# A High-Performance Singularity-Free Rotation Estimator in Geometric Algebra

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**Abstract.** Well known methods for solving the Wahba's problem are formulated in the linear algebra framework, mainly using the SVD or polar decomposition, or in quaternion's framework which leads to solve a max-eigenvalue problem. Those methods are based on well stablished numerical algorithms which on the other hand are iterative and computationally expensive. Recently, closed form solutions has been proposed based on an analytic formula for solving the roots of the quartic polynomial associated with the eigenvalue problem. Closed form methods are fast but they have singularities i.e., they completely fail on certain input data. In this paper we propose a high-performance, singularity-free estimator of the best quaternion aligning two sets of corresponding vectors i.e., equivalent to Wahba's problem. It is based on a new formulation of the problem in the Geometric Algebra representation of rotations which is isomorphic to Hamilton's quaternions. The proposed method converges in a fixed number of iterations, its performance is competitive with closed form solutions reported in literature and at the same time is free of singularities, robust to noise and simple to implement.

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#### 1. Introduction

Wahba's problem has been studied for over half a century since 1965 [15]. The problem looks for the optimal rotation between two sets of corresponding vectors. Many effective methods have been developed to solving the problem [1,6,9,12,20] mainly by formulating it in the quaternions framework, which lead us to solve an eigenvalue problem, or by formulating it in the linear algebra framework and using the Singular Value Decomposition (SVD) and recently by formulating it in the Geometric Algebra framework [3,11] which at some point casts the solution into linear algebra framework and SVD due to

the lack of geometric algebra numerical algorithms. More recently, closed form solutions for computing the optimal quaternion has been proposed [17–19,21] based on solving the roots of the quartic polynomial associated with the eigenvalue problem with an analytic formula.

Accuracy and speed of most methods have been compared in previous works [4, 8, 19] where the trade-off between performance and robustness is assessed. In particular SVD based methods exhibit very good accuracy but low performance and quaternion based methods are in the other end depending on the implementation. Regarding the later methods, the proposed closed form solutions exhibit the best trade-off so far but they have singularities i.e., they completely fail on certain input data.

In this paper we propose a high-performance, singularity-free estimator of the best quaternion aligning two sets of corresponding vectors i.e., equivalent to Wahba's problem. It is based on a new formulation of the problem in the Geometric Algebra representation of rotations which is isomorphic to Hamilton's quaternions. The proposed method converge in a fixed number of iterations being is as fast as the closed form solutions reported in literature and at the same time is free of singularities, robust to noise and simple to implement.

In this work we propose a high-performance, singuarity-free method for solving the Wahba's problem. It is based on a maximizing a convex quadratic energy functional, which is equivalent to Wahba's problem, formulated in geometric algebra framework  $\mathbb{G}_3$ . The proposed method converges in a fixed number of iterations being is as fast as the closed form solutions reported in literature and at the same time is free of singularities and simple to implement.

Applications of Wahba's solutions are diverse from aerospace engineering computation of spacecraft attitude [19] to mesh deformation in computer graphics [13, 14] for accurate motion construction and restoration [10, 11]. An important characteristic of our method is that it is based almost entirely on symmetric-matrix multiplication so it can be hardware-accelerated using vector instructions or graphics hardware without effort. In engineering fields requiring high-performance vector alignment our method can lower down the time by taking advantage of the AVX (Advanced Vector Extensions) support available in modern microprocessors. Modern matrix packages such as Eigen [5] can produce apropriate AVX instructions automatically. In computer graphics applications our method can lower down the time even more by taking advantage of GPU vector instructions obtaining a performance boost not present in other numerical algorithms.

Few work has been done on studying this problem using geometric algebra. Geometric algebra rotors are closely related to quaternions (quaternion algebra can be regarded as a geometric algebra defined on a set of imaginary basis vectors) we find geometric algebra to be a more natural choice for studying this problem since it is defined over a Euclidean vector space  $\mathbb{R}^3$ , where original data is defined. In contrast to previous works we base our

formulation on bivectos instead of vectors for the sake of mathematical convenience. Due to mathematical duality of vector and bivectors in  $\mathbb{G}_3$  our formulation is also valid for vectors. The implementation of our algorithm does not require any geometric algebra library, we present an implementation based on standard matrix and quaternion library.

This paper is arranged as follows: Section II introduces the geometric algebra  $\mathbb{G}_3$ , Section III includes the presentation of our fast rotor estimation algorithm. Section IV demonstrates the experimental results.

