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## DIFFEOMORPHIC B-SPLINE VECTOR FIELDS WITH A TRACTABLE SET OF INEQUALITIES

MICHAËL SDIKA

**ABSTRACT.** B-spline diffeomorphic vector fields are objects of great interest in image processing and analysis, more specifically for the registration of medical images. In this paper, several conditions on the B-spline coefficients ensuring that a given B-spline vector field is a diffeomorphism are proposed. Some properties of vector fields satisfying these conditions are established showing that they are not too restrictive while having a reasonable computational complexity. This work opens the way to the development of practical image registration algorithms in two and three dimensions whose unknowns would be such diffeomorphic B-spline vector fields.

### 1. INTRODUCTION

Image registration is an image processing technique that, given two images, aims at finding the geometric transformation that aligns one image to the other. It is at the core of several medical analysis techniques such as atlas based segmentation [31, 25, 15], heart or lung deformation analysis [17, 20, 29], computational anatomy [10, 3] or slice interpolation [18, 22]. It is usually desired, and sometimes required, that the nonlinear transformation of the space that align the images is invertible.

For the modelization and the implementation of registration algorithms, it is necessary to have an adequate representation of diffeomorphic vector fields. In the literature, numerous methods are based on the flow of diffeomorphism framework [27, 26, 1]: the transformation is defined as the solution at  $t = 1$  of the transport equation  $\frac{\partial \phi}{\partial t}(x, t) = v(\phi(x, t), t)$ . When the new variable  $v$  is a Lipschitz function,  $\phi(., t)$  is a diffeomorphism for all  $t$ . The problem is then discretized and solved numerically [2, 6, 4, 30, 1].

Other works [19, 11, 7] rely on hyperelastic regularization for diffeomorphic image registration. Negative Jacobian determinants are avoided by including a barrier function of the discretized Jacobian determinant term in the regularization. A theorem of Ball [5] ensures the existence of solutions of such problems.

A different but yet popular approach is to assume that the transformation belongs to the vector space of uniform B-spline vector fields. As the analytical expressions of the transformation and its derivatives are known, they can be computed exactly and consistently. This can be of great importance for example if we need to study the Jacobian map that no Jacobian is negative due to numerical errors. The transformation resolution can also be chosen independently from the image resolution. Finally, as we manipulate directly the transformation, additional constraints such as priors on local rigidity [23] or priors on the motion orientation [24]

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can be handled very easily. However, questions regarding invertibility of B-spline vector fields have not been solved yet and, most works simply drop the invertibility requirement. Some only use regularization as a cheap way to penalize singularities, others constrain the Jacobian to be positive on the pixels to avoid strong folding but without guaranteeing that the transformation is a diffeomorphism [21]. Few sufficient conditions on the B-spline coefficients have been proposed: they guarantee that the transformation is a diffeomorphism but are either too restrictive [8, 13, 9] or subject to the curse of dimensionality and only usable on 2D images [22].

In this work, we show that a B-spline vector field can be made a diffeomorphism with a large deformation in  $\mathbb{R}^2$  or  $\mathbb{R}^3$  if its coefficients satisfy a finite and computationally tractable set of inequalities.

The paper is organized as follows. In section 2, basic properties of B-spline vector fields are reminded. In section 3, a new condition on the B-spline coefficients guarantying the invertibility of the 2 dimensional vector field is proposed. The 3-dimensional case is more involved and is studied in section 4. After a first general result on the cross product of 3D cones given in section 4.1, an important object for our derivation, the  $p$ -cone, is introduced and studied in section 4.2. A first set of conditions using 1-cones is then proposed in section 4.3. A second set of conditions, involving 2-cones is proposed in section 4.4. In section 3.3 and 4.5, parameters of the conditions are discussed respectively for the 2D and 3D cases. Section 5 is devoted to study the strength of the conditions: how large are the spaces of B-spline vector fields satisfying the proposed conditions. Computational complexity of the proposed condition is given and compared to the state of the art in section 6.

## 2. B-SPLINE VECTOR FIELD

The following notations and definitions will be used throughout the paper.

In one dimension, the B-spline function of degree 0 is defined as the characteristic function on the real interval  $] - 1/2, 1/2]$ . The B-spline function of degree  $n$  is the repeated convolution of the B-spline of degree 0 with itself  $n + 1$  times. In dimension  $D$ , the B-spline function of degree  $n$ ,  $\beta$ , is defined as the tensor product of 1-dimensional B-spline of degree  $n$ . Basic properties of B-spline functions can be found in [28, 22].

In all this work, we will consider  $\mathcal{B}^D$ , the space of  $D$ -dimensional B-spline vector field  $T$  defined by:

$$T(x) = \sum_{i \in \mathbb{Z}^D} c_i \beta(x/h - i).$$

In this expression,  $x \in \mathbb{R}^D$ ,  $c_i \in \mathbb{R}^D$  are the B-spline coefficients, the node spacing vector  $h$  is in  $\mathbb{R}^D$  and  $x/h$  is the component-wise division of  $x$  by  $h$ . The first order finite difference coefficients in the direction  $l$  of the vector field play an important role:

$$d_i^l = \frac{c_i - c_{i-e_l}}{h_l} \in \mathbb{R}^D,$$

where  $e_l$  is the  $l^{\text{th}}$  vector of the canonical basis.

To prove that a vector field is a diffeomorphism, we rely on the corollary 4.3 of [16] saying that  $T$  is a diffeomorphism if and only if  $J(x) = \det(T'(x))$  never vanishes (where  $T'(x)$  is the  $D \times D$  Jacobian matrix at position  $x$ ) and  $\lim_{|x| \rightarrow \infty} |T(x)| = \infty$ .

A similar results was originally proved by Hadamard in [12] for continuous maps: a locally invertible  $C^0$  map is a homeomorphism if and only if it is proper.

We assume that all the B-spline vector fields in this paper are in the set defined below.

**Definition 2.1.**  $\mathcal{B}_a^D$  is set of  $D$ -dimensional B-spline vector fields that are equal to an affine function with positive determinant when  $|x|$  is large enough:

$$\mathcal{B}_a^D = \left\{ T \in \mathcal{B}^D \mid \begin{array}{l} \exists K > 0, A \in GL^+(D, \mathbb{R}), b \in \mathbb{R}^D \text{ such that} \\ \forall x, |x| > K \text{ then } T(x) = Ax + b \end{array} \right\}.$$

In practice, this condition is not restrictive: as affine transform can be represented exactly using B-splines of degree one or more (with  $c_i = A(hi) + b$ ) and as the vector fields of interest are usually considered over a bounded domain, an extrapolation of the coefficients is often sufficient to fit in our framework. Note that a similar assumption at infinity is also made with the flow of diffeomorphism formalism: the diffeomorphism are assumed to converge to the identity at infinity (see [1], section 2, page 143). B-spline vector fields  $T$  in  $\mathcal{B}_a^D$  enjoy two interesting properties. First, as  $T'(x) = A \in GL^+(D, \mathbb{R})$  is constant for  $x$  large enough, the  $d_i^l$  coefficients are also constant for  $i$  large enough and the values of  $d_i^l$  are in a finite set: this will be useful to prove strict inequalities. Second,  $\lim_{|x| \rightarrow \infty} |T(x)| = \infty$ , which is one of the requirement to prove they are a diffeomorphism.

We also define Jacobian coefficients as:

$$J_{i_1, \dots, i_D} = \det(d_{i_1}^1, \dots, d_{i_D}^D),$$

where for all  $(i_1, \dots, i_D) \in (\mathbb{Z}^D)^D$ . The  $J_{i_1, \dots, i_D}$  are the coefficients of the B-spline expansion of the Jacobian  $J(x)$ . As B-splines have a compact support, this expansion can be made only on a subset  $E_D$  of  $(\mathbb{Z}^D)^D$  (see [22]). The expression of the active indexes sets  $E_D$  is given below: for a B-spline vector field of degree  $n$ , if we define the two integer intervals  $I^- = [-n, n-1]$  and  $I = [-n, n]$ ,  $E_D$  is the set of index D-tuples  $i_1, \dots, i_D \in \mathbb{Z}^{D \times D}$  such that for all  $(a, b) \in [1, D]^2$  with  $a \neq b$ :

$$i_b - i_a \in \prod_{k=1}^D I_k,$$

where

$$I_k = \begin{cases} I^- & \text{if } a = k \\ -I^- & \text{if } b = k \\ I & \text{otherwise.} \end{cases}$$

Therefore, in 2-dimensions, the set of active indexes is

$$E_2 = \{(i, j) \in \mathbb{Z}^2 \times \mathbb{Z}^2 \mid j - i \in I^- \times (-I^-)\}.$$

In 3-dimensions,  $E_3$  is the set of triples  $(i, j, k) \in \mathbb{Z}^3 \times \mathbb{Z}^3 \times \mathbb{Z}^3$  such that

$$\begin{cases} j - i & \in I^- & \times & (-I^-) & \times & I \\ k - i & \in I^- & \times & I & \times & (-I^-) \\ k - j & \in I & \times & I^- & \times & (-I^-) \end{cases}$$

In [22], we derived a sufficient condition involving only the B-spline Jacobian coefficients for the invertibility of the vector field  $T$  by bounding its Jacobian  $J(x) = \det(T'(x))$ . The continuous set of inequalities  $J(x) > 0$  has been replaced by a discrete set. When  $T$  is in  $\mathcal{B}_a^D$ , this set is finite.

**Theorem 2.2.** *Let  $T$  be a  $D$ -dimensional B-spline of degree  $n$  vector field and  $J$  its Jacobian, then, for all  $x$  the following expression holds:*

$$\min_{i_1, \dots, i_D \in E_D} J_{i_1, \dots, i_D} \leq J(x) \leq \max_{i_1, \dots, i_D \in E_D} J_{i_1, \dots, i_D}$$

*Proof.* See [22]. □

As discussed in [22], theorem 2.2 suffers from the curse of dimensionality and in practice, the cardinality of  $E_D$  restricts its use to 2-dimensional vector fields. In this work, we use this theorem to derive conditions for the invertibility of  $T$  in two or three dimensions. These conditions are computationally tractable while still allowing large deformations.

### 3. 2D DIFFEOMORPHIC B-SPLINE VECTOR FIELD CONDITION

**3.1. Cone.** To derive our new condition, we impose some constraints between neighboring node coefficients and prove that these constraints imply the strict positivity of the Jacobian function using the theorem 2.2.

As this theorem relies on sign of determinants, which are invariant to positive scaling, the neighborhood constraints should also be invariant to positive scaling and cones are the object of choice to ensure this property. In short, we will show that if the finite difference coefficients of neighboring nodes belong to the same cone, then the vector field is a diffeomorphism. To do so, we first define the circular cone.

