Rational Orthogonal Approximations to Orthogonal Matrices

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Abstract

Several algorithms are presented for approximating an orthogonal rotation matrix M in three dimensions by an orthogonal matrix with rational entries. The first algorithm generates an approximation $M_2(M,\epsilon)$ with accuracy ϵ and $2b+4$-bit numerators and a common $2b+4$-bit denominator (bit-size $2b+4$), where $b = \lceil -\lg\epsilon \rceil$ ($\epsilon \approx 2^{-b}$). The second algorithm uses basis reduction to generate an approximation $M_\nu(M,\epsilon)$ with accuracy $\epsilon^{\nu/1.5}$ and bit-size νb for some $1.5 \leq \nu \leq 6$ (but ν cannot be controlled except by trial and error). A third algorithm, based on integer programming, generates optimal $M_{\mathrm{opt}}(M,\epsilon)$ with accuracy ϵ and bit-size proven to be no more than $1.5b$. In practice, the second algorithm generates an approximation with $\nu \approx 1.5$ and is much faster than the third algorithm. The best bit-sizes which one could obtain using previously known results in two dimensions [1] are more than $3b$ bits for numerator and denominator. Applications are described for the approximation functions in the area of solid modeling.

1 Introduction

Certain numerical issues must be resolved in order to implement an algorithm of computational geometry as a computer program. The implementation can use exact or rounded arithmetic. If rounded arithmetic is used, it is necessary to deal with topological inconsistencies and numerical error. Exact arithmetic does not present these problems, but it has, in general, much higher cost than rounded arithmetic.

Let us suppose we choose to use exact arithmetic. It is desirable that all operations be within the field of rational numbers. This is difficult to accomplish for constructions or computations involving rotations, such as solids modeling or robotic path planning. Orthogonal rotation matrices[1], often defined in terms of Euler angles ψ, ϕ, θ,

$$M(\psi,\phi,\theta) = \begin{bmatrix} \cos\psi\cos\phi - \sin\psi\cos\theta\sin\phi & -\cos\psi\sin\phi - \sin\psi\cos\theta\cos\phi & \sin\psi\sin\theta \\ \sin\psi\cos\phi + \cos\psi\cos\theta\sin\phi & -\sin\psi\sin\phi + \cos\psi\cos\theta\cos\phi & -\cos\psi\sin\theta \\ \sin\theta\sin\phi & \sin\theta\cos\phi & \cos\theta \end{bmatrix}, \quad (1)$$

have entries which are irrational and non-algebraic except for very special choices of input angles. What is desired is the following: a function $M_{\mathrm{approx}}(M,\epsilon)$ which takes an arbitrary orthogonal matrix M and accuracy $\epsilon > 0$ as input and returns an orthogonal matrix that has rational entries and which approximates M to within ϵ:

$$\max_{|v|=1} |(M - M_{\mathrm{approx}})v| \leq \epsilon. \quad (2)$$

At the ACM geometry conference last year, Canny, Donald, and Ressler [1] presented a technique for generating rational two dimensional rotation matrices. For any two dimensional rotation matrix M, their technique can

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[1] Matrix M is orthogonal if $M^t = M^{-1}$. These are sometimes called *orthonormal.*

generate a rational matrix with accuracy 2^{-b} and rational entries with b-bit numerators and a common b-bit denominator (bit-size b). This is the worst-case behavior of their technique. Given a desired rotation angle θ, they use the standard rational parameterization of the unit circle, $\sin\theta = \frac{2t}{1+t^2}$ and $\cos\theta = \frac{1-t^2}{1+t^2}$, where $t = \tan(\theta/2)$. They then apply a variation of known techniques for finding the solution to the *best approximation problem*[2] (see [10][8]) to find the best rational approximation for t with accuracy ϵ. This leads to the best rational approximation to M. Since their technique generates angles with rational sines and cosines, it can be used to create rational three-dimensional orthogonal matrices through the use of Equation 1 above. However, this results in an increase in bit-size to roughly $3b$ numerator and denominator, which is far from the best possible.

