

# 1 Notations

Let  $d, c \in \mathbb{N}^*$  such that  $d \geq c > 1$ . Let  $m = c - 1$ .

Let  $\mathcal{M}_{m,d}(\mathbb{R})$  be the set of real matrices of dimension  $m \times d$ .

Let  $\mathcal{S}_m^+(\mathbb{R})$  be the set of symmetric positive-definite real matrices of dimension  $m \times m$ .

Let  $\mathcal{S}_d(\mathbb{R})$  be the set of symmetric positive-semidefinite real matrices of dimension  $d \times d$ .

Let  $\text{GL}_m(\mathbb{R})$  be the set of non-singular real matrices of dimension  $m \times m$ .

Let  $\mathcal{O}_m(\mathbb{R})$  be the set of real orthogonal matrices of dimension  $m \times m$ .

The range of a matrix  $M$  is denoted  $\text{rg}(M)$ , its rank is denoted  $\text{rk}(M)$ , and its spectrum is denoted  $\text{sp}(M)$ .

The Euclidean norm is denoted  $\|\cdot\|$ . We use the notation  $\delta_{ij} = 1$  if  $i = j$  and 0 otherwise.

Following the convention in differential geometry, we denote the components of a vector  $v$  by  $v^i$  with a superscript.

# 2 Definitions

**Definition 2.1** (Probability simplex). Define the *probability simplex* of dimension  $m$  by:

$$\Delta^m = \left\{ \theta \in \mathbb{R}^c : \forall k \in \{1, \dots, c\}, \theta^k > 0 \text{ and } \sum_{i=1}^c \theta^i = 1 \right\}.$$

$\Delta^m$  is a smooth submanifold of  $\mathbb{R}^c$  of dimension  $m = c - 1$ .

When we write  $\theta \in \Delta^m$ , we see  $\theta$  as having  $m$  coordinates:  $\theta = (\theta^1, \dots, \theta^m)$ . Then, we define  $\theta^c = 1 - \sum_{i=1}^m \theta^i$ .

**Definition 2.2** (Fisher information metric). We endow  $\Delta^m$  with the *Fisher information metric* (FIM)  $g$ . For each  $\theta \in \Delta^m$ , the FIM defines a *symmetric positive-definite bilinear form*  $g_\theta$  over the tangent space  $T_\theta \Delta^m$ . In the *standard coordinates* of  $\mathbb{R}^c$ , we have, for all  $\theta \in \Delta^m$  and for all *tangent vectors*  $v, w \in T_\theta \Delta^m$ :

$$g_\theta(v, w) = v^T G_\theta w,$$

where  $G_\theta$  is the *Fisher information matrix* for parameter  $\theta \in \Delta^m$  defined by:

$$G_{\theta,ij} = \frac{\delta_{ij}}{\theta^i} + \frac{1}{\theta^c}. \quad (1)$$

For any  $\theta \in \Delta^m$ , the matrix  $G_\theta$  is *symmetric positive-definite and non-singular* (Proposition 1.6.2 in [1]). The FIM induces a distance on  $\Delta^m$  called the *Fisher-Rao distance* denoted  $d(\theta_1, \theta_2)$  for any  $\theta_1, \theta_2 \in \Delta^m$ .

**Definition 2.3** (Euclidean metric). We consider the *Euclidean space*  $\mathbb{R}^d$  endowed with the *Euclidean metric*  $\bar{g}$ . It is defined in the standard coordinates of  $\mathbb{R}^d$  for all  $x \in \mathbb{R}^d$  and for all tangent vectors  $v, w \in T_x \mathbb{R}^d$  by:

$$\bar{g}_x(v, w) = v^T w,$$

thus its matrix is the identity matrix of dimension  $d$  denoted  $I_d$ . The Euclidean metric induces a distance on  $\mathbb{R}^d$  that we will denote with the  $l_2$ -norm:  $\|x_1 - x_2\|_2$  for any  $x_1, x_2 \in \mathbb{R}^d$ .

**From now on, we fix:**

- a smooth map  $f : (\mathbb{R}^d, \bar{g}) \rightarrow (\Delta^m, g)$ . We denote by  $f^i$  the  $i$ -th component of  $f$  in the standard coordinates of  $\mathbb{R}^c$ .
- a point  $x \in \mathbb{R}^d$ .
- a positive real number  $\epsilon > 0$ .

