Matching Paired Sets of Space and Orientation Data

Andrew J. Hanson

hansona@indiana.edu

School of Informatics and Computing

Indiana University

WTC 2018

Champaign-Urbana, IL

16–19 October 2018

Matching Paired Sets of Space and Orientation Data

Why is this interesting ?? **Because -**

(a) It requires *quaternions* (I wrote a 498 page book *Visualizing Quaternions*).

(b) For half a century, **all known solution methods** for the 3D and 4D matching problems have involved numerical approximations.

Exact algebraic solutions in 3D and 4D were known to involve 4th order polynomials, and, so far as I know, were considered to be **intractable**.

I have used quaternions and Mathematica to produce the first exact algebraic solutions of the full 3D and 4D eigenspectra ever written down, and extended the method to orientation frames.

. . . *with a Few Caveats* . . .

- There *are* algebraic formulas, both for Singular Value Decomposition and for eigensystems, that in principle solve this matching problem, but they are hugely complex compared to the equivalent formulas we will exhibit.

- It is *possible* that our formulas were known, say, in the 19th century, and have been lost to current literature. I would be *thrilled* to have someone point out this literature if it exists. No one I know is aware of any such literature.

- Even if there *are* prior solutions to the 3D spatial RMSD problem identical to ours, our 4D solutions are novel, and so are our 3D and 4D orientation frame optimization formulas.

The RMSD Matching Problem

- Our input data are the *reference* data set $\{y_k\}$ and one or more item-by-item matched *test* data sets $\{x_k\}$.

- The task is to **PICK ONE ROTATION MATRIX** $\boxed{R}$ that minimizes the *Root-Mean-Square Deviation* measure

$$\text{RMSD}^{\,2} \rightarrow \mathbf{S}^{\,2} = \sum_{k=1}^{N} \| R \cdot x_k - y_k \|^2$$

Refining the Optimization Problem

Method: *Minimizing* the RMSD is equivalent (dropping constants, for any dimension D) to *maximizing* the simpler cross-term measure Δ:

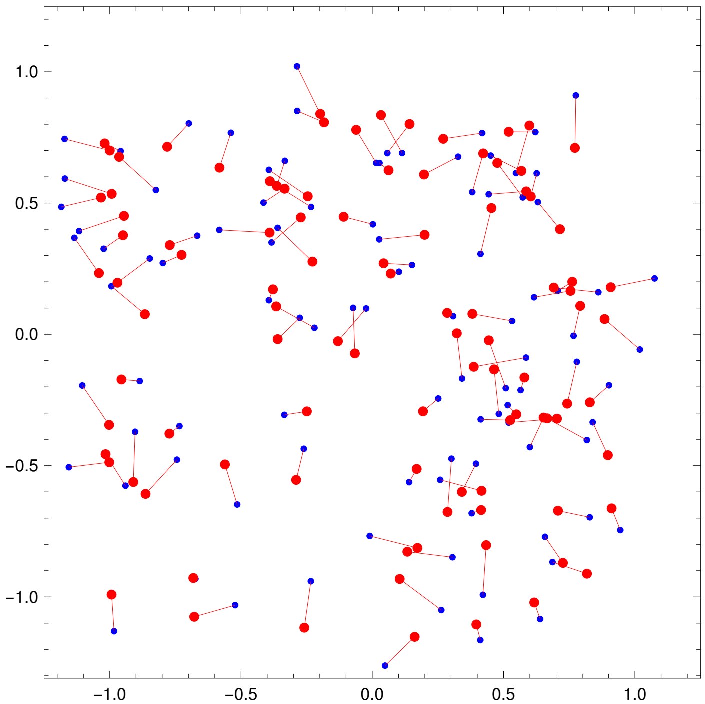
$$\Delta_D = \sum_{k=1}^{N} (R_D \cdot x_k) \cdot y_k = \sum_{a=1,b=1}^{D} {R_D}^{ba} E_{ab} = \mathrm{tr}\,[R_D \cdot E] \ ,$$