In this paper, we present a technique based on quaternion arithmetic for directly generating three dimensional rational orthogonal matrices. This technique reduces the matrix approximation problem to that of finding simultaneous rational approximations, p_1/p_0, p_2/p_0, p_3/p_0 to real numbers $\alpha_1, \alpha_2, \alpha_3$. We prove that the best simultaneous approximation leads to the best rational matrix approximation. A naive approximation, setting $p_0 = 2^b$ and finding the best p_1, p_2, p_3, yields $M_2(M, \epsilon)$ with bit-size $2b + 2$ and accuracy $\epsilon = 2^{-b}$.

Using the *basis reduction* algorithm of Lenstra, Lenstra, and Lovasz [10] [9], we describe a method of approximating α_i by p_i/p_0, $i = 1, 2, 3$ with a "smaller sized" p_0 for a given accuracy. However, it does not give as good a control on the accuracy attained. For any given $\eta > 0$, it finds an integer $p_0 \leq 8\eta^{-3}$ such that there is an approximation to M with accuracy η/p_0 and bit-size $2\lceil \lg p_0 \rceil$. If we set $\eta = \epsilon^{1/4}$ and if p_0 is near its upper bound, then the accuracy will be ϵ and the bit-size close to $1.5b$ for $b = -\lg\epsilon$. If p_0 is small, we do not attain the desired accuracy. In the worst case, we have to set $\eta = \epsilon$ and then we obtain accuracy ϵ^4 (much closer than we wanted) and bit-size $6b$. Thus the approximation is $M_\nu(M, \epsilon)$ with accuracy $\epsilon^{\nu/1.5}$ and bit-size νb for some $1.5 \leq \nu \leq 6$. This method generates good approximations in practice, because it takes only a few tries to find p_0 near its upper bound. This technique yields accuracies of $\epsilon = 10^{-6}$ in a few seconds on a 30 MIPS workstation. The basis reduction algorithm runs in strongly polynomial time.

Finally, we prove that the optimal approximation $M_{\text{opt}}(M, \epsilon)$ has bit-size at most $1.5b$, and we show how to apply integer programming to find an approximation $M_{\text{opt}}(M, \epsilon)$ within one bit of optimal. This can be solved in polynomial time using an algorithm of Lovasz and Scarf [11] which has been implemented by Cook, *et al* [3]. We plan to run tests of the running time, but it is probably most practical to use the older basis reduction method.

1.1 Applications

Currently, there is no reasonable way to implement a computer system that can model polyhedral objects. Such a system would have half-spaces (such as $\{(x, y, z) \mid x \geq 0\}$) as primitives and would allow at least the following operations:

- regularized set operations: union, intersection, complement, difference;
- Euclidean transformations: translation, rotation, scaling;
- convex hull.

There are no known robust algorithms for implementing such a system in rounded floating point arithmetic. Actually, one can describe combinatorially consistent algorithms for these operations, but there are imaginable cases for these algorithms which have unbounded numerical error.

If one implements such a system using exact rational arithmetic in a standard fashion, then there are sequences of operations which have exponential growth in bit-complexity. For instance, intersecting three polyhedra might generate a vertex which is the intersection of three faces. Taking the convex hull will generate a face containing three vertices. Generating a point from three planes and generating a plane from three points in each case trebles the number of bits in the representation. This example is clearly not a proof, but we expect that for any exact algorithm, the bit-complexity will grow exponentially in the worst case.

[2] Given a number $\alpha \in \mathbf{Q}$ and an $\epsilon \in \mathbf{Q}$, $\epsilon > 0$, find a rational number p/q such that $q > 0$, $|\alpha - p/q| < \epsilon$ and q is as small as possible.

We see the design of a practical solid modeler as consisting of three parts: fast integer arithmetic for geometric constructions, rational Euclidean transformations, and geometric rounding.

