On Grioli's minimum property and its relation to Cauchy's polar decomposition

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Every invertible matrix $F \in \mathbb{R}^{n \times n}$ can be uniquely decomposed into a product of a unitary matrix $R \in O(n)$ and a positive definite matrix U:

$$F = R U.$$

The roots of this "polar decomposition theorem" lie in Cauchy's work on elasticity [6]. Finger gave it as an algebraic statement and ideas for a proof [13, Eq (25)], the brothers E. and F. Cosserat proved it [7, §6]. Matrix notation and extension to the complex case are due to Autonne [1], cf. [11, Sect. 43], [34, Sect. 35-37]. (The result also holds for complex matrices and for non-square matrices (then upon loosing the uniqueness property of R), see e.g. [16, ch. 8].)

The unitary polar factor R plays an important role in geometrically exact descriptions of solid materials. In this case $R^T F = U$ is called the right stretch tensor of the deformation gradient $F = \nabla \varphi$ and serves as a basic measure of the elastic deformation [2, 24, 28, 23, 22]. Indeed, it is known that the strain energy density for isotropic materials must depend only on the stretch U in order to be frame-indifferent. Similar reasonings on objectivity lead to the result that the strain energy for isotropic second gradient materials must depend on the stretch U and on its spatial gradient (see [8, 10, 9]). For additional applications and computational issues of the polar decomposition see e.g. [14, Ch. 12] and [21, 5, 19, 20].

The unitary polar factor can be characterized by its best-approximation property. For given F, it is the unique unitary matrix realizing

$$\inf_{Q} \|F - Q\|^{2} = \inf_{Q} \|Q^{T}F - I\|^{2} = \|\sqrt{F^{T}F} - I\|^{2} = \|U - I\|^{2}$$
(1)

over all unitary matrices Q, where $\|\cdot\|$ is an arbitrary unitarily invariant norm [12].

Optimality of the unitary polar factor is presently shown even for the expression $\| \log Q^T F \|$ in [17], a distance measure arising from geometric considerations, connected with geodesic distances on matrix Lie groups (see [31], [3], [25] and [26]). Here, Log is the (possibly multi-valued) matrix logarithm, i.e. a solution of $\exp(X) = Q^T F$. In contrast to $\|F - Q\|$ (cf. [27]), in this logarithmic expression symmetric and skew-symmetric part of the matrix norm can be weighted differently and the optimality of the polar factor still holds:

$$\min_{Q \in \mathrm{SO}(n)} \left(\mu \|\operatorname{sym}\operatorname{Log}(Q^T F)\|^2 + \mu_c \|\operatorname{skew}\operatorname{Log}(Q^T F)\|^2 \right) = \mu \|\log \sqrt{F^T F}\|^2$$

for $\mu > 0, \mu_c \ge 0$, whereas the unitary polar factor fails to minimize the weighted expression

$$\mu \|\operatorname{sym}(Q^T F - I)\|^2 + \mu_c \|\operatorname{skew}(Q^T F - I)\|^2, \quad 0 < \mu_c < \mu$$

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in the Frobenius norm.

In this short note we would like to trace back the development on the optimality of the polar factor to its presumable roots, the work [15] of G. Grioli, who shows the minimization property (1) in the important special case of (some expression equivalent to) the Frobenius matrix norm and dimension 3.

This work seems to have gone nearly unnoticed (but [32], [18], [4] and [34]) and certainly the matrixanalysis community seems not to be aware of it. For example, [16] refers to the work [12] of Fan and Hoffman for the optimality property (this is quite natural when being concerned with all unitarily invariant norms), who in turn seem to be nescient of Grioli's work.

We will juxtapose Grioli's original work [15], carefully translated from the original Italian paper by us, to a version with current notation. It will become clear that Grioli is showing even more: He considers Euclidean movements, not only linear transformations. Therefore, in his framework, it is not possible to consider weighted expressions.

While our paper does not contain new original results it may serve a pedagogical purpose: fundamental results are always older than it appears (see e.g. [33]).

Grioli starts by putting himself in the framework of finitely deforming bodies:

Let C_* be the reference configuration of an arbitrary continuous material system S; C and C' the current configurations of S as a consequence of two different regular displacements S and S', P_* the generic point of C_* ; P the corresponding of P_* .