**Definition 3.1.** If  $u \in \mathbb{R}^D \setminus \{0\}$  and  $\theta_u \in [0, \frac{\pi}{2}]$ , we denote by  $C_{u, \theta_u}$  the circular cone of axis  $u$  and semi-angle  $\theta_u$ :

$$C_{u, \theta_u} = \{x \in \mathbb{R}^D \mid x \neq 0 \text{ and } x^T u \geq |x| |u| \cos \theta_u\}.$$

Note that in our definition, the origin is excluded from the cone. We need also the following technical lemma.

**Lemma 3.2.** *Let  $(\theta_1, \theta_2) \in [0, \frac{\pi}{2}]^2$ , and  $u \in \mathbb{R}^D \setminus \{0\}$ , if  $x \in C_{u, \theta_1}$  and  $y \in C_{u, \theta_2}$  then*

$$x^T y \geq |x| |y| \cos(\theta_1 + \theta_2)$$

*Proof.* see appendix A. □

**3.2. The 2D Diffeomorphic B-spline Vector Field Condition.** If the group of invertible matrices with positive determinant is denoted as  $GL^+(D, \mathbb{R})$ , in two dimension, the new condition is given by the following theorem.

**Theorem 3.3.** *Let  $(\theta_1, \theta_2) \in [0, \frac{\pi}{2}]^2$  such that  $\theta_1 + \theta_2 < \frac{\pi}{2}$ . Let's consider  $T \in \mathcal{B}_a^2$   $(d_i^l)_{i,l}$  its finite difference coefficients and  $J$  its Jacobian. Let also  $(M_i)_i$  be a set of matrices in  $GL^+(D, \mathbb{R})$ . We define the two sets of indexes*

$$\begin{aligned} L^1 &= \{0\} \times I^- \\ L^2 &= I^- \times \{0\} \end{aligned}$$

and the matrix

$$R = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

If for all  $(a, l) \in \mathbb{Z}^2 \times \mathbb{Z}^2$ :

$$\begin{cases} l - a \in L^1 \implies M_a d_l^1 \in C_{M_a d_a^1, \theta_1} \\ l - a \in L^2 \implies R M_a d_l^2 \in C_{M_a d_a^2, \theta_2} \end{cases}$$

then for all  $x \in \mathbb{R}^2$ , we have

$$J(x) > 0.$$

*Proof.* We first note that

$$\forall x, \forall y \quad \det(x, y) = x^T R y.$$

Let's  $(i, j) \in E_2$ . If we define  $a = a(i, j) = (i^1, j^2) \in \mathbb{Z}^2$  then we have  $i - a \in L^1$  and  $j - a \in L^2$  which implies by hypothesis

$$M_a d_i^1 \in C_{M_a d_a^1, \theta_1}$$

and

$$R M_a d_j^2 \in C_{M_a d_a^2, \theta_2}.$$

But using lemma 3.2, this implies that

$$\begin{aligned} \det(d_i^1, d_j^2) &= \frac{\det(M_a d_i^1, M_a d_j^2)}{\det(M_a)}, \\ &= \frac{(M_a d_i^1)^T R M_a d_j^2}{\det(M_a)}, \\ &\geq \cos(\theta_1 + \theta_2) \frac{|M_a d_i^1| |M_a d_j^2|}{\det(M_a)}. \end{aligned}$$

Using theorem 2.2 and  $\theta_1 + \theta_2 < \frac{\pi}{2}$  we obtain:

$$\begin{aligned} J(x) &\geq \min_{i, j \in E_2} \det(d_i^1, d_j^2) \\ &\geq \cos(\theta_1 + \theta_2) \min_{i, j \in E_2} \frac{|M_a(i, j) d_i^1| |M_a(i, j) d_j^2|}{\det(M_a(i, j))} \\ &> 0. \end{aligned}$$

Note that as  $T$  is in  $\mathcal{B}_a^D$ , there is a finite number of different  $d_i^l$  and despite  $E_2$  is infinite, the min in the two lines above is indeed a minimum (and not only an infimum). This allows to deduce the *strict* positivity of the Jacobian.  $\square$

Instead of ensuring the positivity of  $J_{i, j}$  for  $(i, j) \in E_2$ , it is now sufficient to ensure some constraints on neighborhoods defined by  $L^1$  and  $L^2$ . The number of constraint per node is cut down from  $4n^2$  to  $4n$  and we will see that large deformations are still possible.

**3.3. Choosing the  $M_a$  matrices.** The sufficient condition in theorem 3.3 depends on a family of matrices in  $M_a \in GL^+(D, \mathbb{R})$ , where the index  $a$  corresponds to a node index. Each of these matrices defines a metric near the corresponding B-spline node that enables to enlarge the space of acceptable B-spline vector field compared to the trivial case (choosing  $M_a$  as the identity). For example, if used as an additional "slack" variable in an optimisation problem involving invertible B-spline vector fields, it is expected that the  $M_a$  will be chosen by the algorithm to make the condition as strong as possible, *i. e.* to enlarge the search space. An interesting possibility is to fix  $M_a$  as  $M_a = \mathbf{J}_a^{-1}$  where  $\mathbf{J}_a$  is the finite difference B-spline Jacobian matrix on the node  $a$ :  $\mathbf{J}_a = (d_a^1, d_a^2)$ . In this case, the additional condition  $\forall a, \det(\mathbf{J}_a) > 0$  is required. We will see in section 5 that with this choice the set of B-spline diffeomorphism satisfying the invertibility condition is much larger than with  $M_a = I_d$ . The expressions involved in the invertibility theorems

are also simplified. For example,  $M_a d_a^l = e_l$ , the  $l^{\text{th}}$  element of the canonical basis. The following corollary summarize this case.

**Corollary 3.4** (to theorem 3.3). Let  $(\theta_1, \theta_2) \in [0, \frac{\pi}{2}]^2$  such that  $\theta_1 + \theta_2 < \frac{\pi}{2}$ . Let's consider  $T \in \mathcal{B}_a^2$ ,  $(d_i^l)_{i \in \mathbb{Z}^2, l \in \{1,2\}}$  its finite difference coefficients and  $J$  its Jacobian.

If  $\forall a \in \mathbb{Z}^2$ ,  $\det(\mathbf{J}_a) > 0$  and for all  $(a, l) \in \mathbb{Z}^2 \times \mathbb{Z}^2$

$$\begin{cases} l - a \in L^1 & \implies \mathbf{J}_a^{-1} d_l^1 \in C_{e_1, \theta_1} \\ l - a \in L^2 & \implies R\mathbf{J}_a^{-1} d_l^2 \in C_{e_1, \theta_2} \end{cases}$$

then for all  $x \in \mathbb{R}^2$ , we have

$$J(x) > 0.$$

#### 4. 3D DIFFEOMORPHIC B-SPLINE VECTOR FIELD

In 3D, the problem is more involved. Indeed, the determinant is no longer bilinear but trilinear. As it can still be expressed using a dot product:  $\det(x, y, z) = (x \wedge y)^T z$ , the problem is now to find a tractable expression of the cross product of two cones in  $\mathbb{R}^3$ . This raises another question: what cone should we use? As opposed to the 2-dimensional case, cones can have different shapes in  $\mathbb{R}^3$ .

The question of the cross product of convex cones will be solved in section 4.1, in section 4.2, we will introduce  $p$ -cones, a family of cones with interesting properties for the cross product operator. More specifically, we are able to derive the analytical expression of the cross product of 1-cones under certain conditions. In sections 4.3 and 4.4, we propose two sets of conditions on the B-spline coefficients to guarantee that the vector field is invertible.

**4.1. The cross product of convex cones.** In this section, we will find a parameterization of the cross product of two convex cones. Instead of an implicit representation of the cross product of cones, we will find a three parameters explicit expression.

**Theorem 4.1.** *Let  $f : \mathbb{R}^3 \rightarrow \mathbb{R}$  be a real homogeneous function of degree 1, convex and continuous and the convex cone  $C_f = f^{-1}(\mathbb{R}^-) \setminus \{0\}$ , where  $\mathbb{R}^- = (-\infty, 0]$ . We assume it exists  $u \in \mathbb{R}^3$  such that  $C_f \subset \{x \in \mathbb{R}^3 | u^T x > 0\}$  and we define the directrix of  $C_f$  relative to  $u$  as the curve  $D_f = \{x \in \mathbb{R}^3 | f(x) = 0 \text{ and } u^T x = 1\}$ . Let  $g$  and  $v$  be a function and a vector sharing the same properties as  $f$  and  $u$  and let's define the set  $C_g$  and  $D_g$  accordingly.*

*If  $C_f \cap C_g = \emptyset$  and  $C_f \cap -C_g = \emptyset$  then*

$$C_f \wedge C_g = \mathbb{R}^{+*} D_f \wedge D_g.$$

*Proof.* The inclusion  $\mathbb{R}^{+*} D_f \wedge D_g \subset C_f \wedge C_g$  is trivial.

To prove the opposite inclusion, let's consider  $(a, b) \in C_f \times C_g$ . The function  $t \mapsto f((1-t)a + tb)$  is continuous and it takes the value  $f(a) \leq 0$  for  $t = 0$  and  $f(b) > 0$  for  $t = 1$ . So, using the intermediate value theorem, there exists  $t_a \in [0, 1[$  such that  $f(\tilde{a}) = 0$  with  $\tilde{a} = (1-t_a)a + t_a b$ . Note that as  $C_f \cap -C_g = \emptyset$ ,  $\tilde{a}$  cannot be null. Similarly, there exists  $t_b \in ]0, 1]$  such that  $\tilde{b} = (1-t_b)a + t_b b$  is not null and  $g(\tilde{b}) = 0$ .

As  $f(\tilde{a}) = 0$  and  $\tilde{a} \neq 0$  then  $\tilde{a} \in C_f$  and consequently  $a_1 = u^T \tilde{a}$  is strictly positive. Similarly,  $\tilde{b} \in C_g$  and  $b_1 = v^T \tilde{b}$  is also strictly positive.

We can compute the cross product of  $\tilde{a}$  and  $\tilde{b}$ :

$$\begin{aligned}\tilde{a} \wedge \tilde{b} &= [(1-t_a)a + t_ab] \wedge [(1-t_b)a + t_bb] \\ &= (t_b - t_a) a \wedge b.\end{aligned}$$

If  $t_b \leq t_a$ , then  $\tilde{b} \in [a, \tilde{a}]$  and as  $C_f$  is convex then  $\tilde{b} \in C_f \cap C_g = \emptyset$  so  $t_b - t_a > 0$ .

