. The vector \( z_0 \) will be approximately positive, and by replacing negative coefficients by 0, we may assume \( z_0 \geq 0 \). Let \( \delta = c - yA' - zA \) be the error row vector resulting from numerical approximations. Then for any feasible solution \( x \) of the primal, we have

\[
c \cdot x = (\delta + y_0A' + z_0A)x \leq \delta \cdot x + y_0 \cdot b' + z_0 \cdot b.
\]

Using the bounds of the variables \( x_i \), we bound \( \delta \cdot x \leq D \), and thus obtain the rigorous upper bound \( c \cdot x \leq D + y_0 \cdot b' + z_0 \cdot b \) on the primal.

### 3.1.2 Implementation details

The linear programs are solved numerically using a commercial package (CPLEX). The input and output to these numerical programs are processed by a custom Java program, which is linked to CPLEX with a Java API provided by the software manufacturer. Each bound is calculated with interval arithmetic to insure that it is reliable. (We use a simple implementation of interval arithmetic in Java based on the Java BigDecimal implementation of arbitrary precision arithmetic.)

### 3.2 Nonlinear duality

The second general technique is nonlinear duality. Suppose that we wish to show that the maximum of \( \mathfrak{B} \) is at most \( M \).

Let \( x^* = (x_D^*) \) be a guess of the solution to the problem, obtained for example, by numerical nonlinear optimization. We relax the nonlinear optimization by dropping from the matrix \( A \) and the vector \( b \) those inequalities that are not binding at \( x^* \). With this modification, we may assume that \( A x^* = b \). Let \( m \) be the size of the vector \( b \), that is, the number of binding linear conditions. Let \( d \) be the number of local domains \( D \).

We introduce a linear dual problem with real variables \( t, r_\phi : \phi \in \Phi_D \), and \( w \in \mathbb{R}^m \). The variables \( r_\phi \) and \( w \) are constrained to be non-negative.

We consider the linear problem of maximizing \( t \) such that

\[
M + d t - c \cdot x^* \geq 0
\]

and such that for each \( D \) in each \( D \) the linear inequality

\[
c_D \cdot (x_D - x_D^*) + \sum_{\phi \in \Phi_D} r_\phi \phi(x) + wA_D(x_D^* - x_D) + t < 0
\]

is satisfied.

There is no guarantee that a feasible solution exists to this system of inequalities. However, any feasible solution gives an upper bound \( M \). Indeed, let \( x = (x_D) \) be any feasible argument to the primal, and let \( t, r_\phi, w \) be a feasible solution to the dual. Taking the sum of the linear inequalities over \( D \) at \( x \), we have (recall \( \phi \geq 0 \) and \( Ax \leq b \)):

\[
M \geq M + c \cdot (x - x^*) + \sum_D \sum_{\phi_D} r_\phi \phi(x) + wA(x^* - x) + d t,
\]

\[
\geq c \cdot x + (M + d t - c \cdot x^*) + w(b - Ax),
\]

\[
\geq c \cdot x.
\]

Since the dual problem has infinitely many constraints (because of constraints for each \( x \in D \)), we solve the dual problem in two stages. First, we approximate each \( D \) by a finite set of test points, and solve the finitely constrained linear programming problem for \( t, r_\phi, \) and \( w \).

We replace \( t \) with \( t_0 = (-M + c \cdot x^*)/d \) (to make the constraint \( M \) bind). It follows from the feasibility of \( t \) that \( t \geq t_0 \), and that \( t_0, r_\phi, w \) is also feasible on the finitely constrained problem. To show that \( t_0, r_\phi, w \)
satisfies all the inequalities (under the substitution \( t \mapsto t_0 \)), we use interval arithmetic to show that each of these inequalities hold. (To make these interval arithmetic verifications as easy as possible, we have chosen the solution \( t_0, r, w \) to make the closest inequality hold by as large a margin \( t - t_0 \) as possible. This is the meaning of the maximization over \( t \) in the dual problem.) The next section will give further details about interval arithmetic verifications.

3.3 Branch and bound

The third technique is branch and bound. When no feasible solution is found in step (2), it may still be possible to partition \( X \) into finitely many sets \( X = \bigsqcup X_i \), on which feasible solutions to the dual may be found. Although this is an essential part of the solution, the rules for branching in the Kepler conjecture follow the structure of that problem, and we do not give a general branching algorithm.