We consider a domain C_* , an arbitrary point $\vec{p}_* \in C_*$ and diffeomorphisms

$$S: C_* \to C, \qquad \qquad S': C_* \to C'$$

and denote $\vec{p} = S(\vec{p}_*), \vec{p}' = S'(\vec{p}_*)$. We then restrict our investigation to a small ball $c_* = B_{\rho}(\vec{p}_*)$, where the affine approximation (by the first terms of the Taylor expansion)

$$S(\vec{p}_* + h) \approx \vec{p} + \nabla S(\vec{p}_*).h \tag{2}$$

is sufficiently good.

Let then c_* be a sphere with center P_* and radius ρ very small, which must be intended to be fixed independently of P_* .

More precisely, we will consider ρ to be so small that (correspondingly to any P_*) the displacements S and S' in c_* can be identified with the corresponding homogeneous displacements tangent in P_* . If the displacements S and S' were homogeneous, no limitation would exist for ρ .

With reference to the arbitrary point P_* it is common to define "local distance" of the two displacements S and S' the integral:

$$d_{P_*} = \int_{c_*} |Q'Q|^2 \, dC_*,$$

where Q and Q' are the corresponding points in C and C' respectively to the arbitrary point Q_* of c_* .

The distance Grioli uses is

$$d_{\vec{p}_*}(S,S') = \int_{x \in B_{\rho}(\vec{p}_*)} |S(x) - S'(x)|_{\mathbb{R}^3}^2 \, dV = \int_{h \in B_{\rho}(0)} |S(\vec{p}_* + h) - S'(\vec{p}_* + h)|_{\mathbb{R}^3}^2 \, \mathrm{d}V.$$

To understand this distance measure better and demonstrate its connections to the Frobenius norm $||Z||_F = \sqrt{\operatorname{tr} Z^T Z}$, for the moment we assume Z and Z' to be linear. Then

$$d_{\vec{p}_{*}}(Z, Z') = \int_{x \in B_{\rho}(\vec{p}_{*})} \langle Z(x) - Z'(x), Z(x) - Z'(x) \rangle dx$$

$$= \int_{x \in B_{\rho}(\vec{p}_{*})} \langle (Z - Z')^{T} (Z - Z') x, x \rangle dx$$

$$= \frac{4\pi\rho^{5}}{15} \operatorname{tr}((Z - Z')^{T} (Z - Z')) = \frac{4\pi\rho^{5}}{15} \|Z - Z'\|_{F}^{2}.$$

Herein, the Frobenius-norm is obtained, since

$$\int_{h\in B_{\rho}(0)} \langle Zh,h\rangle \,\mathrm{d}V = \int_{h\in B_{\rho}(0)} \sum_{i,j=1}^{3} z_{ij}h_ih_j \,\mathrm{d}V$$

$$= \int_{h\in B_{\rho}(0)} z_{11}h_1^2 + z_{22}h_2^2 + z_{33}h_3^2 \,\mathrm{d}V = \operatorname{tr} Z \int_{h\in B_{\rho}(0)} h_1^2 \,\mathrm{d}V \qquad (3)$$

$$= \operatorname{tr} Z \int_{h\in B_{\rho}(0)} \frac{h_1^2 + h_2^2 + h_3^2}{3} \,\mathrm{d}V = \operatorname{tr} Z \int_{r=0}^{\rho} \int_{\mathbb{S}^2} \frac{r^2}{3} \,\mathrm{d}S \, r^2 \,\mathrm{d}r = \operatorname{tr} Z \,\frac{4\pi\rho^5}{15},$$

where the third equality holds since $\int_h h_i^2 dV = \int_h h_j^2 dV$, i, j = 1, 2, 3 and where we used that $\int_{\mathbb{S}^2} 1 dS = 4\pi$.