As a result, if we set  $\lambda = \frac{a_1 b_1}{t_b - t_a} > 0$ ,  $a' = \frac{\tilde{a}}{a_1} \in D_f$  and  $b' = \frac{\tilde{b}}{b_1} \in D_g$ , we have  $a \wedge b = \lambda a' \wedge b'$  which proves the second inclusion.  $\square$

This theorem provides a global parameterization of the cross product of two convex cones once their directrices are parameterized. The problem is now to find two functions  $x(\alpha)$  and  $y(\beta)$  to describe  $D_f$  and  $D_g$ . In this case, the points of  $C_f \wedge C_g$  are  $\lambda x(\alpha) \wedge y(\beta)$ .

**4.2.  $p$ -cones and their cross product.** In this section, we define and give some properties of the family of cones we will use in the remainder of the paper. These cones have interesting characteristics when it comes to the computation of their cross product.

**Definition 4.2** ( $p$ -cones). If  $U = (u_i)_i$  is an orthonormal basis of  $\mathbb{R}^D$ , we define the  $p$ -cone of semi-angle  $\theta_u \in [0, \frac{\pi}{2}[$  in the basis  $U$  by:

$$C_{U, \theta_u}^p = \left\{ x = \sum_{i=1}^D x_i u_i \mid x_1 > 0 \text{ and } \left( \sum_{i>1} |x_i|^p \right)^{\frac{1}{p}} \leq \tan(\theta_u) x_1 \right\}.$$

Its directrix relative to  $u_1$  is the curve defined as:

$$D_{U, \theta_u}^p = \left\{ x = u_1 + \sum_{i>1} x_i u_i \mid \left( \sum_{i>1} |x_i|^p \right)^{\frac{1}{p}} = \tan(\theta_u) \right\}.$$

Note that 2-cones are simply circular cone, they do not depend on the basis  $U$  but only on the direction of  $u_1$ :

$$C_{u, \theta_u} = C_{U, \theta_u}^2$$

where  $U = (u_i)_i$ ,  $u_1 = \frac{u}{|u|}$  and  $(u_i)_{i>1}$  is any basis of the orthogonal space of  $u \in \mathbb{R}^D \setminus \{0\}$ .

In the proposition below, a few useful properties of  $p$ -cones are given.

**Proposition 4.3** ( $p$ -cones properties). Let  $p \leq q$ . Let  $U = (u_i)_i$  and  $V = (v_i)_i$  be two orthonormal bases of  $\mathbb{R}^D$ ,  $(\theta_u, \theta_v) \in [0, \frac{\pi}{2}[^2$ ,  $\theta'_u = \arctan\left(\left((D-1)^{\frac{1}{p}-\frac{1}{q}} \tan(\theta_u)\right)\right)$  and let  $\theta_{uv} = \arccos\left(\frac{u_1^T v_1}{|u_1||v_1|}\right)$  be the angle between  $u_1$  and  $v_1$ . The following properties hold:

- (1) when  $p \geq 1$ ,  $C_{U, \theta_u}^p$  is convex.
- (2)  $C_{U, \theta_u}^q \subset C_{U, \theta'_u}^p$
- (3)  $C_{U, \theta_u}^p \subset C_{U, \theta_u}^q$
- (4) if  $p \leq 2$  and  $\theta_u + \theta_v < \theta_{uv}$  then  $C_{U, \theta_u}^p \cap C_{V, \theta_v}^p = \emptyset$
- (5) if  $p \leq 2$  and  $\theta_{uv} < \pi - (\theta_u + \theta_v)$  then  $C_{U, \theta_u}^p \cap -C_{V, \theta_v}^p = \emptyset$

*Proof.* see appendix B  $\square$

In  $\mathbb{R}^3$ , we can apply theorem 4.1 to parameterize the cross product of  $p$ -cones.

**Theorem 4.4.** *Let's  $(\theta_u, \theta_v) \in [0, \frac{\pi}{2}[$ ,  $p \in [1, 2]$ , let  $U = (u_i)_i$  and  $V = (v_i)_i$  be two orthonormal bases of  $\mathbb{R}^3$  and  $\theta_{uv} = \arccos\left(\frac{u_1^T v_1}{|u_1||v_1|}\right)$  be the angle between  $u_1$  and  $v_1$ .*

*If  $\theta_u + \theta_v < \theta_{uv} < \pi - (\theta_u + \theta_v)$  then the cross product of the two  $p$ -cones  $C_{U, \theta_u}^p$  and  $C_{V, \theta_v}^p$  can be parameterized by  $D_{U, \theta_u}^p$  and  $D_{V, \theta_v}^p$ , their directrices relative to  $u_1$  and  $v_1$ :*

$$C_{U, \theta_u}^p \wedge C_{V, \theta_v}^p = \mathbb{R}^{+*} D_{U, \theta_u}^p \wedge D_{V, \theta_v}^p$$

*Proof.* As  $\theta_u + \theta_v < \theta_{uv} < \pi - (\theta_u + \theta_v)$ , using the properties 4 and 5 of proposition 4.3, we have  $C_{U, \theta_u}^p \cap C_{V, \theta_v}^p = \emptyset$  and  $C_{U, \theta_u}^p \cap -C_{V, \theta_v}^p = \emptyset$ .

For  $x = \sum x_i u_i$ , we define  $f(x) = (\sum_{i>1} |x_i|^p)^{\frac{1}{p}} - \tan(\theta_u) x_1$ .  $f$  is a continuous real positive homogeneous function of degree 1. As  $p \geq 1$ , it is also convex. We have  $C_{U, \theta_u}^p = f^{-1}(\mathbb{R}^-) \setminus \{0\}$  and if  $x \in C_{U, \theta_u}^p$  then  $u_1^T x = x_1 > 0$ .

Defining similarly the  $g$  function for the  $C_{V, \theta_v}^p$   $p$ -cone, we apply theorem 4.1 and we have

$$C_{U, \theta_u}^p \wedge C_{V, \theta_v}^p = \mathbb{R}^{+*} D_{U, \theta_u}^p \wedge D_{V, \theta_v}^p.$$

□

The directrix of a  $p$ -cone can be easily parameterized using two functions  $c_p$  and  $s_p$  by:  $x(\alpha) = u_1 + \tan(\theta_u)(u_2 c_p(\alpha) + u_3 s_p(\alpha))$

For example, 2-cones can be parameterized using the functions  $c_2(t) = \cos(t)$  and  $s_2(t) = \sin(t)$  on  $[-\pi, \pi]$  and 1-cones can be parameterized using the two 4-periodic functions  $c_1$  and  $s_1$  defined on  $[-2, 2]$  by:

$$(4.1) \quad c_1(t) = 1 - |t|,$$

and

$$(4.2) \quad s_1(t) = \begin{cases} -2 - t & \text{if } t \in [-2, -1] \\ t & \text{if } t \in [-1, 1] \\ 2 - t & \text{if } t \in [1, 2], \end{cases}$$

Note that using these definitions, for  $p \in \{1, 2\}$  and for all  $t$  we have:  $c_p(t) \in [-1, 1]$  and  $s_p(t) \in [-1, 1]$ .

### 4.3. 3D Diffeomorphic B-spline Vector Field Condition with 1-cone.

4.3.1. *The cross product of 1-cones.* Results of the previous section enable the parameterization of the cross product of  $p$ -cones. However, we still need a more explicit representation. In a specific case, the cross product of 1-cones have a simple analytical expression. We first define, given two non zeros vectors, what we called their associated bases and then the expression of the cross product of 1-cones defined in these bases.

**Definition 4.5.** Let  $u \in \mathbb{R}^3$  and  $v \in \mathbb{R}^3$  be two linearly independent vectors, we define  $U$  and  $V$ , the two orthonormal bases associated to  $u$  and  $v$  by

$$U = (u_1, u_2, u_3) = \left( \frac{u}{|u|}, \frac{u \wedge v}{|u \wedge v|}, \frac{u \wedge (u \wedge v)}{|u||u \wedge v|} \right)$$

and

$$V = (v_1, v_2, v_3) = \left( \frac{v}{|v|}, \frac{u \wedge v}{|u \wedge v|}, \frac{v \wedge (u \wedge v)}{|v||u \wedge v|} \right).$$

**Lemma 4.6.** *Let  $(\theta_u, \theta_v) \in [0, \frac{\pi}{4}]^2$ , and  $u$  and  $v$  be two vectors in  $\mathbb{R}^3 \setminus \{0\}$  such that*

$$\theta_u + \theta_v < \theta_{uv} < \pi - (\theta_u + \theta_v).$$

where  $\theta_{uv} = \arccos\left(\frac{u^T v}{|u||v|}\right)$  is the angle between  $u$  and  $v$ . Let  $U$  and  $V$  be the orthonormal bases associated to  $u$  and  $v$ .

If we set  $c_{uv} = \cos \theta_{uv}$ ,  $s_{uv} = \sin \theta_{uv}$ ,  $t_u = \tan \theta_u$  and  $t_v = \tan \theta_v$ , and if we define the two positive numbers  $M_X$  and  $M_Y$  by

$$M_X = \max \left\{ \frac{t_v}{s_{uv}}, \frac{t_u t_v}{s_{uv}(s_{uv} - t_v |c_{uv}|)} \right\},$$

$$M_Y = \max \left\{ \frac{t_u}{s_{uv}}, \frac{t_u t_v}{s_{uv}(s_{uv} - t_u |c_{uv}|)} \right\}$$

and the cone  $B_{u,v,\theta_u,\theta_v}$  by

$$B_{u,v,\theta_u,\theta_v} = \{au_2 + bu_3 + cv_3 \mid a > 0 \text{ and } |b| \leq M_X a \text{ and } |c| \leq M_Y a\}$$

then, we have

$$C_{U,\theta_u}^1 \wedge C_{V,\theta_v}^1 \subset B_{u,v,\theta_u,\theta_v}.$$

If  $M_X = \frac{t_v}{s_{uv}}$  and  $M_Y = \frac{t_u}{s_{uv}}$  then

$$C_{U,\theta_u}^1 \wedge C_{V,\theta_v}^1 = B_{u,v,\theta_u,\theta_v}.$$

*Proof.* As  $\theta_u + \theta_v < \theta_{uv} < \pi - (\theta_u + \theta_v)$ , we can apply theorem 4.4 and we have

$$C_{U,\theta_u}^1 \wedge C_{V,\theta_v}^1 = \mathbb{R}^{+*} D_{U,\theta_u}^1 \wedge D_{V,\theta_v}^1.$$