# 2. Geometric Algebra $\mathbb{G}_3$

A geometric algebra  $\mathbb{G}_3$  is constructed over a real vector space  $\mathbb{R}^3$ , with basis vectors  $\{e_1, e_2, e_3\}$ . The associative geometric product is defined so that the square of any vector is a scalar  $aa = a^2 \in \mathbb{R}$ . From the vector space  $\mathbb{R}^3$ , the geometric product generates the geometric algebra  $\mathbb{G}_3$  with elements  $\{X, R, A...\}$  called multivectors.

For a pair of vectors, a symmetric inner product  $a \cdot b = b \cdot a$  and antisymmetric outer product  $a \wedge b = -b \wedge a$  can be defined implicitly by the geometric product  $ab = a \cdot b + a \wedge b$  and  $ba = b \cdot a + b \wedge a$ . It is easy to prove that  $a \cdot b = \frac{1}{2}(ab + ba)$  is scalar, while the quantity  $a \wedge b = \frac{1}{2}(ab - ba)$ , called a bivector or 2-vector, is a new algebraic entity that can be visualized as the two-dimensional analogue of a direction, that is, a planar direction. Similar to vectors, bivectors can be decomposed in a bivector basis  $\{e_{12}, e_{13}, e_{23}\}$  where  $e_{ij} = e_i \wedge e_j$ .

The outer product of three vectors  $a \wedge b \wedge c$  generates a 3-vector also known as the pseudoscalar, because the trivector basis consist of single element  $e_{123} = e_1 \wedge e_2 \wedge e_3$ . Similarly, the scalars are regarded as 0-vectors whose basis is the number 1. It follows that the outer product of k-vectors is the completely antisymmetric part of their geometric product:  $a_1 \wedge a_2 \wedge ... \wedge a_k = \langle a_1 a_2 ... a_k \rangle_k$  where the angle bracket means k-vector part, and k is its grade. The term grade is used to refer to the number of vectors in any exterior product. This product vanishes if and only if the vectors are linearly dependent. Consequently, the maximal grade for nonzero k-vectors is 3. It follows that every multivector X can be expanded into its k-vector parts and the entire algebra can be decomposed into k-vector subspaces:

$$\mathbb{G}_3 = \sum_{k=0}^n \mathbb{G}_3^k = \{ X = \sum_{k=0}^n \langle X \rangle_k \}$$

This is called a *grading* of the algebra.

Reversing the order of multiplication is called reversion, as expressed by  $(a_1a_2...a_k) = a_k...a_2a_1$  and  $(a_1 \wedge a_2 \wedge ... \wedge a_k) = a_k \wedge ... \wedge a_2 \wedge a_1$ , and the reverse of an arbitrary multivector is defined by  $\tilde{X} = \sum_{k=0}^{n} \langle \tilde{X} \rangle_k$ .

Rotations are even grade multivectors known as rotors. We denote the subalgebra of rotors as  $\mathbb{G}_3^+$ . A rotor R can be generated as the geometric product of an even number of vectors. A reflection of any k-vector X in a

plane with normal n is expressed as the sandwitch product  $(-1)^k nXn$ . The most basic rotor R is defined as the product of two unit vectors a and b with angle of  $\frac{\theta}{2}$ . The rotation plane is the bivector  $B = \frac{a \wedge b}{\|a \wedge b\|}$ .

$$ab = a \cdot b + a \wedge b = \cos\left(\frac{\theta}{2}\right) + B\sin\left(\frac{\theta}{2}\right).$$

Rotors act on all k-vectors using the sandwitch product  $X' = RX\tilde{R}$ , where  $\tilde{R}$  is the reverse of R and can be obtained by reversing the order of all the products of vectors.

### 3. Geometric Algebra Rotor Estimation

Given two sets of n corresponding bivectors  $P = \{p_j\}_{j=1}^n$  and  $Q = \{q_j\}_{j=1}^n$ , we attempt to maximize the following energy function:

$$E(R) = \max_{R \in \mathbb{G}_3^+} \sum_{j} c_j ||p_j + \tilde{R}q_i R||^2$$

s.t. 
$$R\tilde{R} = 1$$

where  $\{c_j\}_{j=1}^n$  are scalar weights such that  $\sum_j^n c_j = 1$ . It is a non-linear quadratic maximization problem with a non-linear constraint in R. Notice that the term  $\|p_j + \tilde{R}q_iR\|^2$  is dual to the traditional least squares error  $\|q_j - Rp_j\tilde{R}\|^2$ . Duality in the sense that the optimal R is a critical point of both energies. Notice also that  $p_j + \tilde{R}q_iR$  is equivalent to  $Rp_j + q_jR$  by multiplying by R on the left and using the fact that  $R\tilde{R} = 1$ . The equivalent problem is:

$$E(R) = \max_{R \in \mathbb{G}_3^+} \sum_j c_j ||Rp_j + q_j R||^2$$

$$s.t. R\tilde{R} = 1$$

which is a linear maximization problem with a non-linear constraint in R.