The integration over the sphere/ball/... is a useful concept in order to average out (homogenize) direction dependent response. For applications in gradient elasticity, see e.g. [30, 29]. It leads in a natural way to an isotropization, at the expense, however, to oversimplify the material response in special cases. This is e.g. the case in linear elasticity theory where it leads to a Poisson number $\nu = \frac{1}{4}$:

Consider a linear elastic body, the strain energy of a small homogeneous sample in response to a displacement u is to be obtained. Locally, the energy should be quadratic in the distance of neighbouring particles. Let x and x + h be two such particles. The elastic interaction in the direction h is governed by a quadratic spring with spring constant $\mu > 0$. Hence, the directional energy is

$$\mathcal{E}_h(x) = \frac{\mu}{2} \langle u(x+h) - u(x), h \rangle_{\mathbb{R}^3}^2.$$
(4)

Since no direction is preferred in an isotropic body, the dependence on the direction can be averaged out and the total energy is obtained as integral over a sphere

$$\mathcal{E}(x) = \frac{\mu}{2} \int_{h \in \mathbb{S}^2} \mathcal{E}_h(x) \,\mathrm{dS}.$$

Assuming a Taylor expansion $u(x+h) = u(x) + \nabla u(x) \cdot h + \dots$ and approximating (4) by $\langle \nabla u(x) \cdot h, h \rangle^2$, i.e.

$$\mathcal{E}(x) \sim \frac{\mu}{2} \int_{h \in \mathbb{S}^2} \langle \nabla u(x).h, h \rangle^2 \,\mathrm{dS}$$

and using (cf. [30])

$$\int_{h\in\mathbb{S}^2} \langle Z.h,h\rangle^2 \,\mathrm{dS} = \frac{4\pi}{15} \left(2\|\operatorname{sym} Z\|^2 + [\operatorname{tr} Z]^2\right),$$

one arrives at

$$\mathcal{E}(x) = \frac{4\pi}{15} \left(\mu \|\operatorname{sym} \nabla u(x)\|^2 + \underbrace{\frac{\mu}{2}}_{=:\frac{\lambda}{2}} [\operatorname{tr} \nabla u(x)]^2 \right),$$

which corresponds to $\nu = \frac{\lambda}{2(\mu + \lambda)} = \frac{1}{4}$.

If one thinks the regular displacement S to be arbitrarily assigned, one can ask himself: corresponding to arbitrary P_* , what is the rigid displacement which has the minimum local distance from S? What is, in other words, the rigid displacement which, locally, best approximates S?

Grioli aims to find a rigid $S'_{r(igid)}$, such that $d_{\vec{p}_*}(S, S'_r)$ is minimal. "Rigid displacement" means that S'_r is of the form $S'_r(x) = t' + R'x$ for some $t' \in \mathbb{R}^3$ and $R' \in SO(3)$, that is a constant rotation followed by a constant translation:

$$\inf_{t'\in\mathbb{R}^3,\overline{R}\in\mathrm{SO}(3)}\int_{h\in B_\rho(0)}|S(\vec{p}_*+h)-[\overline{R}.h+t']|^2_{\mathbb{R}^3}\,\mathrm{d}V$$

This problem becomes simpler if not rotations, but their infinitesimal version, represented by elements of $\mathfrak{so}(3)$, i.e. skew-symmetric matrices, are considered, and Grioli gives a reference:

For an infinitesimal displacement S the answer has already been known for a long time¹: decomposing the displacement (homogeneous, infinitesimal) in a rigid displacement plus a pure deformation, one gets as rigid displacement exactly the one which best approximates the effective displacement of the particle.

For $W \in \mathfrak{so}(3)$ and for an arbitrary matrix ∇u (in linear elasticity theory, usually the displacement gradient ∇u is of interest)