**Definition 2.4** (Euclidean ball). Define the Euclidean open ball centered at  $x$  with radius  $\epsilon$  by:

$$\bar{b}(x, \epsilon) = \{z \in \mathbb{R}^d : \|z - x\|_2 < \epsilon\}.$$

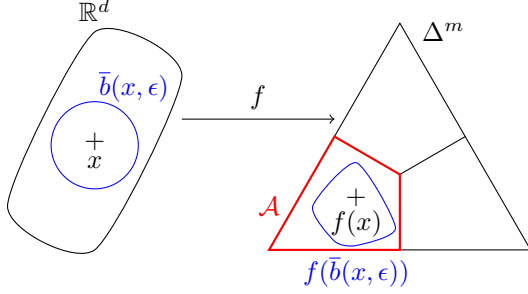


Figure 1:  $\epsilon$ -robustness at  $x$  is enforced if and only if  $f(\bar{b}(x, \epsilon)) \subseteq \mathcal{A}$ .

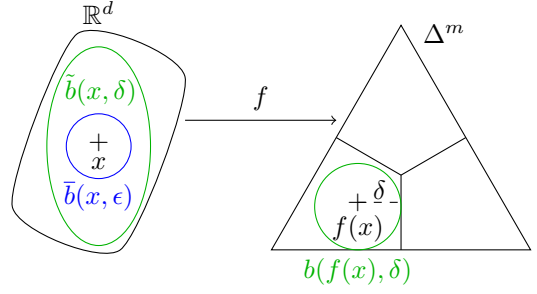


Figure 2:  $\epsilon$ -robustness at  $x$  is enforced if  $\bar{b}(x, \epsilon) \subseteq \tilde{b}(x, \delta)$ .

**Definition 2.5.** Define the set  $\mathcal{A} = \{\theta \in \Delta^m : \arg \max_i \theta^i = \arg \max_i f^i(x)\}$  (Figure 1). For simplicity, assume that  $f(x)$  is not on the “boundary” of  $\mathcal{A}$ , such that  $\arg \max_i f^i(x)$  is well defined.

**Definition 2.6** (Geodesic ball of the FIM). Let  $\delta > 0$  be the Fisher-Rao distance between  $f(x)$  and  $\Delta^m \setminus \mathcal{A}$  (Figure 2).

Define the geodesic ball centered at  $f(x) \in \Delta^m$  with radius  $\delta$  by:

$$b(f(x), \delta) = \{\theta \in \Delta^m : d(f(x), \theta) \leq \delta\}.$$

In section 8, we propose a efficient approximation of  $\delta$ .

**Definition 2.7** (Pullback metric). On  $\mathbb{R}^d$ , define the *pullback metric*  $\tilde{g}$  of  $g$  by  $f$ . In the standard coordinates of  $\mathbb{R}^d$ ,  $\tilde{g}$  is defined for all tangent vectors  $v, w \in T_x \mathbb{R}^d$  by:

$$\tilde{g}_x(v, w) = v^T J_x^T G_{f(x)} J_x w,$$

where  $J_x$  is the Jacobian matrix of  $f$  at  $x$  (in the standard coordinates of  $\mathbb{R}^d$  and  $\mathbb{R}^c$ ). Define the matrix of  $\tilde{g}_x$  in the standard coordinates of  $\mathbb{R}^d$  by:

$$\tilde{G}_x = J_x^T G_{f(x)} J_x. \quad (2)$$

**Definition 2.8** (Geodesic ball of the pullback metric). Let  $\tilde{d}$  be the distance induced by the pullback metric  $\tilde{g}$  on  $\mathbb{R}^d$ . We can define the geodesic ball centered at  $x$  with radius  $\delta$  by:

$$\tilde{b}(x, \delta) = \{z \in \mathbb{R}^d : \tilde{d}(x, z) \leq \delta\}.$$

### 3 Robustness condition

**Definition 3.1** (Robustness). We say that  $f$  is  $\epsilon$ -robust at  $x$  if:

$$\forall z \in \mathbb{R}^d, \|z - x\|_2 < \epsilon \Rightarrow f(z) \in \mathcal{A}. \quad (3)$$

Equivalently, we can write (Figure 1):

$$f(\bar{b}(x, \epsilon)) \subseteq \mathcal{A}. \quad (4)$$

**Proposition 3.2** (Sufficient condition for robustness). *If  $\bar{b}(x, \epsilon) \subseteq \tilde{b}(x, \delta)$ , then  $f$  is  $\epsilon$ -robust at  $x$  (Figure 2).*

Our goal is to start from Proposition 3.2 and make several assumptions in order to derive a condition that can be efficiently implemented.