It is commonly understood that geometric constructions depend on the *signs* of arithmetic expression on the input coordinates, not the actual values. This fact is what makes the use of rounded arithmetic so perilous: the sign function has infinite relative error for inputs near zero. On the other hand, there are ways to compute the sign of integer expressions which are practically and/or theoretically more efficient than determining the actual value. Karasick, Lieber and Nackman [7], Clarkson [2], and Fortune and Van Wyk [5] have given results in this area, of which the latter is perhaps the most practical.

This paper describes how to obtain rational orthogonal matrices in three dimensions. From these, arbitrary rational Euclidean transformations can be constructed.

Even if multiple-precision operations can be made relatively cheap, some means must be developed for overcoming the exponential growth in the bit-complexity of the polyhedra. The first author and Nackman [12] have shown that finding the minimum-perturbation rounding of the coordinates to lower precision, without changing the combinatorial structure, is an NP-complete problem. However, this author has proposed techniques [13] [14] that round to lower precision and change the combinatorial structure in a reasonable way. The first author and Nackman are also working on heuristics for rounding without changing the combinatorial structure.

It is hoped that by combining different techniques, one could offer a solution to the solid modeling problem, which the field of computational geometry has so far failed to provide.

2 Algorithms for Constructing Rational Orthogonal Approximations

Our goal is to construct a rational rotation matrix M_{approx} which approximates an arbitrary rotation matrix M. This section shows how to reduce this problem to that of finding a good simultaneous rational approximation $p_1/p_0, p_2/p_0, p_3/p_0$ to three real values $\alpha_1, \alpha_2, \alpha_3$. It is also shown that the best approximation to the α's yields the best approximation matrix M_{approx}.

2.1 Quaternion Arithmetic

For purposes of this abstract we summarize the quaternion representation of orthogonal matrices by saying that an arbitrary quaternion takes the form, $Q = Q_0 + Q_1 i + Q_2 j + Q_3 k$ where i, j, k are square roots of -1. A theorem by Rodriguez [4] shows that the following matrix is a rotation matrix:

$$M(Q) = (Q_0^2 + Q_1^2 + Q_2^2 + Q_3^2)^{-1} \begin{bmatrix} Q_0^2 + Q_1^2 - Q_2^2 - Q_3^2 & 2(Q_1Q_2 - Q_0Q_3) & 2(Q_1Q_3 + Q_0Q_2) \\ 2(Q_2Q_1 + Q_0Q_3) & Q_0^2 - Q_1^2 + Q_2^2 - Q_3^2 & 2(Q_2Q_3 - Q_0Q_1) \\ 2(Q_3Q_1 - Q_0Q_2) & 2(Q_3Q_2 + Q_0Q_1) & Q_0^2 - Q_1^2 - Q_2^2 + Q_3^2 \end{bmatrix}. \quad (3)$$

Given angle θ and unit vector $u \in \mathbf{R}^3$, we define a unit quaternion

$$q(\theta, u) = \cos\frac{\theta}{2} + \sin\frac{\theta}{2}\hat{u} = \cos\frac{\theta}{2} + \sin\frac{\theta}{2}u_x i + \sin\frac{\theta}{2}u_y j + \sin\frac{\theta}{2}u_z k. \quad (4)$$

$M(q(\theta, u))$ is the rotation with angle θ and axis u.

We note that if the components of Q are b'-bit integers, then the entries of the matrix will have $b = 2b' + 2$ bits in the numerator and a common b-bit denominator.