Using the function  $c_1$  and  $s_1$  defined by the expressions 4.1 and 4.2, we parameterize the directrix  $D_{U,\theta_u}^1$  in the basis  $U$  with

$$x(\alpha) = u_1 + t_u (u_2 c_1(\alpha) + u_3 s_1(\alpha))$$

and  $D_{V,\theta_v}^1$  in the basis  $V$  with

$$y(\beta) = v_1 + t_v (v_2 c_1(\beta) + v_3 s_1(\beta))$$

and define the cross product

$$z(\alpha, \beta) = x(\alpha) \wedge y(\beta).$$

To derive an explicit expression of  $z(\alpha, \beta)$ , one can first remark that  $c_{uv} = \frac{u^T v}{|u||v|}$  and  $s_{uv} = \frac{|u \wedge v|}{|u||v|}$  and that using the double cross product formula, we have:

$$\begin{aligned} u_3 &= u \frac{(u^T v)}{|u||u \wedge v|} - v \frac{|u|^2}{|u||u \wedge v|} \\ &= u_1 \frac{c_{uv}}{s_{uv}} - v_1 \frac{1}{s_{uv}} \end{aligned}$$

and

$$\begin{aligned} v_3 &= u \frac{|v|^2}{|v||u \wedge v|} - v \frac{(u^T v)}{|v||u \wedge v|} \\ &= u_1 \frac{1}{s_{uv}} - v_1 \frac{c_{uv}}{s_{uv}} \end{aligned}$$

One can also notice that:

$$(4.3) \quad u_1^T v_1 = u_3^T v_3 = c_{uv}.$$

We now write the cross product of the vectors of the two bases  $U$  and  $V$ :

$$(4.4) \quad \begin{aligned} u_1 \wedge v_1 &= s_{uv}u_2 & u_2 \wedge v_1 &= -v_3 & u_3 \wedge v_1 &= c_{uv}u_2 \\ u_1 \wedge v_2 &= u_3 & u_2 \wedge v_2 &= 0 & u_3 \wedge v_2 &= -u_1 \\ u_1 \wedge v_3 &= -c_{uv}u_2 & u_2 \wedge v_3 &= v_1 & u_3 \wedge v_3 &= s_{uv}u_2 \end{aligned}$$

and express  $z$  in the (non orthonormal) basis  $(u_2, u_3, v_3)$ :

$$\begin{aligned} z(\alpha, \beta) &= x(\alpha) \wedge y(\beta) \\ &= z_{u_2}(\alpha, \beta)u_2 + z_{u_3}(\alpha, \beta)u_3 + z_{v_3}(\alpha, \beta)v_3 \\ &= (s_{uv} - t_v c_{uv} s_1(\beta) + t_u c_{uv} s_1(\alpha) + t_u t_v s_{uv} s_1(\alpha) s_1(\beta)) u_2 \\ &+ \left( t_u c_1(\beta) - t_u t_v \frac{1}{s_{uv}} c_1(\alpha) s_1(\beta) + t_u t_v \frac{c_{uv}}{s_{uv}} s_1(\alpha) c_1(\beta) \right) u_3 \\ &- \left( t_u c_1(\alpha) - t_u t_v \frac{c_{uv}}{s_{uv}} c_1(\alpha) s_1(\beta) + t_u t_v \frac{1}{s_{uv}} s_1(\alpha) c_1(\beta) \right) v_3 \end{aligned}$$

Let's prove now that for all  $\alpha$  and  $\beta$ ,  $z_{u_2}(\alpha, \beta)$  is strictly positive. We have:

$$\begin{aligned} z_{u_2}(\alpha, \beta) &= (s_{uv} - t_v c_{uv} s_1(\beta) + t_u c_{uv} s_1(\alpha) + t_u t_v s_{uv} s_1(\alpha) s_1(\beta)), \\ &\geq (s_{uv} - t_v |c_{uv}| - t_u |c_{uv}| - t_u t_v s_{uv}), \\ &= s_{uv} (1 - t_u t_v) \left( 1 - \frac{t_v + t_u |c_{uv}|}{1 - t_u t_v s_{uv}} \right), \\ &= s_{uv} (1 - t_u t_v) \left( 1 - \frac{|\cot(\theta_{uv})|}{\cot(\theta_u + \theta_v)} \right). \end{aligned}$$

As  $(\theta_u, \theta_v) \in [0, \frac{\pi}{4}]^2$ ,  $t_u$  and  $t_v$  are in  $[0, 1[$  and as  $\theta_u + \theta_v < \theta_{uv} < \pi - (\theta_u + \theta_v)$   $|\cot(\theta_{uv})| < \cot(\theta_u + \theta_v)$  and then  $\forall \alpha \forall \beta z_{u_2}(\alpha, \beta) > 0$

We can now define

$$\begin{aligned} X^{\theta_u, \theta_v}(\alpha, \beta) &= \frac{z_{u_3}(\alpha, \beta)}{z_{u_2}(\alpha, \beta)} \\ &= \frac{t_u c_1(\beta) - t_u t_v \frac{1}{s_{uv}} c_1(\alpha) s_1(\beta) + t_u t_v \frac{c_{uv}}{s_{uv}} s_1(\alpha) c_1(\beta)}{s_{uv} - t_v c_{uv} s_1(\beta) + t_u c_{uv} s_1(\alpha) + t_u t_v s_{uv} s_1(\alpha) s_1(\beta)} \end{aligned}$$

and

$$\begin{aligned} Y^{\theta_u, \theta_v}(\alpha, \beta) &= -\frac{z_{v_3}(\alpha, \beta)}{z_{u_2}(\alpha, \beta)} \\ &= \frac{t_u c_1(\alpha) - t_u t_v \frac{c_{uv}}{s_{uv}} c_1(\alpha) s_1(\beta) + t_u t_v \frac{1}{s_{uv}} s_1(\alpha) c_1(\beta)}{s_{uv} - t_v c_{uv} s_1(\beta) + t_u c_{uv} s_1(\alpha) + t_u t_v s_{uv} s_1(\alpha) s_1(\beta)}. \end{aligned}$$

As  $c_1$  is even and  $s_1$  is odd, one can first notice that

$$(4.5) \quad Y^{\theta_u, \theta_v}(\alpha, \beta) = X^{\theta_v, \theta_u}(-\beta, -\alpha)$$

and consequently, we can restrict our analysis to the study of  $X^{\theta_u, \theta_v}$ . To simplify the notation, we write  $X$  for  $X^{\theta_u, \theta_v}$  when there is no ambiguity.

As both  $c_1$  and  $s_1$  are 4-periodic, so is  $X$ : the analysis of  $X$  can be restricted to  $(\alpha, \beta) \in [-2, 2]^2$ . To find the extrema of the  $X$  function, let's define  $K = \{-2, -1, 0, 1\}$  and  $K_{i,j} = [i, i+1] \times [j, j+1]$ . As  $c_1$  and  $s_1$  are both piecewise affine, for  $(i, j) \in K^2$ ,  $X_{/K_{i,j}}$  is the ratio of two bilinear functions. The denominator being strictly positive,  $X_{/K_{i,j}}(\alpha, \cdot)$  and  $X_{/K_{i,j}}(\cdot, \beta)$  have no pole and are both monotonic

on  $[i, i + 1]$  and  $[j, j + 1]$ . Consequently, the extrema of  $X_{/K_{i,j}}$  are on the corners of  $K_{i,j}$  and

$$\max_{(\alpha,\beta) \in [-2,2]^2} X(\alpha, \beta) = \max_{(i,j) \in K^2} \max_{(\alpha,\beta) \in K_{i,j}} X(\alpha, \beta) = \max_{(i,j) \in K^2} X(i, j).$$

We can compute the values of  $X(i, j)$  for  $(i, j) \in K^2$  (again, the 4-periodicity of  $X$  allows to avoid computing  $X(., 2)$  and  $X(2, .)$ ):

	$X(., -2)$	$X(., -1)$	$X(., 0)$	$X(., 1)$
$X(-2, .)$	$-\frac{t_v}{s_{uv}}$	$-\frac{t_u t_v \frac{1}{s_{uv}}}{s_{uv} + t_v c_{uv}}$	$\frac{t_v}{s_{uv}}$	$+\frac{t_u t_v \frac{1}{s_{uv}}}{s_{uv} - t_v c_{uv}}$
$X(-1, .)$	$-\frac{t_v}{s_{uv}}$	0	$\frac{t_v}{s_{uv}}$	0
$X(0, .)$	$-\frac{t_v}{s_{uv}}$	$+\frac{t_u t_v \frac{1}{s_{uv}}}{s_{uv} + t_v c_{uv}}$	$\frac{t_v}{s_{uv}}$	$-\frac{t_u t_v \frac{1}{s_{uv}}}{s_{uv} - t_v c_{uv}}$
$X(1, .)$	$-\frac{t_v}{s_{uv}}$	0	$\frac{t_v}{s_{uv}}$	0

As  $t_u > 0$ ,  $t_v > 0$  and the denominator is always strictly positive, the sign of the values of  $X(i, j)$  can be easily deduced. When  $X(i, j)$  is strictly positive, it takes its values in the set:

$$\left\{ \frac{t_u t_v}{s_{uv}(s_{uv} - t_v c_{uv})}, \frac{t_v}{s_{uv}}, \frac{t_u t_v}{s_{uv}(s_{uv} + t_v c_{uv})} \right\}$$

So if  $M_X = \max \left\{ \frac{t_v}{s_{uv}}, \frac{t_u t_v}{s_{uv}(s_{uv} - t_v |c_{uv}|)} \right\}$ , we have

$$\max_{(\alpha,\beta) \in [-2,2]^2} X(\alpha, \beta) = M_X,$$

and similarly, we prove that

$$\min_{(\alpha,\beta) \in [-2,2]^2} X(\alpha, \beta) = -M_X.$$

Using the equation 4.5, we also prove that

$$\max_{(\alpha,\beta) \in [-2,2]^2} Y(\alpha, \beta) = M_Y$$

and

$$\min_{(\alpha,\beta) \in [-2,2]^2} Y(\alpha, \beta) = -M_Y,$$

with  $M_Y = \max \left\{ \frac{t_u}{s_{uv}}, \frac{t_u t_v}{s_{uv}(s_{uv} - t_u |c_{uv}|)} \right\}$ .