We define the commutator product of two bivectors  $p_j$  and  $q_j$  as  $p_j \times q_j = \frac{1}{2}(p_jq_j-q_jp_j)$ . The commutator product of bivectors in  $\mathbb{G}_3$  can be interpreted as a cross-product of bivectors in the sense that the resulting bivector  $B=p_j\times q_j$  is orthogonal to both  $p_j$  and  $q_j$ . The commutator product allow us to define the geometric product of two bivectors as  $AB=A\cdot B+A\times B$ . Recall that the inner product of bivectors is not the same as the inner product of vectors, since the square of bivectors is negative, the inner product of bivectors has the opposite sign e.g.,  $(ae_{12}+be_{13}+ce_{23})\cdot (de_{12}+ee_{13}+fe_{23})=-ad-be-cf$ .

For a pair of unit bivectors, A and B, the rotor R aligning them can be defined as  $R = A\frac{(A+B)}{\|A+B\|}$ . Defining the unit bivector  $C = \frac{A+B}{\|A+B\|}$  the rotor R is also R = AC = w + L where  $w = A \cdot C = \cos(\theta/2)$  and  $L = A \times C = \sin(\theta/2)\frac{A\times B}{\|A\times B\|}$ .

The constraint  $Rp_j + q_jR$  can be rewriten as  $(w + L)p_j + q_j(w + L)$ . Expanding the geometric product of bivectors in terms of the inner product and the communicator product we get:

$$w(p_j + q_j) + L \cdot (p_j + q_j) + (q_j - p_j) \times L$$

In matrix language we can define the following matrix system  $M_i R = 0$ :

$$\begin{split} M_j R = \left[ \begin{array}{cc} 0 & -s_j^T \\ s_j & \left[ d_j \right]_\times \end{array} \right] \left[ \begin{array}{c} w \\ L \end{array} \right] = \left[ \begin{array}{c} -s_j^T L \\ w s_j + d_j \times L \end{array} \right] \\ d_j = q_j - p_j \quad s_j = p_j + q_j \end{split}$$

where  $d_j$  and  $s_j$  are  $3\times 1$  column vectors holding bivector's coefficients,  $M_j$  is a skew-symmetric  $4\times 4$  real matrix, so that  $M_j^T=-M_j$ . The rotor R is represented as  $4\times 1$  column vector made of the scalar w and the  $3\times 1$  column vector L holding the bivector's components. The  $3\times 3$  matrix  $[d_j]_{\times}$  is representing the skew-symmetric cross-product matrix as usually defined for vectors in  $\mathbb{R}^3$ .

Let define the function  $F^{j}$  representing the linear transformation:

$$F^j = \sqrt{c_j} M_j R$$

Let F be a column vector of n stacked functions  $F^{j}$ 

$$F = \left[ \begin{array}{c} F^1 \\ \vdots \\ F^n \end{array} \right]$$

such that the energy E(R) can be expressed as matrix product

$$E(R) = F^T F = \begin{bmatrix} F^{1T} & \cdots & F^{nT} \end{bmatrix} \begin{bmatrix} F^1 \\ \vdots \\ F^n \end{bmatrix}$$

We can express E(R) as the following quadratic form:

$$E(R) = \max_{R} R^{T} M R$$

$$s t R^{T} R = 1$$

where  $M = \sum_{j}^{n} c_{j} M_{j}^{T} M_{j}$ . Note that since  $M_{j}$  is skew-symmetric, the product  $M_{j}^{T} M_{j}$  is symmetric and positive semi-definite. Consequently the matrix M is also symmetric positive semi-definite. It follows that all eigenvalues of M are real and  $\lambda_{i} \geq 0$ .

$$\begin{aligned} M_j^T M_j &= \begin{bmatrix} \|s_j\|^2 & (s_j \times d_j)^T \\ s_j \times d_j & s_j s_j^T - [d_j]_\times^2 \end{bmatrix} \\ d_j &= q_j - p_j \quad s_j = p_j + q_j \end{aligned}$$

By the spectral theorem the maximizer of E(R) is the eigenvector of M associated with the largest eigenvalue which is a positive number. Typically

it can be obtained with great precision using SVD or QR factorization. Nevertheless, in this work we seek for an efficient solution which allow us to take advantage of nowadays computing hardware.