2.2 Constructing $Q(M)$

The first task in the approximation of an orthogonal transformation M is the construction of a quaternion $Q(M)$ which generates M. If the axis u and the rotation angle θ are known, then Equation 4 yields $q(M)$

directly. If M is given as a matrix $(r_{ij})_{1\le i,j\le 3}$, then the following can be shown from Equation 3 (see [16]):

$$\begin{bmatrix} 1+r_{11}+r_{22}+r_{33} & r_{32}-r_{23} & r_{13}-r_{31} & r_{21}-r_{12} \\ r_{32}-r_{23} & 1+r_{11}-r_{22}-r_{33} & r_{12}+r_{21} & r_{13}+r_{31} \\ r_{13}-r_{31} & r_{12}+r_{21} & 1-r_{11}+r_{22}-r_{33} & r_{23}+r_{32} \\ r_{21}-r_{12} & r_{13}+r_{31} & r_{23}+r_{32} & 1-r_{11}-r_{22}+r_{33} \end{bmatrix} =$$

$$4\begin{bmatrix} q_0^2 & q_0q_1 & q_0q_2 & q_0q_3 \\ q_1q_0 & q_1^2 & q_1q_2 & q_1q_3 \\ q_2q_0 & q_2q_1 & q_2^2 & q_2q_3 \\ q_3q_0 & q_3q_1 & q_3q_2 & q_3^2 \end{bmatrix} = 4\begin{bmatrix} q_0 \\ q_2 \\ q_2 \\ q_3 \end{bmatrix}\begin{bmatrix} q_0 & q_2 & q_2 & q_3 \end{bmatrix}, \tag{5}$$

where $q = q_0 + q_1 i + q_2 j + q_3 k$ is a unit quaternion that generates M. As one can see, every row is proportional to the components q. In case we are using floating point arithmetic, it is important to select the row which contains the maximum diagonal element $4q_i^2$. We call the row selected in this fashion $Q(M)$. By this selection, one avoids using a degenerate (all-zero) row. This computation is numerically accurate in floating point since $Q(M) = 4q_i q$, where $|4q_i| \ge 2$. The absolute error of 3μ per component, where μ is the rounding unit, is converted into an absolute error, $3\mu/(4q_i)$, after normalization. This error is bounded by 1.5μ.

Implementation note: If we define $r_{00} = r_{11}+r_{22}+r_{33}$, then each diagonal element can be written $1+2r_{ii}-r_{00}$, $i = 0,1,2,3$. Hence, determining the maximum diagonal element is equivalent to finding $\max\{r_{00}, r_{11}, r_{22}, r_{33}\}$.

2.3 Generating an Approximation

Define $Q_u(M) = Q(M)/Q_i(M)$, where $Q_i(M)$ is the largest magnitude component of $Q(M)$. Suppose, without loss of generality, that $i = 0$, and thus the components of $Q_u(M)$ are $(1, \alpha_1, \alpha_2, \alpha_3)$. We need to find integers p_1, p_2, p_3, p_0 such that,

$$|\alpha_i - \frac{p_i}{p_0}| \le \frac{\epsilon}{2\sqrt{3}} \qquad i = 1,2,3. \tag{6}$$

It can be shown that setting $Q_{\text{approx}} = p_0 + p_1 i + p_2 j + p_3 k$ and then generating the corresponding matrix M_{approx} yields an ϵ approximation to M that satisfies Equation 2. Accuracy ϵ for M_{approx} is equivalent to accuracy ϵ for $Q_{\text{approx}}/|Q_{\text{approx}}|$ and is equivalent to accuracy $\epsilon/2\sqrt{3}$ for the approximation to $\alpha_1, \alpha_2, \alpha_3$.

2.4 Finding the Best Approximation

The following two lemmas show that the best (smallest bit-size) rational approximations p_1/p_0, p_2/p_0, p_3/p_0 to real numbers $\alpha_1, \alpha_2, \alpha_3$ with accuracy $\epsilon/2\sqrt{3}$ have bit-size at most $0.75b$ ($b = -\lg\epsilon$ as usual), and this leads to a $1.5b$-bit approximation to a matrix M. Furthermore, the best rational matrix approximation can be found by determining the best rational approximation $\alpha_1, \alpha_2, \alpha_3$ with accuracy $\epsilon/2\sqrt{3}$. Therefore, the optimal approximation $M_{\text{opt}}(M,\epsilon)$ to M with with accuracy ϵ has bit-size at most $1.5b$.