Working with geodesic balls  $\bar{b}(x, \eta)$  and  $\tilde{b}(x, \delta)$  is intractable, so our first assumption consists in using an “infinitesimal” condition by restating Proposition 3.2 in the tangent space  $T_x \mathbb{R}^d$  instead of working directly on  $\mathbb{R}^d$ .

**Definition 3.3.** In  $T_x\mathbb{R}^d$ , define the Euclidean ball of radius  $\epsilon$  by:

$$\bar{\mathcal{B}}_x(0, \epsilon) = \{v \in T_x\mathbb{R}^d : \bar{g}_x(v, v) = v^T v \leq \epsilon^2\}.$$

**Definition 3.4.** In  $T_x\mathbb{R}^d$ , define the  $\tilde{g}_x$ -ball of radius  $\delta$  by:

$$\tilde{\mathcal{B}}_x(0, \delta) = \left\{v \in T_x\mathbb{R}^d : \tilde{g}_x(v, v) = v^T \tilde{G}_x v \leq \delta^2\right\}.$$

**Assumption 1.** We replace Proposition 3.2 by:

$$\bar{\mathcal{B}}_x(0, \epsilon) \subseteq \tilde{\mathcal{B}}_x(0, \delta). \quad (5)$$

For small enough  $\delta$ , Equation (5) implies  $\epsilon$ -robustness at  $x$ . However, contrary to Proposition 3.2, Equation (5) does not offer any guarantee on the  $\epsilon$ -robustness at  $x$  for arbitrary  $\delta$ .

**Proposition 3.5.** Equation (5) is equivalent to:

$$\forall v \in T_x\mathbb{R}^d, \quad \tilde{g}_x(v, v) \leq \frac{\delta^2}{\epsilon^2} \bar{g}_x(v, v). \quad (6)$$

Since  $m < d$ , the Jacobian matrix  $J_x$  has rank smaller or equal to  $m$ . Thus, since  $G_{f(x)}$  has full rank,  $\tilde{G}_x = J_x^T G_{f(x)} J_x$  has rank at most  $m$  (when  $J_x$  has rank  $m$ ).

**Assumption 2.** The Jacobian matrix  $J_x$  has full rank equal to  $m$ .

## 4 Isometry condition

In order to simplify the notations, we replace:

- $J_x$  by  $J \in \mathcal{M}_{m,d}(\mathbb{R})$ ,
- $G_{f(x)}$  by  $G \in \mathcal{S}_m^+(\mathbb{R})$ ,
- $\tilde{G}_x$  by  $\tilde{G} \in \mathcal{S}_d(\mathbb{R})$ ,

We define  $D = (\ker(\tilde{G}))^\perp$ . We will use the two following facts.

**Fact 4.1.**

$$D = \text{rg}(J^T) = (\ker(J))^\perp = (\ker(J^T G J))^\perp$$

**Fact 4.2.**  $J^T G J$  is symmetric positive semidefinite. Thus, by the spectral theorem, the eigenvectors associated to its nonzero eigenvalues are all in  $D = \text{rg}(J^T)$ .

In particular, since  $\text{rk}(J) = m$ , there exists an orthonormal basis of  $T_x\mathbb{R}^d$ , denoted  $\mathcal{B} = (e_1, \dots, e_m, e_{m+1}, \dots, e_d)$ , such that each  $e_i$  is an eigenvector of  $J^T G J$  and such that  $(e_1, \dots, e_m)$  is a basis of  $D = \text{rg}(J^T)$  and  $(e_{m+1}, \dots, e_d)$  is a basis of  $\ker(J)$ .

The set  $D = \text{rg}(J^T)$  is a  $m$ -dimensional subspace of  $T_x\mathbb{R}^d$ .  $\tilde{g}_x$  does not define an inner product<sup>1</sup> on  $T_x\mathbb{R}^d$  because  $\tilde{G}$  has a nontrivial kernel of dimension  $d - m$ . However, when restricted to  $D$ ,  $\tilde{g}_x|_D$  defines an inner product.

**Definition 4.3.** We define the restriction of  $\tilde{\mathcal{B}}_x(0, \delta)$  to  $D$ :

$$\tilde{\mathcal{B}}_D(0, \delta) = \left\{v \in D : v^T \tilde{G} v \leq \delta\right\}$$

**Definition 4.4.** We define the restriction of  $\bar{\mathcal{B}}_x(0, \epsilon)$  to  $D$ :

$$\bar{\mathcal{B}}_D(0, \epsilon) = \left\{v \in D : v^T v \leq \epsilon^2\right\}.$$

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<sup>1</sup>In particular, the set  $\tilde{\mathcal{B}}_x(0, \delta)$  is not bounded, i.e., it is a cylinder rather than a ball.