# 4. Convexity

The convexity of the energy E(R) can be proof by showing that its Hessian matrix of second partial derivatives is positive semi-definite. The Hessian matrix of E(R) is  $\frac{\partial^2 E(R)}{\partial R} = \sum_j^n c_j M_j^T M_j$  which is symmetric, moreover since  $M_j$  is skew-symmetric matrix, the product  $M_j^T M_j$  is symmetric positive semi-definite. Then follows that  $\sum_j^n c_j M_j^T M_j$  is positive semi-definite and therefore convex, provided that the sum of weights is convex i.e.,  $\sum_j^n c_j = 1$ .

### 5. Numerical Method

The most time consuming task of the estimation is to compute the eigenvector of M associated with the greatest eigenvalue. Sound numerical algorithms for computing eigenvectors of a real symmetric matrix are SVD, QR factorization and Jacobi iteration among others. However those algorithms finds all eigenvectors of a matrix. Since we are interested in finding an eigenvector with greatest eigenvalue, our best choice is to use the Power Iteration. Which have the following form:

$$R_{i+1} = \frac{MR_i}{\|MR_i\|}$$

It has been established that convergence of power iteration is linear or geometric, depending on the ratio of the largest eigenvalue to the second eigenvalue  $\lambda_2/\lambda_{\rm max}$  i.e., the method converges slowly if there is an eigenvalue close in magnitude to the largest eigenvalue. A well-known algorithm for finding dominant eigenvectors of matrices consists of repeatedly squaring a matrix, renormalizing the matrix after each squaring. See [16].

$$M_{i+1} = \frac{M_i M_i}{\|M_i\|_F}$$

In [7] it is showed that the convergence of the repeated squaring is quadratic and for real symmetric  $N\times N$  matrices the average number of iterations required is  $O(\ln N + \ln \|\ln \epsilon\|)$ . Moreover, the following upper bound is provided  $\frac{1}{\ln 2}[\ln(3\sqrt{2}(N(N-1)/2+N))+1+\ln(2\ln N+\|\ln \epsilon\|)]+1$ . Thus for a symmetric  $4\times 4$  matrix, taking a small  $\epsilon=10^{-13}$  the average number of iterations is 6 and upper bound is 12. That can be exploited for creating deterministic algorithms.

Several mathematicians have proved bounds on eigenvalues in terms of the value of the matrix. A simple test in [2], is based on the L1-norm of the columns nd rows. Let  $a_{ij}$  be the elements,  $R_i = \sum_j |a_{ij}|$  be the L1-norm of

the *i*th row and  $C_j = \sum_i |a_{ij}|$  the L1-norm of the *j*th column. Let  $\mathcal{R}$  be the largest  $R_i$  and  $\mathcal{C}$  the largest  $C_j$ . Then for all eigenvalues  $|\lambda| \leq \min(\mathcal{R}, \mathcal{C})$ . Since our matrix is symmetric the upper bound is the same for rows and columns. Going back to the power method, we see that after a small number of repeated matrix squaring, the dominant eigenvector correspond to the *j*th column having the largest  $C_j$  value.

### 6. Optimal Computation of M

The symmetric matrix  $M_i^T M_j$  has a simple form:

$$M_{j}^{T} M_{j} = \begin{bmatrix} \|s_{j}\|^{2} & (s_{j} \times d_{j})^{T} \\ s_{j} \times d_{j} & s_{j} s_{j}^{T} - d_{j} d_{j}^{T} + \|d_{j}\|^{2} I \end{bmatrix}$$
$$d_{j} = q_{j} - p_{j} \quad s_{j} = p_{j} + q_{j}$$

In terms of  $p_j$  and  $q_j$  it is:

$$M_j^T M_j = 2 \begin{bmatrix} p_j^T q_j & (p_j \times q_j)^T \\ p_j \times q_j & p_j q_j^T + q_j p_j^T - p_j^T q_j I_{3 \times 3} \end{bmatrix} + (\|p_j\|^2 + \|q_j\|^2) I_{4 \times 4}$$

All terms of the matrix  $M_j^T M_j$  can be derived from the matrix  $B = p_j q_j^T$  plus the quantity  $||p_j||^2 + ||q_j||^2$ . Since  $M_j^T M_j$  is symmetric, only 10 out of 16 elements need to be actually computed. Notice that the trace of  $M_j^T M_j$  is  $Tr(M_j^T M_j) = 4||p_j||^2 + 4||q_j||^2$  and  $Tr(H) = 4\sum_j (||p_j||^2 + ||q_j||^2)$ .