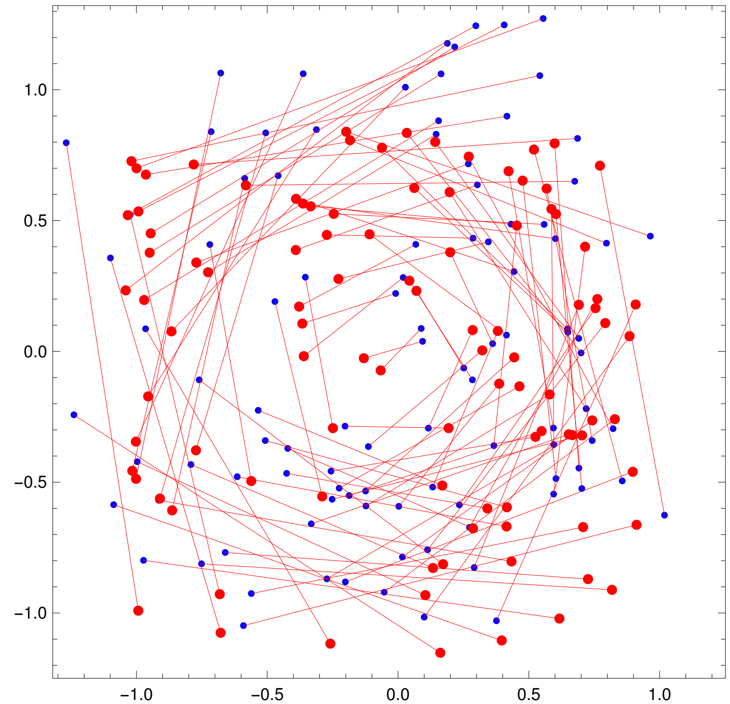
where the "data contents" all reduce to the Euclidean component-wise averages,

$$E_{ab} = \sum_{k=1}^{N} {x_k}^{a} {y_k}^{b} \ .$$

The raw form of the RMSD optimization task is thus to find the rotation matrix R that maximizes Δ.