**Assumption 3.** We replace Equation (5) with:

$$\bar{\mathcal{B}}_D(0, \epsilon) = \tilde{\mathcal{B}}_D(0, \delta). \quad (7)$$

Equation 7 is the limit case of Equation 5, in the sense that if Equation 7 holds, then  $\tilde{\mathcal{B}}_x(0, \delta)$  is the smallest possible  $\tilde{g}_x$ -ball (for the inclusion) such that Equation 5 holds.

**Proposition 4.5.** Equation (7) is equivalent to:

$$\forall v \in D, \quad \tilde{g}_x(v, v) = \frac{\delta^2}{\epsilon^2} \bar{g}_x(v, v). \quad (8)$$

We can rewrite Equation (8) in a matrix form:

$$\forall v \in D, \quad v^T \tilde{G} v = \frac{\delta^2}{\epsilon^2} v^T v. \quad (9)$$

In section 7, we show how to exploit the properties of the FIM to derive a closed-form expression for a matrix  $P \in \text{GL}_m(\mathbb{R})$  such that  $G = P^T P$ . For now, we assume that we can easily access such a  $P$  and we are looking for a condition on  $P$  and  $J$  that is equivalent with Equation 9.

**Proposition 4.6.** The following statements are equivalent:

$$\begin{aligned} (i) \quad & \forall u \in D, \quad u^T J^T G J u = \frac{\delta^2}{\epsilon^2} u^T u, \\ (ii) \quad & P J J^T P^T = \frac{\delta^2}{\epsilon^2} I_m, \end{aligned}$$

where  $I_m$  is the identity matrix of dimension  $m \times m$ .

Finally, we can define a regularization term:

$$\alpha(x, \epsilon, f) = \frac{1}{m^2} \left\| P J J^T P^T - \frac{\delta^2}{\epsilon^2} I_m \right\|, \quad (10)$$

where  $\|\cdot\|$  is any matrix norm, such as the Frobenius norm or the spectral norm. The loss function is:

$$L(y, x, \epsilon, f) = l(y, f(x)) + \lambda \alpha(x, \epsilon, f), \quad (11)$$

where  $l$  is the cross-entropy loss and  $\lambda > 0$ .

## 5 Randomized isometry condition

The backpropagation algorithm is applied by computing the gradient  $\nabla_x f(x)^T v$  where  $v$  is a vector of  $\mathbb{R}^m$ . Thus, in order to compute the Jacobian matrix  $J$ , we need to apply the backpropagation algorithm  $m$  times, by computing each row  $\nabla_x f(x)^T e_i$ , where  $e_i = (\delta_{ij})_{j=1, \dots, m}$  is the canonical basis of  $\mathbb{R}^m$ .

To reduce the computational cost, we propose a randomized version of the isometry condition. Let  $u$  and  $v$  be two vectors sampled uniformly on the sphere of radius 1 in  $\mathbb{R}^m$ . Consider the bilinear form:

$$(u, v) \mapsto F(u, v) = \left(1 - \sqrt{f^c(x)}\right)^2 \nabla((\tau \circ f(x))^T u) \nabla((\tau \circ f(x))^T v) - \frac{\delta^2}{\epsilon^2} u^T v.$$

Then, we can use  $F(u, v)$  as a regularization term.

## 6 Jacobian bound condition

Let us use the same notations simplifications introduced at the beginning of section 4. Let  $P \in \text{GL}_m(\mathbb{R})$  be as in Proposition 7.3.

**Proposition 6.1.** *Let  $\lambda_{max}$  be the largest eigenvalue of  $PJJ^TP^T$ . The following statements are equivalent:*

- (i)  $\bar{\mathcal{B}}_x(0, \epsilon) \subseteq \tilde{\mathcal{B}}_x(0, \delta),$
- (ii)  $\lambda_{max} \leq \frac{\delta^2}{\epsilon^2},$

We use Hölder's inequality to upper-bound the spectral norm:  $\|PJ\|_2^2 \leq \|PJ\|_1 \|PJ\|_\infty$  with  $\|M\|_1 = \max_{1 \leq j \leq n} \sum_{i=1}^m |M_{ij}|$  and  $\|M\|_\infty = \max_{1 \leq i \leq m} \sum_{j=1}^n |M_{ij}|$ . Now, we can define a regularization term:

$$\alpha(x, \epsilon, f) = \max \left\{ \sqrt{\|PJ\|_1 \|PJ\|_\infty} - \frac{\delta}{\epsilon}, 0 \right\}. \quad (12)$$