$$\begin{split} \inf_{t' \in \mathbb{R}^3, \overline{W} \in \mathfrak{so}(3)} \int_{h \in B_{\rho}(0)} |\vec{p} + \nabla u.h - [\overline{W}.h + t']|_{\mathbb{R}^3}^2 \, \mathrm{d}V \\ &= \inf_{t' \in \mathbb{R}^3, \overline{W} \in \mathfrak{so}(3)} \int_{h \in B_{\rho}(0)} |\vec{p} - t'|_{\mathbb{R}^3}^2 + |(\nabla u - \overline{W}).h|_{\mathbb{R}^3}^2 + 2\underbrace{\langle \vec{p} - t', (\nabla u - \overline{W}).h \rangle}_{=0, \text{ after integration (symmetry)}} \, \mathrm{d}V \\ &\stackrel{\mathrm{choose}}{=} t' := \vec{p} \inf_{\overline{W} \in \mathfrak{so}(3)} \int_{h \in B_{\rho}(0)} |(\nabla u - \overline{W}).h|_{\mathbb{R}^3}^2 \, \mathrm{d}V \\ &= \frac{4\pi\rho^5}{15} \inf_{\overline{W} \in \mathfrak{so}(3)} \|\nabla u - \overline{W}\|_F^2 \\ &= \frac{4\pi\rho^5}{15} \|\operatorname{sym} \nabla u\|_F^2, \qquad \overline{W} = \operatorname{skew} \nabla u. \end{split}$$

This development shows one way which allows to motivate the small strain tensor $\varepsilon = \operatorname{sym} \nabla u$ of linearized elasticity theory.

We want to show how an analogous theorem exists also if the deformation S is not infinitesimal, but which is based on the requirement that the homogeneous displacement tangent to C in P_* is decomposed (which is of course possible) into the product of a pure deformation D^* and a rigid displacement S_r^* .

Using the left polar decomposition to express ∇S as a product of a rotation $R \in SO(3)$ and a pure deformation D with eigenvalues $1 + \Delta_1, 1 + \Delta_2, 1 + \Delta_3$, that is

$$\nabla S = R D,$$

Grioli sets out to deduce a lower bound for $d_{\vec{p}_*}(S, S'_r)$ in terms of Δ_i , that is, in terms of the positive definite polar factor of ∇S .

More precisely, if we indicate by $\Delta_1, \Delta_2, \Delta_3$ the principal coefficients of the linear dilatation in P_* , we will show that (with reference to P_*) the local difference of S to any rigid displacement S'_r is always such that

$$d_{P_*} \geq rac{4}{15} \pi
ho^5 \, (\Delta_1^2 + \Delta_2^2 + \Delta_3^2),$$

where equality holds if and only if S'_r coincides with S^*_r .

$$\inf_{t' \in \mathbb{R}^3, \overline{R} \in \mathrm{SO}(3)} \int_{h \in B_{\rho}(0)} |S(\vec{p}_* + h) - [\overline{R}.h + t']|^2 \,\mathrm{d}V = \frac{4}{15} \pi \rho^5 \left(\Delta_1^2 + \Delta_2^2 + \Delta_3^2\right)$$

Also in the proof we will keep using the notations used by prof. SIGNORINI in different publications² and in his current course on finite elastic transformations held at the National Institute of High Mathematics.

Grioli starts his proof by choosing an appropriate coordinate system: the coordinate axes are the eigenvectors of the positive definite part in the polar decomposition of $\nabla S = RD$.

¹ Sobrero, Lezioni di Fisica Matematica, Roma, 1935-36

² A. Signorini: Atti Accad. Naz. Lincei. Rendiconti 1930, vol. XII, p. 312: Sulle deformazioni finite dei sistemi continui.

With reference to a specific but arbitrary point P_* we choose the Cartesian reference frame $T = P_*i_1, i_2, i_3$ with the condition that it is a principal system for deformation (in P_*) and, with respect to this system, we denote by y_1, y_2, y_3 the coordinates of the generic Q_* and by x_1, x_2, x_3 those of the corresponding Q. We also set

$$lpha \equiv egin{bmatrix} rac{\partial x_1}{\partial y_1} & rac{\partial x_1}{\partial y_2} & rac{\partial x_1}{\partial y_3} \ rac{\partial x_2}{\partial y_1} & rac{\partial x_2}{\partial y_2} & rac{\partial x_2}{\partial y_3} \ rac{\partial x_2}{\partial y_1} & rac{\partial x_2}{\partial y_2} & rac{\partial x_3}{\partial y_3} \ rac{\partial x_3}{\partial y_1} & rac{\partial x_3}{\partial y_2} & rac{\partial x_3}{\partial y_3} \ \end{pmatrix}$$

where all the $\frac{\partial x_r}{\partial y_s}(r,s=1,2,3)$ are meant to be calculated in P_* .