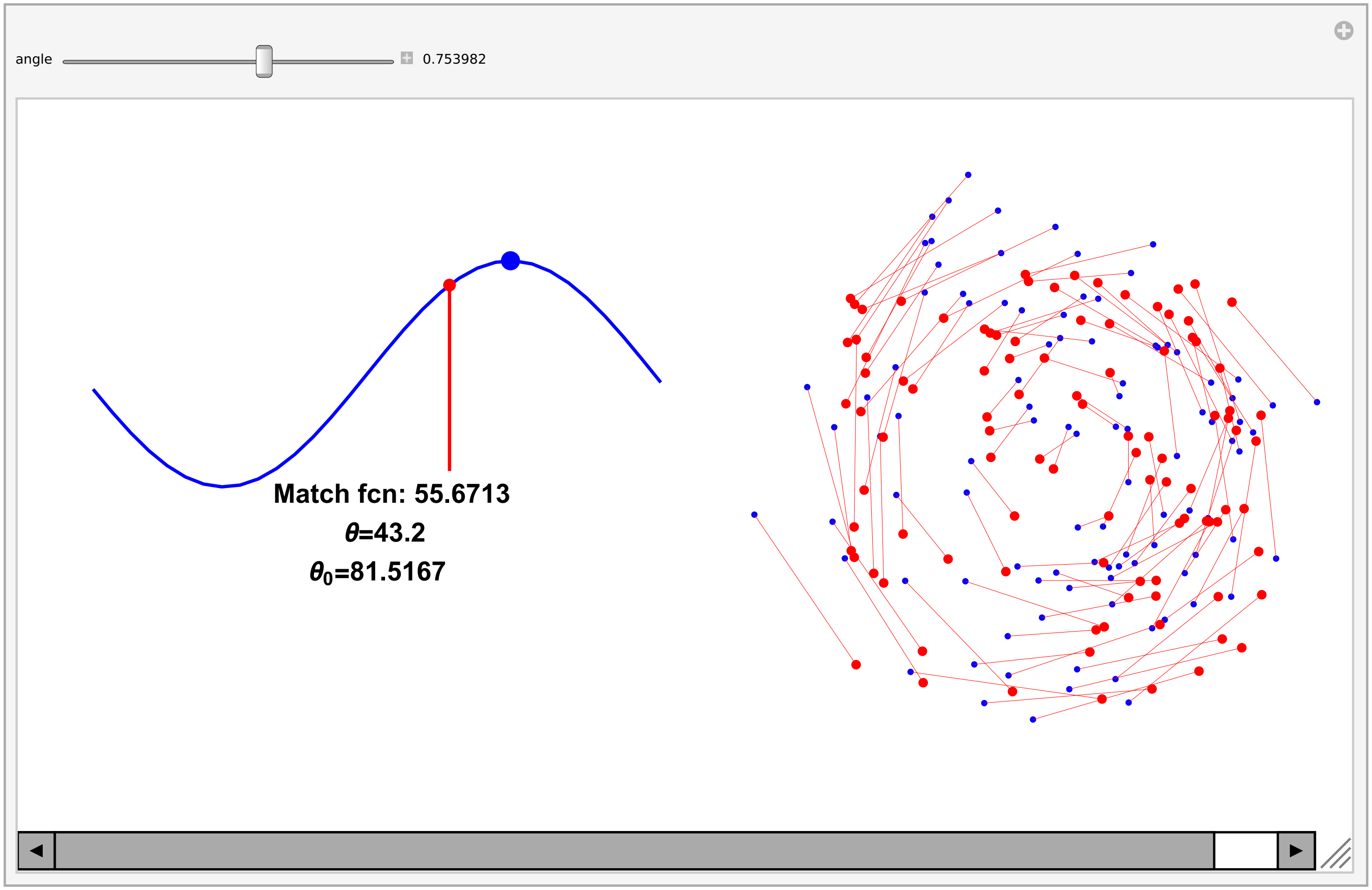
DEMO: Collections of $\|x_k - y_k\|^2$





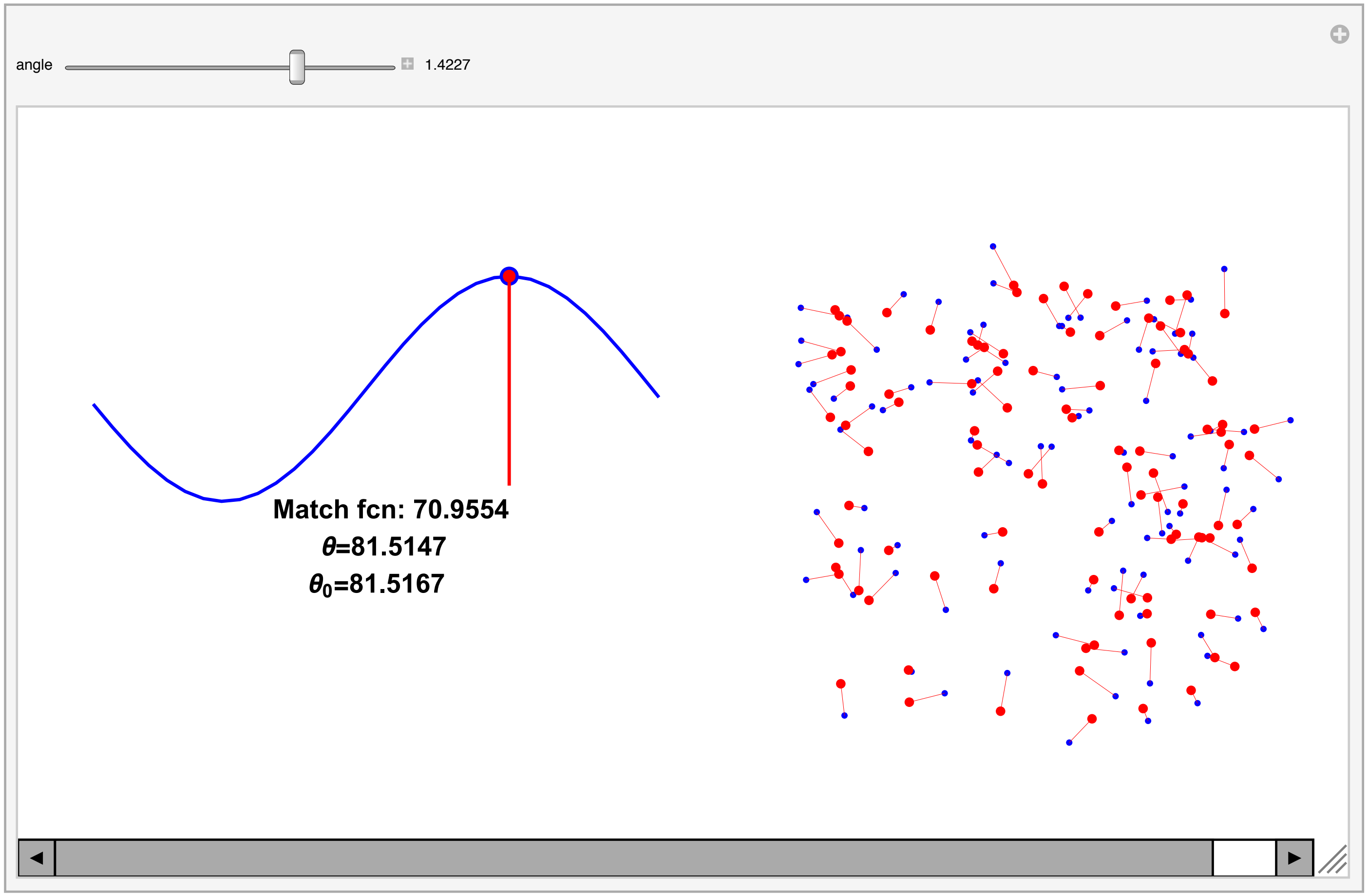
Left: *Reference* data $\{y_k\}$ are in red, noisy *test* data $\{x_k\}$ in blue, *before* global rotation. **Right:** What happens to the incremental distances after a **global rotation** of the noisy blue test data around the mutual center of mass.

Solving – how the optimization looks!



Partway through the rotation from mismatched state, still lots of space between the blue and red points.

At the Solution!



The matrix R_0 rotates the blue points to optimal alignment with red points.

Quaternion Version of 3D Spatial RMSD Problem

- It was discovered independently, in at least three different literatures, and at least four different non-co-citing published papers, that the 3D problem reduces to a 4D **quaternion eigenvalue problem**, and that finding that *numerical solution* is relatively easy.

- **We now show how to exploit quaternions in Mathematica to algebraically solve this 4D problem, in principle a very difficult quartic algebraic equation.**

First, We Need Some Quaternion Properties

- **Quaternions are Unit four-vectors.**

  Take $q = (q_0, q_1, q_2, q_3) = (q_0, \vec{\mathbf{q}})$ to obey the constraint $q \cdot q = 1$.