## 7 Coordinate change

In this section, we show how to compute the matrix  $P$  introduced for Corollary 4.6. To this end, we isometrically embed  $\Delta^m$  into the Euclidean space  $\mathbb{R}^c$  using the following inclusion map:

$$\begin{aligned} \mu : \Delta^m &\longrightarrow \mathbb{R}^c \\ (\theta^1, \dots, \theta^m) &\longmapsto 2 \left( \sqrt{\theta^1}, \dots, \sqrt{\theta^m}, \sqrt{1 - \sum_{i=1}^m \theta^i} \right) \end{aligned}$$

We can easily see that  $\mu$  is an embedding. If  $\mathcal{S}^m(2)$  is the sphere of radius 2 centered at the origin in  $\mathbb{R}^c$ , then  $\mu(\Delta^m)$  is the subset of  $\mathcal{S}^m(2)$  where all coordinates are strictly positive (using the standard coordinates of  $\mathbb{R}^c$ ).

**Proposition 7.1.** *Let  $g$  be the Fisher information metric on  $\Delta^m$  (Definition 2.2), and  $\bar{g}$  be the Euclidean metric on  $\mathbb{R}^c$ . Then  $\mu$  is an isometric embedding of  $(\Delta^m, g)$  into  $(\mathbb{R}^c, \bar{g})$ .*

Now, we use the stereographic projection to embed  $\Delta^m$  into  $\mathbb{R}^m$ :

$$\begin{aligned} \tau : \mu(\Delta^m) &\longrightarrow \mathbb{R}^m \\ (\mu^1, \dots, \mu^m, \mu^c) &\longmapsto 2 \left( \frac{\mu^1}{2 - \mu^c}, \dots, \frac{\mu^m}{2 - \mu^c} \right), \end{aligned}$$

with  $\mu^c = 2\sqrt{1 - \sum_{i=1}^m \theta^i}$ .

**Proposition 7.2.** *In the coordinates  $\tau$ , the FIM is:*

$$G_{\tau, ij} = \frac{4}{(1 + \|\tau/2\|^2)^2} \delta_{ij}. \quad (13)$$

Let  $\tilde{J}$  be the Jacobian matrix of  $\tau \circ \mu : \Delta^m \rightarrow \mathbb{R}^m$  at  $f(x)$ . Then we have:

$$G = \tilde{J}^T G_\tau \tilde{J} = \frac{4}{(1 + \|\tau/2\|^2)^2} \tilde{J}^T \tilde{J}.$$

Thus, we can choose:

$$P = \frac{2}{1 + \|\tau/2\|^2} \tilde{J}. \quad (14)$$

Write  $f(x) = \theta = (\theta^1, \dots, \theta^m)$  and  $\theta_c = 1 - \sum_{i=1}^m \theta^i$ . For simplicity, write  $\tau^i(\theta) = \tau^i(\mu(\theta)) = 2\sqrt{\theta^i}/(1 - \sqrt{\theta^c})$  for  $i = 1, \dots, m$ . More explicitly, we have:

**Proposition 7.3.** *For  $i, j = 1, \dots, m$ :*

$$P_{ij} = \frac{\delta_{ij}}{\sqrt{\theta^i}} - \frac{\tau^i(\theta)}{2\sqrt{\theta^c}}. \quad (15)$$

## 8 The Fisher-Rao distance

As stated in Proposition 7.1, the probability simplex  $\Delta^m$  endowed with the FIM can be isometrically embedded into the  $m$ -sphere of radius 2. Thus, the angle  $\beta$  between two distributions of coordinates  $\theta_1$  and  $\theta_2$  in  $\Delta^m$  with  $\mu_1 = \mu(\theta_1)$  and  $\mu_2 = \mu(\theta_2)$  is:

$$\cos(\beta) = \frac{1}{4} \sum_{i=1}^c \mu_1^i \mu_2^i = \sum_{i=1}^c \sqrt{\theta_1^i \theta_2^i}.$$

The Riemannian distance between these two points is the arc length on the sphere:

$$d(\theta_1, \theta_2) = 2 \arccos \sum_{i=1}^c \sqrt{\theta_1^i \theta_2^i}.$$

In the regularization terms, we replace  $\delta$  by the following upper bound:

$$\delta = d(f(x), \Delta^m \setminus \mathcal{A}) \leq d(f(x), O),$$

where  $O = \frac{1}{c}(1, \dots, 1)$  is the center of the simplex  $\Delta^m$ . Thus:

$$\delta \leq 2 \arccos \sum_{i=1}^c \sqrt{\frac{f(x)^i}{c}}. \quad (16)$$

## 9 Proofs

*Proof of Proposition 3.5.* (6)  $\Rightarrow$  (5)]. Assume (6). Let  $v \in \bar{\mathcal{B}}_x(0, \epsilon)$ . Thus  $\bar{g}_x(v, v) \leq \epsilon^2$ . We have:

$$\tilde{g}_x(v, v) \leq \frac{\delta^2}{\epsilon^2} \bar{g}_x(v, v) \leq \frac{\delta^2}{\epsilon^2} \epsilon^2 = \delta^2.$$

Thus  $v \in \tilde{\mathcal{B}}_x(0, \delta)$ .