Lemma 2.1 *Given $0 \le \alpha_1, \alpha_2, \alpha_3 \le 1$ and $\epsilon/2\sqrt{3} \approx 2^{-b}$, there exists $0.75b$-bit integers p_1, p_2, p_3, p_0 such that $|\alpha_i - p_i/p_0| \le \epsilon/2\sqrt{3}$, $i = 1,2,3$.*

Proof. Ignoring the factor of $2\sqrt{3}$ for simplicity (it changes things by at most two bits), for $-2^{0.75b} \le p_1, p_2, p_3, p_0 \le 2^{0.75b}$, there are roughly 2^{3b} lattice points of the form $(p_1 - p_0\alpha_1, p_2 - p_0\alpha_2, p_3 - p_0\alpha_3)$ inside a cube of size $2^{0.75b}$. Therefore two lattice points must lie distance $2^{-0.25b}$ apart (under L_∞ norm). Their difference is also a lattice point. Dividing through by p_0 yields a point of the form $(p_1/p_0 - \alpha_1, p_2/p_0 - \alpha_2, p_3/p_0 - \alpha_3)$ at distance 2^{-b} from the origin. Thus the resulting p_1, p_2, p_3, p_0 satisfy the theorem. □

These $0.75b$-bit p's yield a $1.5b$-bit approximation matrix. We can turn this around to show that a good approximation matrix implies a small bit-size integer $Q(M)$.

Lemma 2.2 *A rational $2b$-bit sized rotation matrix M_{approx} corresponds to a b-bit or smaller sized integer quaternion Q_{approx}.*

Proof. Given a rational matrix, we can clear fractions and solve for $2q_0, 2q_1, 2q_2, 2q_3$, using Equation 5 above (the 1's on the left are replaced by the common denominator in the matrix). Each $2q_i$ is the square root of an integer: $2q_i = Q_i\sqrt{m_i}$, where m_i is square-free for $i = 0, 1, 2, 3$. However, the fact that $4q_iq_j$ is integral for each pair implies that $m_1 = m_2 = m_3 = m_4$. Therefore, the quaternion $Q_0 + Q_1 i + Q_2 j + Q_3 k$ generates the rational matrix by Equation 3, and the Q's have at most half the bit-size of the entries of M. □

Comment: What if the rational matrix does not have a b-bit *common* denominator, as this proof requires? The answer is that rotating an integer vector by the matrix (which is the eventual application) requires that the entries be adjusted to have a common denominator anyway so that the fractions can be summed. In other words, it is only fair to compute the bit-size of a rotation matrix if its entries have a common denominator.

3 Generating Simultaneous Rational Approximations

We have reduced the problem of finding an approximating rational rotation matrix to that of finding rational approximations with a common denominator to three real values $\alpha_1, \alpha_2, \alpha_3$. As pointed out in Section 3, it is easy to generate an ϵ-accurate ($\epsilon \approx 2^{-b}$) set of rationals by setting the denominator $p_0 = 2^b$ and choosing the best numerators p_1, p_2, p_3. The resulting approximation matrix $M_2(M, \epsilon)$ has bit-size $2b + 2$. This section explores algorithms for finding smaller bit-size approximations. The first algorithm using basis reduction yields a $1.5b$-bit matrix in practice, but is not guaranteed to find the best approximation. A second method, based on integer programming, can find a near optimal approximation. Both algorithms run in polynomial time, but the first is probably the most practical.