We can conclude that

$$C_{U,\theta_u}^1 \wedge C_{V,\theta_v}^1 \subset B_{u,v,\theta_u,\theta_v}.$$

Let's now make the additional assumption that  $M_X = \frac{t_v}{s_{uv}}$  and  $M_Y = \frac{t_u}{s_{uv}}$ . In this case, one can notice that for all  $\alpha$ :

$$X(\alpha, 0) = \frac{t_v}{s_{uv}} = M_X$$

and

$$X(\alpha, 2) = -\frac{t_v}{s_{uv}} = -M_X$$

Using the equation 4.5, we also prove that  $Y(0, \beta) = M_Y$  and  $Y(2, \beta) = -M_Y$ . With these results on the  $[0, 2]^2$  square border, the Poincaré-Miranda theorem can be use to prove that for all  $(x, y) \in [-M_X, M_X] \times [-M_Y, M_Y]$ , there exists  $(\alpha, \beta) \in [0, 2]^2$  such that  $X(\alpha, \beta) = x$  and  $Y(\alpha, \beta) = y$  and consequently, when  $M_X = \frac{t_v}{s_{uv}}$  and  $M_Y = \frac{t_u}{s_{uv}}$ , we have  $C_{U, \theta_u}^1 \wedge C_{V, \theta_v}^1 = B_{u, v, \theta_u, \theta_v}$ .  $\square$

Once we know  $B_{u, v, \theta_u, \theta_v}$ , the cross product of two 1-cones, we need to find the vectors having a positive dot product with all the elements of  $B_{u, v, \theta_u, \theta_v}$ . This is by definition the dual cone of  $B_{u, v, \theta_u, \theta_v}$  and its expression is given below.

**Lemma 4.7.** *Let  $u, v, \theta_u, \theta_v, M_X$  and  $M_Y$  defined as in lemma 4.6, the dual cone of  $B_{u, v, \theta_u, \theta_v}$  is given by*

$$B_{u, v, \theta_u, \theta_v}^+ = \{z \mid z^T(u_2 \pm M_X u_3 \pm M_Y v_3) \geq 0\}$$

*Proof.*  $B_{u, v, \theta_u, \theta_v}$  is a polyhedral cone with its four edges generated by  $u_2 \pm M_X u_3 \pm M_Y v_3$ . Its dual cone is given by the vectors  $z$  such that the scalar products between  $z$  and the four edges are positives.  $\square$

4.3.2. *The  $\theta_u = \theta_v$  case.* When  $\theta_u = \theta_v$ , the different mathematical expressions involved can be considerably simplified.

**Proposition 4.8.** For  $\theta_u = \theta_v \in [0, \frac{\pi}{4}[$ , we have

$$M_X = M_Y = \frac{t_u}{s_{uv}}.$$

*Proof.* see appendix C.  $\square$

4.3.3. *3 Dimensional Diffeomorphic Condition with 1-cone.* In 3-dimension, according to theorem 2.2, diffeomorphicity can be obtained by ensuring the positivity of the Jacobian coefficients  $J_{i, j, k}$  for  $(i, j, k) \in E_3$ . We will see in the theorem below that the positivity condition of  $J_{i, j, k}$  on  $E_3$  can be replaced by constraints between each node and its neighbors. The neighborhoods in question are defined by the three squares  $P^1, P^2$  and  $P^3$ :

$$\begin{aligned} P^1 &= \{0\} \times I^- \times I^- \\ P^2 &= I^- \times \{0\} \times I^- \\ P^3 &= I^- \times I^- \times \{0\} \end{aligned}$$

**Theorem 4.9.** *Let  $T \in \mathcal{B}_a^3, (d_i^l)_{i, l}$  its finite difference coefficients and  $J$  its Jacobian.*

*Let  $(\theta_1, \theta_2) \in [0, \frac{\pi}{4}]^2, (M_a)_{a \in \mathbb{Z}^3}$  a set of matrices in  $GL^+(D, \mathbb{R})$  and let  $U_a$  and  $V_a$  be the bases associated with  $M_a d_a^1$  and  $M_a d_a^2$  according to definition 4.5.*

*If  $\forall a \in \mathbb{Z}^3,$*

$$\theta_1 + \theta_2 < \theta_{M_a d_a^1, M_a d_a^2} < \pi - (\theta_1 + \theta_2)$$

*and  $\forall (a, l) \in \mathbb{Z}^3 \times \mathbb{Z}^3$*

$$\begin{cases} l - a \in P^1 & \implies M_a d_l^1 \in C_{U_a, \theta_1}^1 \\ l - a \in P^2 & \implies M_a d_l^2 \in C_{V_a, \theta_2}^1 \\ l - a \in P^3 & \implies M_a d_l^3 \in B_{M_a d_a^1, M_a d_a^2, \theta_1, \theta_2}^+ \end{cases}$$

where  $\mathring{B}_{M_a d_a^1, M_a d_a^2, \theta_1, \theta_2}^+$  is the interior of the dual cone of  $B_{M_a d_a^1, M_a d_a^2, \theta_1, \theta_2}$  then for all  $x \in \mathbb{R}^3$

$$J(x) > 0.$$

*Proof.* Let  $(i, j, k) \in E_3$ . If we define  $a = (i^1, j^2, k^3) \in \mathbb{Z}^3$  then we have  $i - a \in P^1$ ,  $j - a \in P^2$  and  $k - a \in P^3$ . Consequently, we have  $M_a d_i^1 \in C_{U_a, \theta_1}^1$ ,  $M_a d_j^2 \in C_{V_a, \theta_2}^1$  and  $M_a d_k^3 \in \mathring{B}_{M_a d_a^1, M_a d_a^2, \theta_1, \theta_2}^+$ .

But using lemma 4.6,  $M_a d_i^1 \wedge M_a d_j^2 \in B_{M_a d_a^1, M_a d_a^2, \theta_1, \theta_2}$  and as  $M_a d_k^3 \in \mathring{B}_{M_a d_a^1, M_a d_a^2, \theta_1, \theta_2}^+$ , lemma 4.7 implies

$$\begin{aligned} \det(d_i^1, d_j^2, d_k^3) &= \frac{\det(M_a d_i^1, M_a d_j^2, M_a d_k^3)}{\det(M_a)}, \\ &= \frac{(M_a d_i^1 \wedge M_a d_j^2)^T M_a d_k^3}{\det(M_a)}, \\ &> 0. \end{aligned}$$

Using theorem 2.2, we have  $\forall x \in \mathbb{R}^3$ :

$$\begin{aligned} J(x) &\geq \min_{i,j,k \in E_3} \det(d_i^1, d_j^2, d_k^3) \\ &> 0. \end{aligned}$$

As  $T$  is in  $\mathcal{B}_a^D$ , there is a finite number of different  $d_i^l$  and despite  $E_3$  is infinite, the min in the lines above is indeed a minimum (and not only an infimum). This allows to deduce the *strict* positivity of the Jacobian.  $\square$

**4.4. 3D Diffeomorphic B-spline Vector Field Condition with 2-cone.** In this section, we derive a set of conditions valid for 2-cones. 2-cones have the advantages over others  $p$ -cones that they can be defined using a single smooth inequality constraint and are symmetric about their axis. These properties can be useful when the conditions are used within a numerical algorithm.

In the following lemma, we will find a circular cone enclosing the  $B_{u,v,\theta_u,\theta_v}$  cone.

**Lemma 4.10.** *Let  $u$  and  $v$  be two vectors of  $\mathbb{R}^3 \setminus \{0\}$  and  $(\theta_u, \theta_v) \in [0, \frac{\pi}{4}]^2$  where  $\theta_{uv} = \arccos\left(\frac{u^T v}{|u||v|}\right)$  such that  $\theta_u + \theta_v < \theta_{uv} < \pi - (\theta_u + \theta_v)$ . Let also  $M_X$  and  $M_Y$  be defined as in lemma 4.6. We have:*

$$B_{u,v,\theta_u,\theta_v} \subset C_{u \wedge v, \bar{\theta}_{uv}}$$

with

$$\begin{aligned} \bar{\theta}_{uv} &= \bar{\theta}(\theta_u, \theta_v, \theta_{uv}) \\ &= \arctan\left(\sqrt{M_X^2 + M_Y^2 + 2M_X M_Y |c_{uv}|}\right). \end{aligned}$$

*Proof.* see appendix D.  $\square$

4.4.1. *The cross product of circular cones.*

**Proposition 4.11.** Let  $(\theta_u, \theta_v) \in [0, \frac{\pi}{4}]^2$ ,  $\theta'_u = \arctan(\sqrt{2} \tan \theta_u)$ ,  $\theta'_v = \arctan(\sqrt{2} \tan \theta_v)$  and let  $u$  and  $v$  be two non zero vectors such that

$$\theta'_u + \theta'_v < \theta_{uv} < \pi - (\theta'_u + \theta'_v).$$

where  $\theta_{uv} = \arccos\left(\frac{u^T v}{|u||v|}\right)$  is the angle between  $u$  and  $v$ .

If we set  $\bar{\theta}'_{uv} = \bar{\theta}(\theta'_u, \theta'_v, \theta_{uv})$ , we have

$$C_{u, \theta_u} \wedge C_{v, \theta_v} \subset C_{u \wedge v, \bar{\theta}'_{uv}}.$$

*Proof.* Let's define the basis  $U = (u_1, u_2, u_3)$  and  $V = (v_1, v_2, v_3)$  as in the hypothesis of the lemma 4.6. Using property 2 of proposition 4.3, the circular cone can be bounded:  $C_{u, \theta_u} = C_{U, \theta_u}^2 \subset C_{U, \theta'_u}^1$  and  $C_{v, \theta_v} = C_{V, \theta_v}^2 \subset C_{V, \theta'_v}^1$ .

As  $\theta'_u + \theta'_v < \theta_{uv} < \pi - (\theta'_u + \theta'_v)$ , lemma 4.6 can be applied:

$$C_{U, \theta'_u}^1 \wedge C_{V, \theta'_v}^1 \subset B_{u, v, \theta'_u, \theta'_v}.$$

Using lemma 4.10, we have

$$C_{u, \theta_u} \wedge C_{v, \theta_v} \subset B_{u, v, \theta'_u, \theta'_v} \subset C_{u \wedge v, \bar{\theta}'_{uv}}.$$

□

4.4.2.  $\bar{\theta}$  extrema. The range of  $\bar{\theta}$  is important for the practical use of our condition. It is given by the following proposition.

**Proposition 4.12** ( $\bar{\theta}$  extrema). Let  $(\theta_u, \theta_v) \in [0, \frac{\pi}{4}[^2$  then the function  $\bar{\theta}(\theta_u, \theta_v, \cdot)$  is decreasing on  $] \theta_u + \theta_v, \frac{\pi}{2} ]$  and increasing on  $[\frac{\pi}{2}, \pi - (\theta_u + \theta_v) [$ .

*Proof.* see appendix E

□

The extrema of  $\bar{\theta}$  can be deduced from the last proposition:

$$(4.6) \quad \min_{\theta_{uv} \in ] \theta_u + \theta_v, \pi - (\theta_u + \theta_v) [} \bar{\theta}(\theta_u, \theta_v, \theta_{uv}) = \bar{\theta}\left(\theta_u, \theta_v, \frac{\pi}{2}\right)$$

$$(4.7) \quad = \arctan\left(\sqrt{\tan^2 \theta_u + \tan^2 \theta_v}\right)$$

and

$$\sup_{\theta_{uv} \in ] \theta_u + \theta_v, \pi - (\theta_u + \theta_v) [} \bar{\theta}(\theta_u, \theta_v, \theta_{uv}) = \bar{\theta}(\theta_u, \theta_v, \theta_u + \theta_v).$$

4.4.3. *The  $\theta_u = \theta_v$  case.* When  $\theta_u = \theta_v$ , the different mathematical expressions involved can be simplified. These expressions are given in the following proposition.