(5)  $\Rightarrow$  (6)]. Assume (5). Let  $v \in T_x \mathbb{R}^d$ . Define  $w = \epsilon v / \sqrt{\bar{g}_x(v, v)}$ . Then  $\bar{g}_x(w, w) = \epsilon^2$ . Thus,  $w \in \bar{\mathcal{B}}_x(0, \epsilon)$ . Hence,  $w \in \tilde{\mathcal{B}}_x(0, \delta)$ . Thus,  $\tilde{g}_x(w, w) < \delta^2$ . Finally, we have:

$$\tilde{g}_x(w, w) = \frac{\epsilon^2}{\bar{g}_x(v, v)} \tilde{g}_x(v, v) < \delta^2.$$

We obtain Equation (6) by multiplying by  $\bar{g}_x(v, v)/\epsilon^2$ . □

*Proof of Fact 4.1.* We prove the third equality (the second equality is a well-known fact of linear algebra).

Let  $u \in \ker J$ . Then  $J^T G J u = 0$ , thus  $u \in \ker(J^T G J)$ . Hence  $(\ker(J^T G J))^\perp \subseteq (\ker(J))^\perp$ .

Let  $v \in \ker J^T G J$ . Since  $G$  is symmetric positive-definite, the function  $w \mapsto N(w) = \sqrt{w^T G w}$  is a norm. We have  $0 = v^T J^T G J v = N(Jv)^2$ . The positive-definiteness of the norm  $N$  implies  $Jv = 0$ . Thus,  $v \in \ker J$ . Hence  $(\ker(J))^\perp \subseteq (\ker(J^T G J))^\perp$ . □

*Proof of Proposition 4.5.* The implication (8)  $\Rightarrow$  (7)] is immediate (by double inclusion).

Now, assume (7)] holds. Let  $v \in D$ . Define  $w_1 = \epsilon v / \sqrt{\bar{g}_x(v, v)}$  and  $w_2 = \epsilon v / \sqrt{\tilde{g}_x(v, v)}$ . Then, with a similar argument as in the proof of Proposition 3.5, we can obtain Equation (8). Note that  $w_2$  is well defined because  $v \notin \ker(J)$ . □

*Proof of Proposition 4.6.* **Let us first introduce the polar decomposition.**

Let  $A$  be a  $m \times d$  matrix.

Define the absolute value<sup>2</sup> of  $A$  by  $|A| = (A^T A)^{\frac{1}{2}}$ .

Define the linear map  $u : \text{rg}(|A|) \rightarrow \text{rg}(A)$  by  $u(|A|x) = Ax$  for any  $x \in \mathbb{R}^d$ .

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<sup>2</sup>The square root of  $A^T A$  is well defined because it is a positive semidefinite matrix.

Using the fact that  $|A|$  is symmetric, we have that  $\|Ax\|^2 = x^T A^T A x = (A^T A x)^T x = (|A|^2 x)^T x = x^T |A|^T |A| x = \| |A| x \|^2$ , thus  $u$  is an isometry<sup>3</sup>.

Let  $U$  be the matrix associated to  $u$  in the canonical basis.

**We now prove the main result.**

Let  $A = PJ$ . Using the polar decomposition, we have

$$PJ = U|PJ|,$$

where  $U$  is an isometry from  $\text{rg}(|PJ|) = (\ker|PJ|)^\perp = (\ker(PJ))^\perp = (\ker(J))^\perp = D$  to  $\text{rg}(PJ) = \mathbb{R}^m$  (using our assumption that  $\text{rk}(J) = m$ ). Transposing this relation, we obtain:

$$J^T P^T = |PJ| U^T.$$

Hence, by multiplying both relations, we have:

$$PJ J^T P^T = U|PJ|^2 U^T = U J^T P^T P J U^T$$

Assume that (ii) holds, i.e.,  $PJ J^T P = I_m$ . Then:

$$J^T G J = J^T P^T P J = U^T P J J^T P^T U = U^T U.$$

Since  $U$  is an isometry from  $D$  to  $\mathbb{R}^m$ , then  $U^T U$  is the projection onto  $D$ , denoted  $\Pi_D$ . Thus, we have  $J^T G J = \Pi_D$  which is (i).