This mapping α corresponds to $\nabla S(\vec{p}_*)$ in our notation. As already announced, he then decomposes

$$\nabla S(\vec{p}_*) = RD:$$

By virtue of the regularity conditions for the displacement S, the α can be of course decomposed in the left product of a dilatation α_d with principal coefficients which are all positive and a rotation, α_r : α_d characterizes (the dilatation) D while S_r^* is the product of the rigid rotation characterized by α_r and the translation P_*P .

In other terms we have

$$P_*Q = P_*P + PQ = P_*P + \alpha_r\alpha_d(P_*Q_*),$$

that is

$$S(x) - \vec{p}_* = S(\vec{p}_*) - \vec{p}_* + \nabla S(\vec{p}_*)(x - \vec{p}_*) = \vec{p} - \vec{p}_* + RD(x - \vec{p}_*)$$

(Of course, the first equality sign uses hypothesis (2).)

The substraction of \vec{p}_* is due to his notation for vectors as vectors from one point to another; we would maybe rather write the equivalent

$$S(x) = S(\vec{p}_*) + \nabla S(\vec{p}_*)(x - \vec{p}_*) = \vec{p} + R D(x - \vec{p}_*)$$

Also for the wanted rigid movement such an expression can be given: a rotation R' centered in \vec{p}_* followed by a translation by some t':

$$S'_r(x) - \vec{p}_* = t' + R'(x - \vec{p}_*)...$$

while if we consider also S'_r as the product of a rigid rotation characterized by α'_r and of a translation t' we can set

$$P_*Q'=t'+lpha_r'(P_*Q_*)$$

and hence

$$Q'Q = P_*P - t' + \alpha_r \alpha_d(P_*Q_*) - \alpha'_r(P_*Q_*).$$
(5)

... which leads to this representation of the difference between S and S'_r .

$$S(x) - S'_r(x) = \vec{p} - \vec{p}_* - t' + RD(x - \vec{p}_*) - R'(x - \vec{p}_*)$$

D is positive definite and, according to the choice of the coordinate system, diagonal:

$$D = \begin{pmatrix} 1 + \Delta_1 & & \\ & 1 + \Delta_2 & \\ & & 1 + \Delta_3 \end{pmatrix}.$$
 (6)

Moreover, for the way in which we chose T, we have

$$\alpha_d \equiv \begin{vmatrix} 1 + \Delta_1 & 0 & 0 \\ 0 & 1 + \Delta_2 & 0 \\ 0 & 0 & 1 + \Delta_3 \end{vmatrix}$$
(7)

with

$$1 + \Delta_r > 0, \quad (r = 1, 2, 3)$$
 (2)

and also

$$\int_{c_*} y_r \, dC_* = 0, \quad \int_{c_*} y_r \, y_s \, dC_* = 0, \quad \int_{c_*} y_r^2 \, dC_* = \frac{4}{15} \pi \rho^5, \tag{8}$$
$$(r, s = 1, 2, 3; r \neq s).$$

Since the local distance only depends on the length of the vectors Q'Q, d_{P_*} is not changed if we replace Q'Q with $\alpha_r^{-1}(Q'Q)$, since the invertible linear mapping α_r^{-1} is also a rotation and hence does not affect the distances.

Grioli then notes that $d_{\vec{p}_*}(S, S'_r) = d_{\vec{p}_*}(R^T S, R^T S'_r)$, since $|y|_{\mathbb{R}^3} = |R^T y|_{\mathbb{R}^3}$ and therefore obtains

$$d_{\vec{p}_*}(S, S'_r) = d_{\vec{p}_*}(R^T S, R^T S'_r) = \int_{B_\rho(\vec{p}_*)} |\underbrace{R^T(\vec{p} - \vec{p}_* - t')}_{=:t''} + D(x - \vec{p}_*) - \underbrace{R^T R'_r(x - \vec{p}_*)}_{=:\tilde{R}}|_{\mathbb{R}^3} dV$$

where he defines (what we will call) t'' and \widetilde{R} .

We set

$$t'' = \alpha_r^{-1}(P_*P - t'), \qquad \alpha_r'' = \alpha_r^{-1}\alpha_r',$$
(9)
so that also the invertible linear mapping α_r'' turns out to be a rotation.