- **They have a Multiplication Rule.** The quaternion product of q and p is

  $q * p = (q_0 p_0 - \vec{\mathbf{q}} \cdot \vec{\mathbf{p}},\ q_0 \vec{\mathbf{p}} + p_0 \vec{\mathbf{q}} + \vec{\mathbf{q}} \times \vec{\mathbf{p}})$,

  or, alternatively,

$$\begin{bmatrix} [q*p]_0 \\ [q*p]_1 \\ [q*p]_2 \\ [q*p]_3 \end{bmatrix} = \begin{bmatrix} q_0 p_0 - q_1 p_1 - q_2 p_2 - q_3 p_3 \\ q_0 p_1 + q_1 p_0 + q_2 p_3 - q_3 p_2 \\ q_0 p_2 + q_2 p_0 + q_3 p_1 - q_1 p_3 \\ q_0 p_3 + q_3 p_0 + q_1 p_2 - q_2 p_1 \end{bmatrix}$$

3D Rotations Have a Quaternion Form

Any 3D rotation matrix has a quaternion quadratic form

$$R(q) = \begin{bmatrix} q_0^2+q_1^2-q_2^2-q_3^2 & 2q_1q_2-2q_0q_3 & 2q_1q_3+2q_0q_2 \\ 2q_1q_2+2q_0q_3 & q_0^2-q_1^2+q_2^2-q_3^2 & 2q_2q_3-2q_0q_1 \\ 2q_1q_3-2q_0q_2 & 2q_2q_3+2q_0q_1 & q_0^2-q_1^2-q_2^2+q_3^2 \end{bmatrix} .$$

$R(q)$ converts $\Delta = \mathrm{tr}(R \cdot E) \to \Delta(q)$ having this matrix form

$$\Delta(q) = \sum_{i,j=0}^{3} q_i \mathrm{M}_{ij} q_j \;=\; q \cdot \mathrm{M} \cdot q \;,$$

where M is a novel linear combination of the E_{ab} defined as …

. . . the 3D RMSD Profile Matrix $M(E)$

$$\begin{bmatrix} E_{xx}+E_{yy}+E_{zz} & E_{yz}-E_{zy} & E_{zx}-E_{xz} & E_{xy}-E_{yx} \\ E_{yz}-E_{zy} & E_{xx}-E_{yy}-E_{zz} & E_{xy}+E_{yx} & E_{zx}+E_{xz} \\ E_{zx}-E_{xz} & E_{xy}+E_{yx} & -E_{xx}+E_{yy}-E_{zz} & E_{yz}+E_{zy} \\ E_{xy}-E_{yx} & E_{zx}+E_{xz} & E_{yz}+E_{zy} & -E_{xx}-E_{yy}+E_{zz} \end{bmatrix}$$

Observe that this 4D matrix is **traceless and symmetric**, which simplifies some aspects of the 3D problem.

(It turns out we can also solve the **4D** Euclidean RMSD problem analytically, where the matrix M is completely general, with no constraints whatever.)

Eigenvalues of the Profile Matrix M

The maximum value of

$$\Delta = \mathrm{tr}\,(R \cdot E) = q \cdot \mathbf{M} \cdot q$$

is given by the *maximal eigenvalue* ϵ_{opt} of $\mathbf{M}$ (corresponding to the quaternion eigenvector q_{opt}).

Thus we must solve $\det[\mathbf{M} - eI_4] = 0$, where e denotes a generic eigenvalue and I_4 is the 4D identity matrix. We can write this in two ways:

$$e^4 + e^3 p_1 + e^2 p_2 + e p_3 + p_4 = 0\ ,$$

$$(e - \epsilon_1)(e - \epsilon_2)(e - \epsilon_3)(e - \epsilon_4) = 0\ .$$

where ϵ_i are the eigenvalues, $p_1 = 0$ is the trace, $p_4(E)$ is the determinant, and $p_2(E)$ and $p_3(E)$ are polynomials in the data averages E_{ab}.