**Proposition 4.13.** For  $\theta_u \in [0, \frac{\pi}{4}[$  We have

$$\begin{aligned} \bar{\theta}_{uv} &= \bar{\theta}(\theta_u, \theta_u, \theta_{uv}) \\ &= \arctan\left(\frac{\sqrt{2}t_u}{\sqrt{1 - |c_{uv}|}}\right). \end{aligned}$$

*Proof.* see appendix F.

□

These expressions allow us for example to compute the extrema of the  $\bar{\theta}$  function.

**Corollary 4.14** ( $\bar{\theta}$  extrema). For  $\theta \in [0, \frac{\pi}{4}[$ , we have

$$\min_{2\theta < t < \pi - 2\theta} \bar{\theta}(\theta, \theta, t) = \bar{\theta}\left(\theta, \theta, \frac{\pi}{2}\right) = \arctan\left(\sqrt{2} \tan \theta\right)$$

and

$$\sup_{2\theta < t < \pi - 2\theta} \bar{\theta}(\theta, \theta, t) = \bar{\theta}(\theta, \theta, 2\theta) = \arctan\left(\frac{\tan \theta}{\cos \theta}\right).$$

*Proof.* These expressions are given by a direct application of propositions 4.12 and 4.13 and by using that  $1 - \cos(2\theta) = 2 \cos^2(\theta)$ .

□

4.4.4. *3D Diffeomorphic B-spline Vector Field Condition with 2-cone.* The following theorem is the 2-cone counterpart of theorem 4.9. It shows that, under conditions, if neighbors node finite difference coefficients belong to the same circular cone, invertibility can be guaranteed.

**Theorem 4.15.** *Let  $(\theta_1, \theta_2) \in [0, \frac{\pi}{4}]^2$ ,  $\theta_3 \in [0, \frac{\pi}{2} - \arctan(\sqrt{2}\sqrt{\tan^2 \theta_1 + \tan^2 \theta_2})]$ , and let's define the angles  $\theta'_i = \arctan(\sqrt{2}\tan(\theta_i))$ . Let  $T \in \mathcal{B}_a^3$ ,  $(d_i^l)_{i \in \mathbb{Z}^3, l \in \{1,2,3\}}$  its finite difference coefficients and  $J$  its Jacobian. We also consider  $(M_i)_{i \in \mathbb{Z}^3}$ , a set of matrices in  $GL^+(D, \mathbb{R})$ .*

*If for all index  $(a, l) \in \mathbb{Z}^3 \times \mathbb{Z}^3$ , we have*

$$\begin{cases} l - a \in P^1 & \implies M_a d_l^1 \in C_{M_a d_a^1, \theta_1} \\ l - a \in P^2 & \implies M_a d_l^2 \in C_{M_a d_a^2, \theta_2} \\ l - a \in P^3 & \implies M_a d_l^3 \in C_{M_a d_a^1 \wedge M_a d_a^2, \theta_3} \end{cases}$$

*and if for all  $a \in \mathbb{Z}^3$*

$$\theta'_1 + \theta'_2 < \theta_{M_a d_a^1, M_a d_a^2} < \pi - (\theta'_1 + \theta'_2)$$

*and*

$$\bar{\theta}(\theta'_1, \theta'_2, \theta_{M_a d_a^1, M_a d_a^2}) < \frac{\pi}{2} - \theta_3$$

*then for all  $x \in \mathbb{R}^3$*

$$J(x) > 0.$$

*Proof.* Let  $(i, j, k) \in E_3$ . If we define  $a = (i^1, j^2, k^3)\mathbb{Z}^3$  then we have  $i - a \in P^1$ ,  $j - a \in P^2$  and  $k - a \in P^3$ . Consequently, we have

$$\begin{aligned} M_a d_i^1 &\in C_{M_a d_a^1, \theta_1}, \\ M_a d_j^2 &\in C_{M_a d_a^2, \theta_2}, \\ M_a d_k^3 &\in C_{M_a d_a^1 \wedge M_a d_a^2, \theta_3} \end{aligned}$$

By using proposition 4.11, if we set  $\phi_a = \bar{\theta}(\theta'_1, \theta'_2, \theta_{M_a d_a^1, M_a d_a^2})$  we have

$$M_a d_i^1 \wedge M_a d_j^2 \in C_{M_a d_a^1, \theta_1} \wedge C_{M_a d_a^2, \theta_2} \subset C_{M_a d_a^1 \wedge M_a d_a^2, \phi_a}$$

and  $J_{i,j,k}$  can be bounded below:

$$\begin{aligned} \det(d_i^1, d_j^2, d_k^3) &= \frac{\det(M_a d_i^1, M_a d_j^2, M_a d_k^3)}{\det(M_a)}, \\ &= \frac{(M_a d_i^1 \wedge M_a d_j^2)^T M_a d_k^3}{\det(M_a)}, \\ &\geq \cos(\phi_a + \theta_3) \frac{|M_a d_i^1 \wedge M_a d_j^2| |M_a d_k^3|}{\det(M_a)}, \\ &> 0 \end{aligned}$$

where lemma 3.2 was used on the third line. Consequently, using theorem 2.2, one can deduce that  $\forall x \in \mathbb{R}^3$ :

$$\begin{aligned} J(x) &\geq \min_{i,j,k \in E_3} \det(d_i^1, d_j^2, d_k^3) \\ &> 0 \end{aligned}$$

As  $T$  is in  $\mathcal{B}_a^D$ , there is a finite number of different  $d_i^l$  and despite  $E_3$  is infinite, the min in the lines above is indeed a minimum (and not only an infimum). This allows to deduce the *strict* positivity of the Jacobian.  $\square$

The condition  $\theta_3 \in \left[0, \frac{\pi}{2} - \arctan\left(\sqrt{2}\sqrt{\tan^2\theta_1 + \tan^2\theta_2}\right)\right]$  is an admissibility condition for the values of the  $\theta_i$ . Indeed, to be able to find coefficients satisfying the condition

$$\bar{\theta}(\theta'_1, \theta'_2, \theta_{M_a d_a^1, M_a d_a^2}) < \frac{\pi}{2} - \theta_3$$

of the hypothesis,  $\theta_3$  should be chosen at least such that

$$\min_{\theta} \bar{\theta}(\theta'_1, \theta'_2, \theta) = \arctan\left(\sqrt{2}\sqrt{\tan^2(\theta_1) + \tan^2(\theta_2)}\right) < \frac{\pi}{2} - \theta_3.$$

The three angles  $\theta_1$ ,  $\theta_2$  and  $\theta_3$  enable to control the degree of regularization in a direction or another. When there is no known anisotropy in the problem the B-spline vector field is involved in, the three  $\theta_i$  should be equal. The value of the angle should in this case be strictly lower than  $\theta^{\max}$ , defined as the solution of the equation:

$$\theta^{\max} = \frac{\pi}{2} - \arctan\left(\sqrt{2}\sqrt{2\tan^2\theta^{\max}}\right),$$

which is given by  $\theta^{\max} = \arctan\left(\frac{1}{\sqrt{2}}\right)$ .

**4.5. Choosing the  $M_a$  matrices.** Similarly to the 2D case presented in section 3.3, the matrices  $M_a$  can be let as free variables or fixed. If they are fixed, we will consider the possibility to choose them all equal to the 3D identity matrix or as  $M_a = \mathbf{J}_a^{-1}$  where  $\mathbf{J}_a = (d_a^1, d_a^2, d_a^3)$ . As we will see in section 5, choosing  $M_a = \mathbf{J}_a^{-1}$  the set of B-spline diffeomorphisms satisfying the invertibility condition is much larger than  $M_a = I_d$ . Furthermore, as  $M_a d_a^l = e_l$ , the  $l^{\text{th}}$  element of the canonical basis, the angle between  $M_a d_a^1$  and  $M_a d_a^2$  is constant and equal to  $\frac{\pi}{2}$  and consequently, the angular conditions can be removed from theorems 4.9 and 4.15 hypothesis. One can also note that the bases associated with  $M_a d_a^1$  and  $M_a d_a^2$  are constant and composed of vectors of the canonical basis. Regarding lemma 4.6, one can remark that  $M_X = t_v$  and  $M_Y = t_u$  and consequently that we are in the equality case of the lemma: lemma 4.6 gives the exact expression of two cones cross products.

The case  $M_a = \mathbf{J}_a^{-1}$  is given by the following corollaries.

**Corollary 4.16** (to theorem 4.9). Let  $T \in \mathcal{B}_a^3$ ,  $(d_i^l)_{i \in \mathbb{Z}^3, l \in \{1,2,3\}}$  its finite difference coefficients and  $J$  its Jacobian.

Let  $(\theta_1, \theta_2) \in \left[0, \frac{\pi}{4}\right]^2$ ,  $U = (e_1, e_3, -e_2)$  and  $V = (e_2, e_3, e_1)$  be the basis associated with  $e_1$  and  $e_2$  and  $\mathring{B}^+ = \{z = \sum_i z_i e_i \mid z_3 > \max(t_u |z_1|, t_v |z_2|)\}$ .

If  $\forall a \in \mathbb{Z}^3$ ,  $\det(\mathbf{J}_a) > 0$  and for all  $(a, l) \in \mathbb{Z}^3 \times \mathbb{Z}^3$

$$\begin{cases} l - a \in P^1 & \implies \mathbf{J}_a^{-1} d_l^1 \in C_{U, \theta_1}^1 \\ l - a \in P^2 & \implies \mathbf{J}_a^{-1} d_l^2 \in C_{V, \theta_2}^1 \\ l - a \in P^3 & \implies \mathbf{J}_a^{-1} d_l^3 \in \mathring{B}^+ \end{cases}$$

then for all  $x \in \mathbb{R}^3$

$$J(x) > 0.$$

**Corollary 4.17** (to theorem 4.15). Let  $(\theta_1, \theta_2) \in \left[0, \frac{\pi}{4}\right]^2$  and the angle  $\theta_3 \in \left[0, \frac{\pi}{2} - \arctan\left(\sqrt{2}\sqrt{\tan^2\theta_1 + \tan^2\theta_2}\right)\right]$  such that

$$\arctan\left(\sqrt{2}\tan(\theta_1)\right) + \arctan\left(\sqrt{2}\tan(\theta_2)\right) < \frac{\pi}{2}.$$

Let  $T \in \mathcal{B}_a^3$ ,  $(d_i^l)_{i,l}$  its finite difference coefficients and  $J$  its Jacobian.