# 7. Algorithms

Our algorithm is based on the repeated squaring method, which is an iterative algorithm, although it always performs a fixed number of matrix squaring operations. Since the upper bound of iterations has been established and numerical tests confirms that no more iterations are needed to achieve the required accuracy. In contrast to the power iteration our method doesn't need a random initial guess i.e., the best R is always calculated by matrix squaring.

The proposed method is shown in Algorithm 1.

The C++ code using the Eigen library [5] can be found in Listing 1.

# 8. Comparisons

We select several representative methods e.g. FLAE [19], SVD [6] and QUEST [12] to implement the algorithm. The Eigen library [5] is employed to implement the SVD and QUEST. Another version of QUEST using the Newton iteration is also added for comparison. The tests are ran on a MacBook Pro 13' 2017 computer with the CPU of Intel 3.1GHz 4-core i5. The Visual Studio 2019 C++ compiler is used in our experiments.

### Algorithm 1 Fast Rotor Estimation

```
Require: P = \{p_i\}_{i=1}^n, Q = \{q_i\}_{i=1}^n, C = \{c_i\}_{i=1}^n
  1: for j = 1 to n do
          S = S + c_j(p_j + q_j)
          B = B + c_i p_i q_i^T
  4: end for
 4: end for  5: M = \begin{bmatrix} 0 & B_{12} - B_{21} & B_{20} - B_{02} & B_{01} - B_{10} \\ B_{12} - B_{21} & 0 & B_{01} + B_{10} & B_{20} + B_{02} \\ B_{20} - B_{02} & B_{01} + B_{10} & 0 & B_{12} + B_{21} \\ B_{01} - B_{10} & B_{20} + B_{02} & B_{12} + B_{21} & 0 \end{bmatrix} 
  6: M_{00} = S^T S + Tr(B)
  7: M_{11} = 2B_{00} + S^T S - Tr(B)
  8: M_{22} = 2B_{11} + S^T S - Tr(B)
  9: M_{33} = 2B_{22} + S^T S - Tr(B)
10: for i = 1 to 12 do
         M^{i+1} = \frac{M^i M^i}{Tr(M^i)}
11:
12: end for
13: C_i = M_{i0}, \forall j = 0, ..., 3
14: R = normalize(C_i)
15: return R(0) + R(1)e_{12} + R(2)e_{13} + R(3)e_{23}
```

### 9. Conclusion

In this paper, we solve the problem of estimating the best rotation for the alignment of two sets of corresponding 3D vectors. It is based on solving the linear equations derived from the formulation of the problem in Geometric Algebra. The method is fast, robust to noise, accurate and simpler than most other methods. Experimental validation of the performance of the proposed algorithm is presented. The results show that the slightly losing accuracy of the proposed method is well worth the huge advance in execution time consumption. For many applications the vector datasets are very huge i.e. the computation time would be more important than slight change of accuracy. Therefore, we hope that the proposed algorithm would be of benefit to such applications.

### 10. C++ code

Listing 1. C++ code for rotor estimation

```
Quaterniond GAFastRotorEstimator(
    const vector<Vector3d>& P,
    const vector<Vector3d>& Q,
    const vector<double>& w)
{
    Matrix4d M;
    Matrix3d B;
    Vector3d S;
    const size_t N = P.size();
```

```
const size_t MAX_STEPS = 12;
   B. setZero();
    S. setZero();
    for (size_t j = 0; j < N; ++j) {
        S.noalias() += w[j] * (P[j] + Q[j]);
        B. noalias() += (w[j] * P[j]) * Q[j]. transpose();
    double diag = S.dot(S);
   M(3, 3) = diag + B.trace();
    diag = diag - B.trace();
   M(3, 0) = (B(1, 2) - B(2, 1));
   M(3, 1) = (B(2, 0) - B(0, 2));
   M(3, 2) = (B(0, 1) - B(1, 0));
   M(0, 0) = 2.0 * B(0, 0) + diag;
   M(1, 0) = (B(0, 1) + B(1, 0));
   M(2, 0) = (B(2, 0) + B(0, 2));
   M(1, 1) = 2.0 * B(1, 1) + diag;
   M(2, 1) = (B(1, 2) + B(2, 1));
   M(2, 2) = 2.0 * B(2, 2) + diag;
   M. selfadjointView < Eigen :: Lower > (). evalTo(H);
    for (size_t j = 0; j < MAX\_STEPS; ++j) {
        M *= M;
       M *= 1.0 / M. trace();
    return Quaterniond (M. col (0). normalized ());
}
```

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