Using (5) we get

$$d_{P_*} = \int_{c_*} dC_* |t + \alpha_d(P_*Q_*) - \alpha_r''(P_*Q_*)|^2.$$
(10)

He then computes this integral $d_{\vec{p}_*}(S, S'_r)$.

Using (7) and (8) and the trivial equality

$$|\alpha_r''(P_*Q_*)|^2 = |P_*Q_*|^2,$$

equation (10) is easily simplified in

$$d_{P_*} = rac{4}{3} \pi
ho^3 t^{\prime\prime 2} + \left| \sum_{s=1}^3 (1+\Delta_s)^2 + 3
ight| \; rac{4}{15} \pi
ho^5 - 2 \int_{c_*} dC_* \; lpha_d(P_*Q_*) \cdot lpha_r^{\prime\prime}(P_*Q_*).$$

Here he has used

$$\begin{aligned} |t'' + D(x - \vec{p}_*) - \widetilde{R}(x - \vec{p}_*)|_{\mathbb{R}^3}^2 \\ &= |t''|_{\mathbb{R}^3}^2 + |D(x - \vec{p}_*)|_{\mathbb{R}^3}^2 + |\widetilde{R}(x - \vec{p}_*)|_{\mathbb{R}^3}^2 \\ &+ 2\langle t'', (D - \widetilde{R})(x - \vec{p}_*)\rangle - 2\langle D(x - \vec{p}_*), \widetilde{R}(x - \vec{p}_*)\rangle, \end{aligned}$$

where the first scalar product term vanishes upon integration (because of symmetry) and as rotation and therefore isometry \widetilde{R} in $|\widetilde{R}(x - \vec{p}_*)|^2$ can be neglected. What remains, is

$$\int_{B_{\rho}(\vec{p}_{*})} |t''|_{\mathbb{R}^{3}}^{2} \,\mathrm{d}V + \int_{B_{\rho}(\vec{p}_{*})} |D(x-\vec{p}_{*})|_{\mathbb{R}^{3}}^{2} \,\mathrm{d}V + \int_{B_{\rho}(\vec{p}_{*})} |(x-\vec{p}_{*})|_{\mathbb{R}^{3}}^{2} \,\mathrm{d}V - 2 \int_{B_{\rho}(\vec{p}_{*})} \langle D(x-\vec{p}_{*}), R(x-\vec{p}_{*}) \rangle \,\mathrm{d}V.$$

Herein,

$$\int_{B_{\rho}(\vec{p}_{*})} |t''|_{\mathbb{R}^{3}}^{2} \,\mathrm{d}V = \frac{4}{3}\pi\rho^{3} |t''|_{\mathbb{R}^{3}}^{2},$$

and (confer (3) and (6))

$$\int_{B_{\rho}(\vec{p}_{*})} |D(x - \vec{p}_{*})|_{\mathbb{R}^{3}}^{2} \, \mathrm{d}V = ||D||_{F}^{2} \frac{4\pi}{15} \rho^{5} = \sum_{s=1}^{3} (1 + \Delta_{s})^{2} \frac{4\pi}{15} \rho^{5}.$$

Analogously, $\int_{B_{\rho}} |(x - \vec{p_*})|^2 = ||I||_F^2 \frac{4\pi}{15} \rho^5 = 3\frac{4\pi}{15} \rho^5$. Next we compute the value of the integral over the scalar product term:

On the other hand, if we call c_{rs} the coefficients of the invertible linear mapping α''_r with respect to T, we have [cfr. again (7) and (8)]

$$egin{aligned} &\int_{c_*} dC_*lpha_d(P_*Q_*) imeslpha_r''(P_*Q_*) = \ &= \int_{c_*} dC_* \left|\sum_{s=1}^3 (1+\Delta_s) y_s i_s imes\sum_{r,s=1}^3 c_{rs} y_s i_r
ight| = &rac{4}{15} \pi
ho^5 \sum_{s=1}^3 (1+\Delta_s) c_{ss}, \end{aligned}$$