If  $\forall a \in \mathbb{Z}^3$ ,  $\det(\mathbf{J}_a) > 0$  and for all  $(a, l) \in \mathbb{Z}^3 \times \mathbb{Z}^3$

$$\begin{cases} l - a \in P^1 & \implies \mathbf{J}_a^{-1} d_l^1 \in C_{e_1, \theta_1} \\ l - a \in P^2 & \implies \mathbf{J}_a^{-1} d_l^2 \in C_{e_2, \theta_2} \\ l - a \in P^3 & \implies \mathbf{J}_a^{-1} d_l^3 \in C_{e_3, \theta_3} \end{cases}$$

then for all  $x \in \mathbb{R}^3$

$$J(x) > 0.$$

### 5. ANALYSIS OF THE CONDITIONS

Choi, Lee [8]	Kim, Chun, Fessler [13, 9]	Sdika [22]	New	
			$I_d$	$\mathbf{J}_a^{-1}$
$A \simeq I_d, b \simeq 0$	$A \simeq I_d$	$\det(A) > 0$	$A \simeq Q\Lambda$	$\det(A) > 0$

TABLE 1. Restrictions when the transformation is the affine transform  $T(x) = Ax + b$ .  $Q$  is a rotation matrix,  $\Lambda$  is a diagonal matrix with strictly positive diagonal coefficients.

As in [22], we will use affine transforms to compare the sharpness of our condition to the state of the art. As it does not investigate nonlinear transforms, this criterion is not fully satisfying. However, the analysis using affine transforms is still interesting. First, affine transforms can be exactly represented by B-splines:

$$Ax + b = \sum_i c_i \beta \left( \frac{x}{h} - i \right)$$

when the B-spline coefficients are  $c_i = A(hi) + b$ . Finite difference coefficients in the direction  $l$  are  $d_i^l = \frac{c_i - c_{i-e_l}}{h_l} = Ae_l = A_l$ , the  $l^{\text{th}}$  column vector of the matrix  $A$ . The other reason is that, as B-splines have a local support, our analysis also provides an insight on the local behavior allowed for more general nonlinear transforms. The results of this section are summarized in the table 1.

In the literature, three other sufficient conditions have been proposed.

In [8], Choi and Lee proposed to bound the displacement coefficients:

$$|c_i^l - i_l h_l| < \frac{h_l}{K},$$

where  $K$  is a given constant. This condition constrains  $A$  to be close to the identity and  $b$  to be very small.

In [13, 9], Kim, Chun and Fessler guaranteed the invertibility by keeping the finite differences coefficients close to the canonical basis:

$$\|d_i^l - e_l\|_\infty < K,$$

where  $K = \frac{1}{D}$ . When applied to the affine transform  $Ax + b$ , the condition becomes

$$\|(A - I)e_l\|_\infty < K.$$

All translations are now accepted, however,  $A$  must be close enough to the identity.

In [22], the invertibility is guaranteed by keeping the Jacobian coefficients positive:

$$J_{i_1, \dots, i_D} > 0.$$

When applied to  $Ax + b$ , this last condition simply becomes  $\det(A) > 0$  and is satisfied by all the affine transforms of interest. While this last condition is sharp within the affine transform subspace, it has a very high complexity.

The conditions proposed in this work are studied below. We will differentiate the cases  $M_a = I_a$  from the case  $M_a = \mathbf{J}_a^{-1}$ .

### 5.1. Case $M_a = I_a$ .

5.1.1. *Analysis of the 2D conditions.* According to theorem 3.3, a 2-dimensional B-spline vector field  $T(x) = Ax + b$  is a diffeomorphism when for given  $\theta_1 + \theta_2 < \frac{\pi}{2}$ :

$$\begin{aligned} A_1 &\in C_{A_1, \theta_1} \\ RA_2 &\in C_{A_1, \theta_2} \end{aligned}$$

and one can see that the first condition is always true when  $A_1 \neq 0$ . The second condition can be expressed as

$$\det(A) \geq |A_1| |A_2| \cos \theta_2$$

or

$$\left| \theta_{A_1, A_2} - \frac{\pi}{2} \right| \leq \theta_2.$$

The two column vectors of the matrix  $A$  should be sufficiently orthogonal. One can remark that if  $T(x) = Q\Lambda x + b$  with  $Q$  a rotation and  $\Lambda$  a diagonal matrix with strictly positive diagonal coefficients, it always satisfies the hypothesis of theorem 3.3.

5.1.2. *Analysis of the 3D condition with 1-cones.*  $T(x) = Ax + b$  satisfies the hypothesis of the theorem 4.9 when:

$$(5.1) \quad A_1 \in C_{U_a, \theta_1}^1$$

$$(5.2) \quad A_2 \in C_{V_a, \theta_2}^1$$

$$(5.3) \quad A_3 \in \dot{B}_{A_1, A_2, \theta_1, \theta_2}^+$$

$$(5.4) \quad \theta_1 + \theta_2 < \theta_{A_1, A_2} < \pi - (\theta_1 + \theta_2)$$

The conditions 5.1 and 5.2 are always true when  $A_1 \neq 0$  and  $A_2 \neq 0$ . The two other conditions constrain  $A_1$  and  $A_2$  to be sufficiently orthogonal and  $A_3$  to be sufficiently collinear to  $A_1 \wedge A_2$ . In words, the matrix  $A$  should be sufficiently invertible. As in the 2D case, transforms of the type  $T(x) = Q\Lambda x + b$  satisfy the conditions.

5.1.3. *Analysis of the 3D condition with 2-cones.* When  $T(x) = Ax + b$ , the conditions of theorem 4.15 become:

$$(5.5) \quad A_1 \in C_{A_1, \theta_1}$$

$$(5.6) \quad A_2 \in C_{A_2, \theta_2}$$

$$(5.7) \quad A_3 \in C_{A_1 \wedge A_2, \theta_3}$$

$$(5.8) \quad \theta'_1 + \theta'_2 < \theta_{A_1 A_2} < \pi - (\theta'_1 + \theta'_2)$$

$$(5.9) \quad \bar{\theta}(\theta'_1, \theta'_2, \theta_{A_1, A_2}) < \frac{\pi}{2} - \theta_3.$$

Conditions 5.5 and 5.6 are both always true when  $A_1 \neq 0$  and  $A_2 \neq 0$ . Conditions 5.8 and 5.9 enforce the linear independence of  $A_1$  and  $A_2$ . The condition 5.7 ensures that  $A_3$  is sufficiently orthogonal to  $A_1$  and  $A_2$ .

5.2. **Case  $M_a = \mathbf{J}_a^{-1} = A^{-1}$ .** When  $M_a = \mathbf{J}_a^{-1}$ , we have  $M_a A_l = e_l$ , the  $l^{\text{th}}$  element of the canonical basis. This makes almost all the hypothesis of the corollaries 3.4, 4.16 and 4.17 unconditionally satisfied. The only remaining condition is  $\det(\mathbf{J}_a) = \det(A) > 0$ .

When  $M_a = \mathbf{J}_a^{-1}$ , all the affine transforms with positive determinant satisfy the proposed conditions set with either the 1-cone or the 2-cone.

### 6. COMPLEXITY

We define the complexity of a set of conditions as the number of smooth inequalities that need to be satisfied for each node. The complexity for the different conditions proposed in this work as well as our previous condition given in [22] are reported in the table 2 for dimension up to three and B-spline degree up to four for a general  $M_a$  matrices family. When  $M_a = I_d$  and 2-cone are used, the symmetry of the relation  $u\mathcal{R}v \Leftrightarrow v \in C_{u,\theta}$  can be used to divide the number of constraint by two.

Degree	1D	2D		3D		
		[22]	New	[22]	1-cone	2-cone
n	1	$4n^2$	$4n$	NA	$48n^2 + 1$	$12n^2 + 2$
1	1	4	4	64	49	13
2	1	16	8	2744	193	49
3	1	36	12	27000	433	109
4	1	64	16	140608	769	193

TABLE 2. Number of constraints per node for a general  $M_a$  given the dimension and the degree of the vector field.

As one can see, if the complexity is noticeably reduced in 2D, the reduction is very important in 3D. From the huge set of conditions of [22], we end up with a tractable set of condition, opening the way to a practical software implementation.

### 7. NUMERICAL EXPERIMENTS

The proposed condition has been visually evaluated on a classical 2D synthetic image registration problem. The version with a fixed  $M_a = \mathbf{J}^{-1}$  (corollary 3.4) has been used for our implementation. A disk is deformed to match a C shape by solving the following optimization problem:

$$(7.1) \quad \min_{c \in \mathcal{C}} \frac{1}{N} \sum_x |I_m(T(c, x)) - I_f(x)|^2,$$

where  $c$  are the B-spline coefficients,  $N$  the number of pixels,  $I_m$ , the moving image,  $I_f$  the fixed image and  $\mathcal{C}$ , the domain of the B-spline coefficients. The problem was solved for different  $\mathcal{C}$ : in the first experiment, our condition is compared to other sufficient conditions of the literature, in the second experiment, we observe the behaviour of the registration when the  $\theta_1$  and  $\theta_2$  parameters vary. As in [22], the problem 7.1 is solved by the multipliers method. The inequality constrained problem is solved by solving a succession of unconstrained problems: alternately, the augmented Lagrangian is minimized with respect to the B-spline coefficients and the Lagrange multipliers and the penalization coefficient are updated. The