Eigenvalues of the Profile Matrix **M**

Observe the following:

- The data coefficients $\{p_1(E), p_2(E), p_3(E), p_4(E)\}$ are known: *they are just numbers.*

- The equations above give the *unknown eigenvalues* ϵ_i in terms of the *known data coefficients:*

$$
\begin{aligned}
p_1(E) &= -\epsilon_1 - \epsilon_2 - \epsilon_3 - \epsilon_4 \\
p_2(E) &= \epsilon_1\epsilon_2 + \epsilon_1\epsilon_3 + \epsilon_2\epsilon_3 + \epsilon_1\epsilon_4 + \epsilon_2\epsilon_4 + \epsilon_3\epsilon_4 \\
p_3(E) &= -\epsilon_1\epsilon_2\epsilon_3 - \epsilon_1\epsilon_2\epsilon_4 - \epsilon_1\epsilon_3\epsilon_4 - \epsilon_2\epsilon_3\epsilon_4 \\
p_4(E) &= \epsilon_1\epsilon_2\epsilon_3\epsilon_4
\end{aligned}
$$

- **Therefore our task is to invert this equation for** $\boxed{\epsilon_i(p_1, p_2, p_3, p_4)}$.

Approach to Exact Quaternion Soln

Studying the apparently intractable algebraic expressions for M's symbolic eigensystem in Mathematica, I eventually discovered that it was useful to *change the variables* in the above (traceless) equation to express the 4 eigenvalues of M in the following form:

$$
\begin{aligned}
\epsilon_1 &= +\sqrt{X} + \sqrt{Y} + \sqrt{Z} \\
\epsilon_2 &= +\sqrt{X} - \sqrt{Y} - \sqrt{Z} \\
\epsilon_3 &= -\sqrt{X} + \sqrt{Y} - \sqrt{Z} \\
\epsilon_4 &= -\sqrt{X} - \sqrt{Y} + \sqrt{Z}
\end{aligned}
$$

This is a peculiarly advantageous form of the 4D symmetric, traceless matrix M that is adapted to machine algebra.

Approaching the Quaternion RMSD Solution

Now the equations for the eigenvalues reduce to the following form, where of course *knowing* $(X(p), Y(p), Z(p))$ *means knowing the eigenvalues* ϵ_i*:*

$$\mathrm{Eqns} = \left\{ \begin{array}{rcl} p_4(E) & = & X^2 - 2XY + Y^2 - 2XZ - 2YZ + Z^2 \\ [p_3(E)]^2 & = & 64\,XYZ \\ p_2(E) & = & -2(X + Y + Z) \end{array} \right\}$$

Then `Solve[ Eqns,{X, Y, Z}]` runs for a minute, giving 6 sets of solutions with this `ByteCount[ ]` list:

$$\{\{4584, 19544, 21552\},\ \{4584, 19448, 21552\},\ \{5224, 22232, 28640\},$$
$$\{5224, 22400, 28736\},\ \{5224, 22256, 28632\},\ \{5224, 22392, 28728\}\}$$

Exact Quaternion Soln to 3D RMSD, contd

Each of the *short* expressions looks like this, e.g., for the first $X(p)$, while the other expressions are pages of algebra that do not respond to `Simplify[]` :

$$-\frac{p_2}{6}$$

$$-\frac{\sqrt[3]{-p_2^3+36p_4p_2+\frac{3}{2}\left(\sqrt{-48p_4p_2^4+12p_3^2p_2^3+384p_4^2p_2^2-432p_3^2p_4p_2+81p_3^4-768p_4^3}-9p_3^2\right)}}{12}$$

$$-\frac{p_2^2+12p_4}{12\sqrt[3]{-p_3^3+36p_2p_4+\frac{3}{2}\left(\sqrt{-48p_4p_2^4+12p_3^2p_2^3+384p_4^2p_2^2-432p_3^2p_4p_2+81p_3^4-768p_4^3}-9p_3^2\right)}}$$

Exact Quaternion Soln to 3D RMSD

So *what happens* is that 2/3 of every solution is pages of impenetrable symbols, 20Kb each, but the FIRST one is only 5Kb, as on the previous slide.

If you plug in random numbers, you find that each of the short ones matches one of the long ones, so if you assemble them like a puzzle, you have a completely usable algebraic solution.