We let $\widetilde{R} = \begin{pmatrix} r_{11} & r_{12} & r_{13} \\ r_{21} & r_{22} & r_{23} \\ r_{31} & r_{32} & r_{33} \end{pmatrix}$, where $|r_{ij}| \le 1$, because \widetilde{R} is orthogonal, $(r_{ij} = c_{ij}$ in Grioli's terminology)

and observe

$$-2\int\limits_{B_{\rho}(\vec{p}_{*})} \langle D(x-\vec{p}_{*}), \widetilde{R}(x-\vec{p}_{*})\rangle \,\mathrm{d}V = -2\int\limits_{h\in B_{\rho}(0)} \langle \begin{pmatrix} (1+\Delta_{1})h_{1}\\ (1+\Delta_{2})h_{2}\\ (1+\Delta_{3})h_{3} \end{pmatrix}, \begin{pmatrix} r_{11}h_{1}+r_{12}h_{2}+r_{13}h_{3}\\ r_{21}h_{1}+r_{22}h_{2}+r_{23}h_{3}\\ r_{31}h_{1}+r_{32}h_{2}+r_{33}h_{3} \end{pmatrix} \rangle \,\mathrm{d}V.$$

As Grioli has computed earlier (cf. (9)), the mixed terms h_1h_2 etc. yield 0. We are left with

$$-2\int_{h\in B_{\rho}(0)}(1+\Delta_{1})r_{11}h_{1}^{2}+(1+\Delta_{2})r_{22}h_{2}^{2}+(1+\Delta_{3})r_{33}h_{3}^{2}\,\mathrm{d}V=\frac{4\pi}{15}\rho^{5}\sum_{s=1}^{3}(-2(1+\Delta_{s})r_{ss}).$$

Combining all these, up to now it is shown that

$$d_{\vec{p}_*}(S, S'_r) = \frac{4}{3}\pi\rho^3 |t''|^2 + \frac{4\pi}{15}\rho^5 \left(\sum_{s=1}^3 (1+\Delta_s)^2 + 3 - 2\sum_{s=1}^3 (1+\Delta_s)r_{ss}\right).$$

and hence we have the expression

$$d_{P_*} = \frac{4}{3}\pi\rho^3 t''^2 + \frac{4}{15}\pi\rho^5 |\sum_{s=1}^3 (1+\Delta_s)^2 + 3 - 2(1+\Delta_s)c_{ss}|. \tag{11}$$

This expression obviously becomes minimal if t'' vanishes $(t' = \vec{p} - \vec{p}_*)$ and r_{ss} is maximal - that is, if $r_{ss} = 1$. The conditions $r_{11} = r_{22} = r_{33} = 1$ is not only, as Grioli remarks, contained in but equivalent to the condition that \tilde{R} is the identity. (\tilde{R} is orthogonal, so each column has to be a unit vector.) The minimal value attained then is

$$d_{\vec{p}_*}(S, S'_r) = \frac{4}{3}\pi\rho^3 |0|^2 + \frac{4\pi}{15}\rho^5 \left(\sum_{s=1}^3 \left((1+\Delta_s)^2 - 2(1+\Delta_s)1\right) + 3\right)$$
$$= \frac{4\pi}{15}\rho^5 (\Delta_1^2 + \Delta_2^2 + \Delta_3^2) = \frac{4\pi}{15}\rho^5 ||D-I||_F^2.$$

Let us now consider (2') and the fact that, since c_{rs} are all direction cosines it must be

$$c_{ss} \le 1$$
 $(s = 1, 2, 3).$

This is sufficient to deduce from (11)

$$d_{P_*} \geq rac{4}{15} \pi
ho^5 \, \left| \sum_{s=1}^3 (1+\Delta_s)^2 + 3 - 2(1+\Delta_s)
ight|,$$

and hence

$$d_{P_*} \ge \frac{4}{15} \pi \rho^5 |\Delta_1^2 + \Delta_2^2 + \Delta_3^2|.$$
(12)

The equality sign holds if and only if one simultaneously has

$$t''=0, \qquad c_{ss}=1, \qquad (s=1,2,3).$$

It is evident that the three conditions $c_{ss} = 1(s = 1, 2, 3)$ are contained in the condition according to which the rotation α''_r reduces to the identity.