4 Automated Inequality Proving

What we would like is a general, efficient algorithm for proving inequalities of several real variables. Each inequality \( f < 0 \) of a continuous function on a compact domain can be expressed as a maximization problem:

\[
\max f < 0.
\]  

Generally efficient algorithms are not possible because NP hard problems can be encoded as optimization problems of quadratic functions \[10\].

This section describes an inequality proving procedure that has worked well in practice, and which could be automated to provide a method of general interest. This section assumes some general familiarity with issues of floating-point and interval arithmetic, such as can be found in \[1\], \[3\]. Our methods are similar to those in \[12\].

To prove \( f < 0 \), it is enough to show that the maximum of \( f \) is less than 0. For this reason, we use interval arithmetic to bound the maximum of functions. Through interval arithmetic, an interval \([a, b]\) containing the range of \( f \) can be obtained. By verifying that \( b < 0 \), it follows that the range of \( f \) is negative, and hence that \( f < 0 \).

All our functions can be built from arithmetic operations. (Transcendental functions are replaced with explicit rational approximations with known error bounds.)

Often, the functions \( f \) are twice continuously differentiable. To obtain additional speed and accuracy, we use interval arithmetic to obtain rigorous bounds on the second partial derivatives of \( f \). (We obtain formulas for the second partials through symbolic and automatic differentiation of the function \( f \).) With bounds on the second partials, we obtain rigorous bounds on \( f \) through its Taylor approximation.

The accuracy of the Taylor approximation improves as the domain shrinks in size. We chop the domain into a collection of small rectangles and check on each rectangle whether the Taylor bound implies \( f < 0 \). If Taylor bound is too crude to give \( f < 0 \), we divide it into smaller rectangles and recompute the Taylor bounds. By a process of adaptive subdivision of rectangles, the inequality \( f < 0 \) is eventually established.

Derivative information can be used to speed up the algorithm. Taylor bounds can also be applied to the first partial derivatives of \( f \). If a partial derivative of a variable \( x \) is of fixed sign on a rectangle, then the function is maximized along an edge \( x = a \) of the rectangle. If this edge is shared with an adjacent rectangle, the maximization of \( f \) is pushed to an adjacent rectangle. If this edge lies on the boundary of the domain, the dimension of the optimization problem is reduced by one.

The method outline above works extremely well for simple functions in a small number of variables. The complexity grows rapidly with the number of variables. We are able to obtain satisfactory results for many inequalities that depend on a single simplex \( S \), that is, functions of six variables parameterized by the edge lengths of a simplex.
4.1 Generative Programming

Most of the computer code for the proof of the Kepler conjecture implements the Taylor approximations of the nonlinear functions. The computer code for proving \( f < 0 \) is obtained as follows.

First, an expression for \( f \) is derived. The formulas for the first and second partial derivatives of the function are obtained (say by a symbolic algebra system) from the expressions for \( f \).

These symbolic expressions are then converted to an interval arithmetic format. In a language such as C++ with operator overloading, this can be achieved by defining a class for intervals and overloading arithmetic operations so that they may be applied to instances of the class. In languages without operator overloading, the conversion from the symbolic expression to computer source code is more involved.

There are other considerations to bear in mind in producing the interval code. In practice, there is a substantial degradation of performance when the rounding mode on the computer is frequently switched, and often it is necessary to rearrange the code substantially to reduce the number of changes in rounding mode. Also, floating point arithmetic is not associative, so that in order to obtain rigorous results based on interval arithmetic, great care must be paid to the placement of parentheses. Another issue is the input of floating point constants. In C++, the line of code in (12) sets \( x = 1.0 \), no matter the rounding flags. (The constant is parsed at compile time and truncated to 16 digits, and there is no control over rounding modes until later, when the program executes.) The code must insure that no errors are introduced through compiler constant truncation.

\[
x = 1.000000000000000000001; // set x=1.0, regardless of rounding flags
\]

There are many such perils in the production of reliable interval arithmetic code. Overall, a great deal of effort must be expended to produce the computer code for rather simple inequalities. This effort must be expended every time a new function is introduced into an inequality. This simple fact has kept the inequality-proving software developed for the proof of the Kepler conjecture from having more widespread applicability to more general inequality proving.

Figure 4 shows a snippet of C++ code that computes the arctangent of a linear germ of a function.