THAT solution in turn breaks up magically into a sum of **cube roots of unity**, hugely simplifying our task.

The Solution

By comparing the numerical values to the assortment of algebraic expressions using the tricks above, I was ultimately able to reduce the algebra for the **all eigenvalues of M** to the following form for $(X(p), Y(p), Z(p)) = F_{(x,y,z)}$:

$$F_f(p_2, p_3, p_4) \;=\; \tfrac{1}{6}\left(r(p_2, p_3, p_4) \cos_f(p_2, p_3, p_4) - p_2\right)$$

where we define

$$\begin{aligned}
\cos_x(p_2, p_3, p_4) &= \cos\left(\frac{\arg(a + i\, b)}{3}\right) \\
\cos_y(p_2, p_3, p_4) &= \cos\left(\frac{\arg(a + i\, b)}{3} - \frac{2\pi}{3}\right) \\
\cos_z(p_2, p_3, p_4) &= \cos\left(\frac{\arg(a + i\, b)}{3} + \frac{2\pi}{3}\right)
\end{aligned}$$

Exact Quaternion Soln to 3D RMSD

In this expression $\mathrm{arg}(u+i\,v) = \mathrm{atan2}(v,u) = \mathrm{ArcTan}(u,v)$, $F_f(p)$ corresponds to $X(p)$, $Y(p)$, and $Z(p)$ for $f = \{x,y,z\}$, and the utility functions reduce to

$$\begin{aligned}
a(p_2,p_3,p_4) &= {p_2}^3 + \tfrac{1}{2}\left(27{p_3}^2 - 72p_2p_4\right) \\
n(p_2,p_3,p_4) &= {p_2}^2 + 12p_4 \\
b(p_2,p_3,p_4) &= \sqrt{n^3 - a^2} \\
r(p_2,p_3,p_4) &= \sqrt[6]{a^2 + b^2} = \sqrt{n}\ .
\end{aligned}$$

Exact Quaternion Soln to 3D RMSD

The (all real) 3D eigenvalues in order of descending magnitude are now written in terms of the three phases of $F_f(p)$ for $f = \{x, y, z\}$ corresponding to $\{X, Y, Z\}$:

$$\begin{aligned}
\epsilon_1 &= +\sqrt{X} + \sqrt{Y} + \sqrt{Z} \\
\epsilon_2 &= +\sqrt{X} - \sqrt{Y} - \sqrt{Z} \\
\epsilon_3 &= -\sqrt{X} + \sqrt{Y} - \sqrt{Z} \\
\epsilon_4 &= -\sqrt{X} - \sqrt{Y} + \sqrt{Z} \,.
\end{aligned}$$

Eigenvectors for 3D RMSD

The eigenvector formulas corresponding to ϵ_k can be generically computed by solving the bottom three rows of

$$[\mathbf{M}(E) \cdot \mathbf{v} - e\mathbf{v}] = 0$$

for the elements of $\mathbf{v} = (1, v_1, v_2, v_3)$ as a function of some eigenvalue e, so we just use the exact algebraic solution for $e_{\text{opt}} = \epsilon_1$ and we are done!

Caveat - rearrange $\mathbf{v}$ if any element of M is already diagonal!

DEMO of running the solutions if time permits...

Summary: Quaternion RMSD Solns

- **This solution is unknown to the best of our knowledge.** All previous literature solves *numerically* using, e.g., Newton's method, for the maximal quaternion eigenvalue, giving the quaternion solution for the optimal aligning rotation via the quadratic formula for $R(q)$. In fact, we get **all four** eigenvalues, not just the maximal one.

- **Using similar methods, we have solved the** *3D frame alignment problem* and the 6 DOF *combined problem* in closed form as well.

- Using still further nontrivial quaternion-driven algebraic manipulations, we have also solved the *4D spatial data problem*, the *4D orientation-frame problem*, and the corresponding *combined 10 DOF problem*.