3.1 Approximation by Basis Reduction

Basis reduction is a process that finds a "short" set of basis vectors for a lattice. To find an approximation to $\alpha_1, \alpha_2, \alpha_3$, one reduces the basis,

$$(1,0,0,0),\ (0,1,0,0),\ (0,0,1,0),\ (\alpha_1, \alpha_2, \alpha_3, -x),$$

where x is a parameter chosen to control the accuracy and bit-size of the approximation. Each reduced basis vector is some integer combination, $(p_1 - p_0\alpha_1, p_2 - p_0\alpha_2, p_3 - p_0\alpha_3, p_0 x)$ of the four original vectors. Assuming one can find a reduced basis vector such that the first three components are roughly equal to or smaller than the fourth component in magnitude, then $|p_i/p_0 - \alpha_i| \leq x$. One can set x equal to the desired accuracy $\epsilon/2\sqrt{3}$. Incidentally, it is required that $\alpha_1, \alpha_2, \alpha_3$ be rational, so that one must replace them with rational approximations $\alpha_1^{\text{rat}}, \alpha_2^{\text{rat}}, \alpha_3^{\text{rat}}$. It is easy to generate these rational approximations using continued fractions since they do not have to have a common denominator. If $|\alpha_i^{\text{rat}} - \alpha_i| \leq \epsilon/4\sqrt{3}$ for $i = 1, 2, 3$, we must set $x = \epsilon/4\sqrt{3}$ to obtain the desired accuracy.

The Lenstra, Lestra, Lovasz [9] algorithm for basis reduction is a part of MAPLE and other mathematical packages. It is not known how to determine the value of x that leads to the smallest p_0. However, in practice after a few tries with slightly different x, one can generate a good approximation.

As far as guaranteed behavior, Lovasz [10] indicates that basis reduction leads to a polynomial-time algorithm that takes $\eta > 0$ and a rational vector $(\alpha_1, \alpha_2, \ldots \alpha_n)$ as input and returns integers $p_1, p_2, \ldots, p_n, p_0$ such that $|\alpha_j - \frac{p_j}{p_0}| \leq \frac{\eta}{p_0}$ for $j = 1, 2, \ldots, n$, and $0 < p_0 \leq 2^{n(n+1)/4}\eta^{-n}$.

For $n = 3$, $0 < p_0 \leq 8\eta^{-3}$, and for some $\eta \in \left[\frac{\epsilon}{4\sqrt{3}}, \left(\frac{4}{3}\right)^{\frac{1}{8}} \epsilon^{\frac{1}{4}}\right]$, Lovasz's algorithm will return a value of p_0 such that $\frac{\eta}{p_0} \leq \frac{\epsilon}{4\sqrt{3}}$. Setting $\eta = \epsilon/4\sqrt{3}$ will always work, but may result in $3b$-bit p_0. It is best if η is as large as possible so that p_0 is as small as possible. In practice, one finds solutions for $\eta \approx \epsilon^{\frac{1}{4}}$ and thus p_0 has bit-size about $0.75b$.

3.2 Finding an Optimal Approximation

For any given accuracy ϵ, a near optimal[3] set of p_1, p_2, p_3, p_0 can be found in polynomial time using integer programming. Let ϵ' be a close rational approximation to $\epsilon/4\sqrt{3}$. It is sufficient to solve,

$$-\epsilon' p_0 \leq p_i - \alpha_i^{\mathrm{rat}} p_0 \leq \epsilon' p_0, \qquad i = 1, 2, 3,$$

for integers p_1, p_2, p_3 and minimum integer p_0. Recent results by Cook *et al* [3] show that integer programs of this type can be solved for up to 100 variables using a polynomial-time algorithm of Lovasz and Scarf [11], and we plan to test the practicality of finding optimal approximations with this system.

4 Conclusion

If one is willing to use a few seconds of running time on a typical modern workstation, then the basis reduction scheme is a practical method for finding close $1.5b$-bit rational approximations to 3D rotation matrices. If not, a larger $2b$-bit approximation can be found using a few dozen floating point operations.

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[3] *Near* optimal because the use of rational approximations might lead to a solution that is one bit larger than actual optimum.