If the Kepler conjecture is eventually to be proved by generic tools, we must find a less cumbersome way to produce the computer code. Indeed, a fundamental principle of software design is that there should be no manual procedures (Pragmatic Programmer, Tip 61) [11]. Generative programming gives methods to automate the production of computer code [4]. There is nothing about the interval arithmetic computer code for a new function that requires human thought or effort in an essential way. For example, an examination of the code for the arctangent in Figure 4 reveals that it is a shallow reformatting of the formula for the derivative of the arctangent, combined with the quotient rule in calculus. Why should the code be produced by hand, if it the process is entirely mechanical?

A generative program could be written that takes as its input a function and produces as output the interval arithmetic computer code for the Taylor series bounds of that function. The program would parse the definition of the function, generate symbolic derivatives of the function, convert the derivative information to computer code for calculating the derivatives, and so forth.

What advantages would this bring? First of all, it would no longer be necessary to read 40K lines of check to check the correctness of the proof of the Kepler conjecture. It would be enough to check the code on the much smaller generator. Also, the same generator could be used to prove many other inequalities.

4.1.1 Implementation details

The generative program has not been written. Some feasibility tests have been made with javaCC for parsing and XSLT for abstract syntax tree transformations.
Figure 4: Code to calculate an interval version of the arctangent function

```cpp
/**
 * A lineInterval is an interval version of a linear approximation to a
 * function in 6 variables.
 * The linear approximation is +f + Df[0] x0 + Df[1] x1 + Df[2] x2 +...+ Df[5] x5.
 */
class lineInterval {
    public:
        interval f,Df[6];
        // rest of class omitted
};

/**
 * Sample implementation of the arctangent function.
 * This computes the linear approximation only. The second derivatives
 * are much more involved.
 */
static lineInterval atan(lineInterval a,lineInterval b) // atan(a/b);
{
    static const interval one("1");
    lineInterval temp;
    temp.f = interMath::atan(a.f/b.f); // computes interval-valued arctangent
    interval rden = one/(a.f*a.f+b.f*b.f);
    for (int i=0;i<6;i++) temp.Df[i]= rden*(a.Df[i]*b.f-b.Df[i]*a.f);
    return temp;
}
```

5 Plane Graph Generation

A sphere graph is a graph together with an embedding of it into the unit sphere. We discuss a simple
sphere graph generating algorithm in this section.

Figure 5 shows a sequence of sphere graphs, giving a sequence of faces that are added to a square to
produce the graph dual to the edge graph of the rhombic dodecahedron. We can represent the sequence
abstractly as a directed graph with vertices $v_1, \ldots, v_{11}$ with edges from $v_i$ to $v_{i+1}$. Figure 6 shows that the
sequence of faces can be generated in different orders, and that all different sequences can be represented
as a directed graph whose root is the square $v_1$. Call this the derivation graph. The terminal vertices of
the directed graph represent sphere graphs isomorphic to $v_{11}$.

In going from a parent to a child, we always add one face. Each sphere graph in the derivation
graph has two types of faces – those such as the pentagon in $v_2$ that does not survive unmodified in the
terminal nodes, and those such as the triangle in $v_2$ that do. Call these two types of faces **modifiable** and
**unmodifiable** respectively.

Let us generalize this construction to generate all the sphere graphs that are needed for the proof of
the Kepler conjecture. Fix a natural number $N$.

Consider the set $V_0$ of nonempty sphere graphs with at most $N$ vertices, and no loops or multiple
joins. All faces of the sphere graph are assumed to be polygons, and all polygons are assumed to be
simple. We give each face one of the two attributes **modifiable** or **unmodifiable** and call a graph with these
attributes a **decorated** graph. Let $V$ be the set of all decorated graphs of $V_0$.

Let $P$ be a polygon. We say that a simple polygon $Q$ is an **admissible refinement** of $P$ if every vertex
of $Q$ is either a vertex of $P$ or an interior point of $P$ and if $Q$ shares at least one edge with $P$. An
Some Algorithms in the Kepler Conjecture

Figure 5: The first few stages and the final few stages of drawing the graph dual to the rhombic dodecahedron

Figure 6: The same graphs can be generated by different sequences of adding faces

Let $v$ be a decorated sphere graph in $V$. We say that $v'$ is an admissible refinement of $v$ if there is a modifiable face $P$ of $v'$ and an admissible refinement $Q$ of $P$ such that the graph obtained by adding $Q$ is $v'$ that is compatibly decorated. We say that $v'$ is compatibly decorated if the unmodifiable faces of $v'$ are $Q$ together with the unmodifiable faces of $v$. A special case occurs, when $P = Q$, and in this case, we simply change the attribute of $P$ to unmodifiable.