Now, assume that (i) holds, i.e.,  $J^T P^T P J = \Pi_D$  where  $\Pi_D$  is the projection onto  $D$ . We have:

$$P J J^T P^T = U J^T P^T P J U^T = U \Pi_D U^T.$$

Since  $\text{rg}(U^T) = D$ , then  $\Pi_D U^T = U^T$ . Since  $U$  is an isometry from  $D$  to  $\mathbb{R}^m$ , then  $U U^T = I_m$ . Thus,  $P J J^T P^T = I_m$  which is (ii).  $\square$

*Proof of Proposition 7.1.* We need to show that  $\mu^* \bar{g} = g$ . Using the coordinates  $\theta$  on  $\Delta^m$  (Definition 2.1) and the standard coordinates on  $\mathbb{R}^c$ , and writing  $f(x) = \theta_0 = (\theta_0^1, \dots, \theta_0^m)$  we have:

$$G_{ij} = G_{\theta_0, ij} = \sum_{\alpha=1}^c \sum_{\beta=1}^c \frac{\partial \mu^\alpha(\theta_0)}{\partial \theta^i} \frac{\partial \mu^\beta(\theta_0)}{\partial \theta^j} \delta_{\alpha\beta} = \sum_{\alpha=1}^c \frac{\partial \mu^\alpha(\theta_0)}{\partial \theta^i} \frac{\partial \mu^\alpha(\theta_0)}{\partial \theta^j}.$$

For  $i = 1, \dots, m$  and  $\alpha = 1, \dots, m$  we have:

$$\frac{\partial \mu^\alpha(\theta_0)}{\partial \theta^i} = \frac{\delta_{i\alpha}}{\sqrt{\theta_0^i}},$$

and for  $\alpha = c$ :

$$\frac{\partial \mu^c(\theta_0)}{\partial \theta^i} = -\frac{1}{\sqrt{\theta_0^c}},$$

with  $\theta_0^c = \sqrt{1 - \sum_{i=1}^m \theta_0^i}$ . Thus:

$$G_{\theta_0, ij} = \frac{\delta_{ij}}{\theta_0^i} + \frac{1}{\theta_0^c},$$

which is the FIM as defined in Definition 2.2.  $\square$

*Proof of Proposition 7.2.* For  $i = 1, \dots, m$ , the inverse transformation of  $\tau(\mu)$  is (proof below):

$$\mu^i(\tau) = \frac{2\tau^i}{1 + \|\tau/2\|^2}, \quad (17)$$

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<sup>3</sup>We can arbitrarily extend  $u$  on the entire  $\mathbb{R}^d$ , e.g., by setting  $\ker(u) = \ker(|A|)$ .

and:

$$\mu^c(\tau) = 2 \frac{\|\tau/2\|^2 - 1}{\|\tau/2\|^2 + 1}. \quad (18)$$

Moreover, according to Proposition 7.1, the FIM in the coordinates  $(\mu^1, \dots, \mu^m)$  is the metric induced on  $\mu(\Delta^m)$  by the identity matrix (i.e., the Euclidean metric) of  $\mathbb{R}^c$ . Hence, we have:

$$G_{\tau,ij} = \sum_{\alpha=1}^c \sum_{\beta=1}^c \frac{\partial \mu^\alpha(\tau)}{\partial \tau^i} \frac{\partial \mu^\beta(\tau)}{\partial \tau^j} \delta_{\alpha\beta} = \sum_{\alpha=1}^c \frac{\partial \mu^\alpha(\tau)}{\partial \tau^i} \frac{\partial \mu^\alpha(\tau)}{\partial \tau^j}.$$

For  $i = 1, \dots, m$  and  $\alpha = 1, \dots, m$  we have:

$$\frac{\partial \mu^\alpha(\tau)}{\partial \tau^i} = \frac{2}{1 + \|\tau/2\|^2} \left( \delta_{i\alpha} - \frac{\tau^\alpha \tau^i}{2(1 + \|\tau/2\|^2)} \right),$$

and for  $\alpha = c$ :

$$\frac{\partial \mu^c(\tau)}{\partial \tau^i} = \frac{2\tau^i}{(1 + \|\tau/2\|^2)^2},$$