Hence, simply recalling (9), we can conclude that in (12) the equality sign holds if and only if one has simultaneously

$$t = P_*P, \qquad \alpha'_r = \alpha_r,$$

i.e. if and only if S'_r coincides with S^*_r , qed.

Thus, Grioli has shown that

$$\inf_{t' \in \mathbb{R}^3, \overline{R} \in SO(3)} \int_{h \in B_{\rho}(0)} |S(\vec{p}_*) + \nabla S(\vec{p}_*).h - [\overline{R}.h + t']|^2_{\mathbb{R}^3} \, \mathrm{d}V \\
= \frac{4\pi\rho^5}{15} \|D - I\|^2_F = \frac{4\pi\rho^5}{15} \|\sqrt{\nabla S^T \nabla S} - I\|^2_F$$

where D is unitarily similar to the Hermitian polar factor $\sqrt{\nabla S^T \nabla S}$ of $\nabla S(\vec{p}_*)$.

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1 Appendix

Let $Y = (Z - Z')^T (Z - Z')$, then

$$d_{p*}(Z, Z') = \int_{B_{\rho(p*)}} Y_{ij} x_j x_i$$

$$Y_{11} \int_{B_{\rho(p*)}} x_1 x_1 + Y_{22} \int_{B_{\rho(p*)}} x_2 x_2 + Y_{33} \int_{B_{\rho(p*)}} x_3 x_3$$

$$+Y_{12}\int_{B_{\rho(p^*)}} x_1x_2 + Y_{13}\int_{B_{\rho(p^*)}} x_1x_3 + Y_{21}\int_{B_{\rho(p^*)}} x_2x_3$$

$$+Y_{23}\int_{B_{\rho(p^*)}} x_2 x_3 + Y_{31}\int_{B_{\rho(p^*)}} x_3 x_1 + Y_{32}\int_{B_{\rho(p^*)}} x_3 x_2$$

We know that to pass from cartesian to spherical coordinates one must set

 $x_1 = r \sin\theta \cos\phi$ $x_2 = r \sin\theta \sin\phi$ $x_3 = r \cos\theta$

and that the Jacobian of the transformation is $J = r^2 \sin \theta$, so that

$$\int_{B_{\rho(p*)}} x_1 x_1 = \int_0^{\rho} r^4 dr \int_0^{2\pi} \cos^2 \phi \, d\phi \int_0^{\pi} \sin^3 \theta \, d\theta = \frac{\rho^5}{5} \pi \frac{4}{3} = \frac{4\pi\rho^5}{15}$$

$$\int_{B_{\rho(p*)}} x_2 x_2 = \int_0^{\rho} r^4 dr \int_0^{2\pi} \sin^2 \phi \, d\phi \int_0^{\pi} \sin^3 \theta \, d\theta = \frac{\rho^5}{5} \pi \frac{4}{3} = \frac{4\pi\rho^5}{15}$$

$$\int_{B_{\rho(p*)}} x_3 x_3 = \int_0^{\rho} r^4 dr \int_0^{2\pi} d\phi \int_0^{\pi} \cos^2 \theta \sin \theta \, d\theta = \frac{\rho^5}{5} 2\pi \frac{2}{3} = \frac{4\pi\rho^5}{15}$$

$$\int_{B_{\rho(p*)}} x_1 x_2 = \int_{B_{\rho(p*)}} x_2 x_1 = \int_0^{\rho} r^4 dr \int_0^{2\pi} \sin \phi \cos \phi \, d\phi \int_0^{\pi} \sin^3 \theta \, d\theta = \frac{\rho^5}{5} 0 \frac{4}{3} = 0$$

$$\int_{B_{\rho(p*)}} x_1 x_3 = \int_{B_{\rho(p*)}} x_3 x_1 = \int_0^{\rho} r^4 dr \int_0^{2\pi} \cos \phi \, d\phi \int_0^{\pi} \sin^2 \theta \cos \theta \, d\theta = \frac{\rho^5}{5} 0 0 = 0.$$

Hence, we finally have

$$d_{p*}(Z, Z') = (Y_{11} + Y_{22} + Y_{33}) \frac{4\pi\rho^5}{15}$$

which is Eq. at the end of pag. 2.

A short version of this calculation can be found in (3).