The set $V$ becomes a directed graph $\Gamma$ with an edge from each $v$ to all of the admissible refinements of $v$. The root of the directed graph is an empty node. The children of the root are graphs consisting of a single polygon dividing the sphere into an interior and exterior, one side modifiable and the other not. The terminal vertices in this directed graph are decorated graphs, with no modifiable faces. Thus, terminal vertices are in natural bijection with $V_0$.

If we take any graph in $V_0$, it can be reached from the root as follows. Pick a face of $V_0$ and draw its edges as the initial polygon. Make the interior of the polygon modifiable. Then continue to pick faces that have at least one edge already drawn, and draw all remaining edges of that face, marking the completed face as unmodifiable. This corresponds to following a edge in the directed graph $\Gamma$. 

admissible refinement of $P$ partitions the region $P$ into the region $Q$ and finitely many other polygons.
This gives us an algorithm to generate all sphere graphs in $V_0$: begin with the children of the root vertex (polygons with at most $N$ vertices) and generate all admissible refinements (that is, follow all possible directed edges) until terminal vertices are reached.

We can improve on this algorithm by fixing for each $v \in \Gamma$ a modifiable face $P$ and an edge on that face, and then taking only admissible refinements $Q$ of $P$ that share the given edge. Each sphere graph in $V_0$ is still generated under this restriction. We can also assume without loss of generality that the initial polygon is chosen to be one with the most edges.

There is an enormous combinatorial explosion as all admissible refinements are generated. As fortune has it, we are not interested in all sphere graphs $V_0$, but rather only those that arise as a potential counterexample to the Kepler conjecture. Let $V_1 \subset V_0$ denote this smaller set of relevant graphs. This allows us to combine the general graph-generating algorithm with pruning operations that keep the combinatorics from getting out of hand.

What is needed are criteria on $v \in \Gamma$ that allows us to conclude that $v$ has no no admissibly refined descendents in $V_1$, that is, to conclude there is no directed path from $v$ to $v_1 \in V_1$. The proof of the Kepler conjecture gives a long list of properties of graphs in $V_1$ and this avoids the combinatorial explosion. The implementation of the graph generator includes many other minor tricks to keep the execution time manageable. Pruning and the other tricks are rather mundane, and we refer the reader to the source code for details.

6 Conclusion

We will not try to list all of the places where the algorithms of this article would bring a simplification of the 1998 proof of the Kepler conjecture. The list would be extensive. To give a rough indication, we list a few places these algorithms are relevant to the two shortest articles of the proof [6] and [9].

In the article [6] alone, low-dimensional quantifier elimination problems are the subject of Lemma 1.2, Lemma 1.3, Lemma 1.4, Lemma 1.5, Lemma 1.6, Lemma 1.7, Lemma 1.8, Lemma 1.9, Lemma 1.11, Lemma 2.1, and Lemma 2.2. In [9], an additional low-dimensional quantifier elimination problem appears in Lemma 2.2. In general, the parts of the 1998 proof that rely on what that proof calls geometric considerations are amenable to preprocessed quantifier elimination.

Linear assembly algorithms generalize the algorithm presented in [9], Appendix 2. Some examples where linear assembly would simplify the 1998 proof are [6] Section 4, and [9] Proposition 4.1, Proposition 4.2, Proposition 5.2, Proposition 5.3, Appendix 1 (A.5 and A.7).

Interval arithmetic inequalities are used throughout the 1998 proof, in sections such as [6] Appendix 3.13.1–4.7.5 and [9] Section 10, Appendix 1. In the early articles in the series, interval arithmetic Taylor approximations are not used [9]. As a result, these early papers only prove very limited types of inequalities. The entire strategy of the proof of the Kepler conjecture in [9] is shaped by these algorithmic limitations. This profoundly affects the structure of the optimization problem in [9], because a scoring function within the reach of the early primitive algorithms was chosen, although such a function was highly suboptimal. With improved automated inequality proving algorithms, it should be possible to make a fresh start and devise a much more efficient scoring function.

Graph generation is carried out in [9] Section 8.

We have not yet reached the fundamental objective of avoiding all manual procedures; some parts of the proof remain hand-made (even after taking account of the algorithms of this article). A fully automated proof would have to develop additional algorithms to prove these estimates. Nevertheless, this article brings us one step closer to that objective.

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Acknowledgments

The interval-arithmetic algorithms were developed in collaboration with S. Ferguson.