Thus:

$$\begin{aligned} G_{\tau,ij} &= \frac{4}{(1 + \|\tau/2\|^2)^2} \left( \sum_{\alpha=1}^m \left\{ \delta_{i\alpha} \delta_{j\alpha} - \frac{\delta_{i\alpha} \tau^j \tau^\alpha}{2(1 + \|\tau/2\|^2)} - \frac{\delta_{j\alpha} \tau^i \tau^\alpha}{2(1 + \|\tau/2\|^2)} + \frac{\tau^i \tau^j (\tau^\alpha)^2}{4(1 + \|\tau/2\|^2)^2} \right\} + \frac{\tau^i \tau^j}{(1 + \|\tau/2\|^2)^2} \right) \\ &= \frac{4}{(1 + \|\tau/2\|^2)^2} \left( \delta_{ij} - \frac{\tau^i \tau^j}{1 + \|\tau/2\|^2} + \frac{\tau^i \tau^j \|\tau/2\|^2}{(1 + \|\tau/2\|^2)^2} + \frac{\tau^i \tau^j}{(1 + \|\tau/2\|^2)^2} \right) \\ &= \frac{4}{(1 + \|\tau/2\|^2)^2} \left( \delta_{ij} - \frac{\tau^i \tau^j}{1 + \|\tau/2\|^2} + \frac{\tau^i \tau^j}{1 + \|\tau/2\|^2} \right) \\ &= \frac{4}{(1 + \|\tau/2\|^2)^2} \delta_{ij} \end{aligned}$$

□

*Proof of Equations 17 and 18.* We have  $\tau^i(\mu) = \lambda \mu^i$  with  $\lambda = 2/(2 - \mu^c)$ . Let us express  $\mu^c$  as a function of  $\tau$ . We have:

$$\|\tau\|^2 = \sum_{i=1}^m (\tau^i)^2 = \lambda^2 \|\mu\|^2.$$

Since  $\mu$  belongs to the sphere of radius 2, we have  $\|\mu\|^2 + (\mu^c)^2 = 4$ . Thus:

$$\|\tau\|^2 = \lambda^2 (4 - (\mu^c)^2) = 4 \frac{4 - (\mu^c)^2}{(2 - \mu^c)^2} = 4 \frac{2 + \mu^c}{2 - \mu^c}.$$

Isolating  $\mu^c$ , we get:

$$\mu^c(\tau) = \frac{2\|\tau\|^2 - 8}{\|\tau\|^2 + 4} = 2 \frac{\|\tau/2\|^2 - 1}{\|\tau/2\|^2 + 1}.$$

Now, we can replace  $\mu^c$  into the expression of  $\lambda$ . We obtain  $\lambda = (1 + \|\tau/2\|^2)/2$ , and thus:

$$\mu^i(\tau) = \frac{\tau^i}{\lambda} = \frac{2\tau^i}{1 + \|\tau/2\|^2}$$

□



*Proof of Proposition 7.3.* We have  $\tau^i(\theta) = 2\sqrt{\theta^i}/(1 - \sqrt{\theta^c})$ . Thus:

$$\left\| \frac{\tau(\theta)}{2} \right\|^2 = \sum_{i=1}^m \frac{\tau^i(\theta)^2}{4} = \frac{\sum_{i=1}^m \theta^i}{(1 - \sqrt{\theta^c})^2} = \frac{1 - \theta^c}{(1 - \sqrt{\theta^c})^2} = \frac{1 + \sqrt{\theta^c}}{1 - \sqrt{\theta^c}}.$$

Hence, for any  $i = 1, \dots, m$ :

$$\frac{2}{1 + \|\tau(\theta)/2\|^2} = 1 - \sqrt{\theta^c} = \frac{2\sqrt{\theta^i}}{\tau^i(\theta)}. \quad (19)$$

Now, we compute  $\tilde{J}$ . Let  $i$  and  $j$  in  $\{1, \dots, m\}$ :

$$\frac{\partial \tau^i(\theta)}{\partial \theta^j} = \frac{\delta_{ij}}{\sqrt{\theta^i}(1 - \sqrt{\theta^c})} - \frac{\sqrt{\theta^i}}{\sqrt{\theta^c}(1 - \sqrt{\theta^c})^2} = \frac{\tau^i(\theta)}{2} \left( \frac{\delta_{ij}}{\theta^i} - \frac{\tau^i(\theta)}{2\sqrt{\theta^i}\theta^c} \right) \quad (20)$$

Replacing Equations 19 and 20 into Equation 14 yields the result. □

*Proof of Proposition 6.1.* **TBD** □

## References

- [1] O. Calin and C. Udrişte, *Geometric Modeling in Probability and Statistics*. Springer International Publishing, 2014.