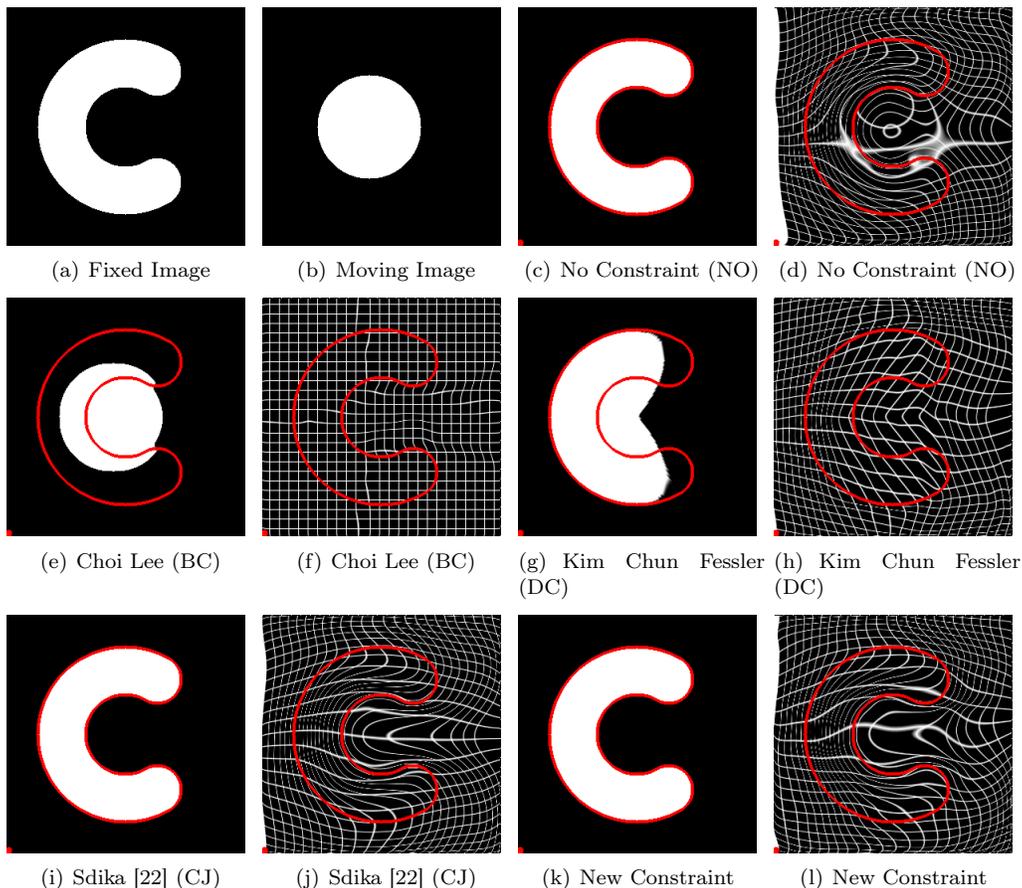


FIGURE 1. Results of the registration for different methods: the floating image and a grid are mapped through the transformation. A contour image of the fixed image is overlaid on these images.

algorithm is run until convergence and the inequalities are strictly satisfied at the end of the algorithm. The LBGFS algorithm [14], which is able to handle large scale problems, is used for unconstrained minimization. More details can be found in [22].

**7.1. Comparison to state of the art.** In this experiment, the problem was solved for different  $\mathcal{C}$ : without constraint (NO), with the bound constraints on the displacement coefficients of [8] (BC), with the bound constraints on the finite difference coefficients of [13, 9] (DC), our condition on the Jacobian coefficients [22] (JC) and the proposed 2D condition (New). For the New condition, we used  $\theta_1 = \theta_2 = \frac{\pi}{4} - 0.001$ . For all the problems, the input images are both  $300 \times 300$ , the node spacing is 6 pixels in each direction, the same multiresolution pattern is used.

The fixed and moving images as well as the deformation of the moving image and a regular grid for each  $\mathcal{C}$  have been presented in figure 1. Without constraints, the match is perfect but lots of folds are visible on the deformed grid. The unconstrained

resolution gives Jacobian values as low as -7. As expected, for all other  $\mathcal{C}$ , all the Jacobian values are strictly positive. As one can see, BC and DC produce a very regular deformation but are too restrictive to match the two shapes. In accordance to the results of section 5, DC allows more freedom in the deformation than BC. Both CJ and the new constraint enable a perfect match of the two shapes and produce regular deformation. Note however that the new constraint produces a grid that seems more distorted and less symmetric than the grid produced with CJ in the black region inside the C shape. As we are working with binary images, there is not much information to drive the registration in regions away from image edges: the cost function is flat in these regions which makes the output of the registration somewhat variable.

**7.2.  $\theta_1$  and  $\theta_2$  parameters.** In this experiment, the same problem has been solved using the corollary 3.4 to ensure invertibility. For the New condition,  $\theta_1$  was set in the range  $[0, \frac{\pi}{2}]$  and  $\theta_2$  was set as  $\theta_2 = \frac{\pi}{2} - \theta_1 - 0.001$ .

The results of the registration are presented in figure 2. One can first notice that the range of  $\theta_1$  producing acceptable registration is quite large. As one can see, for small  $\theta_1$ , not enough freedom is allowed for the deformation in the vertical direction. For large  $\theta_1$  (and small  $\theta_2$ ), the opposite behaviour is obtained: the constraint is too restrictive in the horizontal direction. These two parameters allow to control the regularization in one direction or another in the very specific case where something is known about the anisotropy of the problem.

## 8. CONCLUSION

In this work, we proposed several new sets of conditions on the coefficient of a B-spline vector field to guarantee that it is a diffeomorphism. The new conditions, while still allowing large deformations are now computationally tractable in 3D.

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## APPENDIX A. PROOF OF LEMMA 3.2

We first prove a small lemma.

**Lemma A.1.** *Let  $(\theta_1, \theta_2) \in [0, \frac{\pi}{2}]^2$ , and*

$$f(\lambda) = \lambda \cos \theta_1 - \sqrt{1 - 2\lambda \cos \theta_2 + \lambda^2}$$

*then*

$$\sup_{\lambda \geq 0} f(\lambda) = \cos(\theta_1 + \theta_2).$$

*Proof.* We will prove this lemma by first showing that  $\cos(\theta_1 + \theta_2)$  is a upper bound of  $f$  over  $\mathbb{R}^+$  and then showing that this bound is either attained for a positive  $\lambda$  when  $\theta_1 > 0$  or is the limit of  $f$  at infinity when  $\theta_1 = 0$ . Note first that  $\forall \theta_2 \forall \lambda$  then  $1 - 2\lambda \cos \theta_2 + \lambda^2 \geq 0$  and  $f$  is well defined.

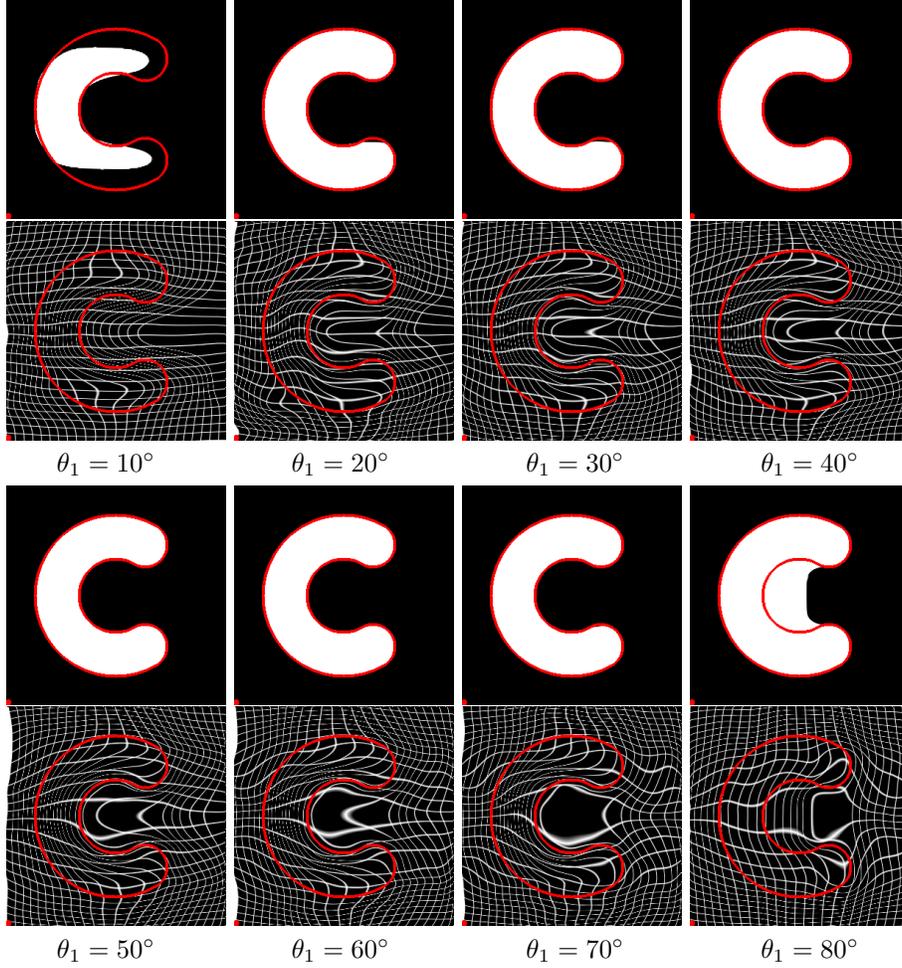


FIGURE 2. Results of the registration for our new condition (corollary 3.4) for different values of  $\theta_1$  (in degree). A contour image of the fixed image is overlaid on these images.

If there exists  $\lambda$  such that  $f(\lambda) > \cos(\theta_1 + \theta_2)$  then

$$\lambda \cos \theta_1 - \cos(\theta_1 + \theta_2) > \sqrt{1 - 2\lambda \cos \theta_2 + \lambda^2}$$

which implies

$$\begin{aligned} \lambda^2 \cos^2 \theta_1 - 2\lambda \cos(\theta_1) \cos(\theta_1 + \theta_2) + \cos^2(\theta_1 + \theta_2) &> 1 - 2\lambda \cos \theta_2 + \lambda^2 \\ \lambda^2 \sin^2 \theta_1 + 2\lambda [\cos \theta_1 \cos(\theta_1 + \theta_2) - \cos \theta_2] + \sin^2(\theta_1 + \theta_2) &< 0 \end{aligned}$$

but as

$$\begin{aligned} \cos \theta_1 \cos(\theta_1 + \theta_2) - \cos \theta_2 &= \cos^2 \theta_1 \cos \theta_2 - \cos \theta_1 \sin \theta_1 \sin \theta_2 - \cos \theta_2 \\ &= -\sin^2 \theta_1 \cos \theta_2 - \cos \theta_1 \sin \theta_1 \sin \theta_2 \\ &= -\sin \theta_1 \sin(\theta_1 + \theta_2), \end{aligned}$$

we have

$$\begin{aligned}\lambda^2 \sin^2(\theta_1) - 2\lambda \sin \theta_1 \sin(\theta_1 + \theta_2) + \sin^2(\theta_1 + \theta_2) &< 0 \\ [\lambda \sin \theta_1 - \sin(\theta_1 + \theta_2)]^2 &< 0\end{aligned}$$

which is not possible. So  $\forall \lambda \geq 0$

$$f(\lambda) \leq \cos(\theta_1 + \theta_2).$$

Let's now assume that  $\theta_1 > 0$  and let's define  $\lambda_1 = \frac{\sin(\theta_1 + \theta_2)}{\sin(\theta_1)}$ , then:

$$\begin{aligned}1 - 2\lambda_1 \cos \theta_2 + \lambda_1^2 &= (\lambda_1 - \cos(\theta_2))^2 + 1 - \cos^2(\theta_2) \\ &= \left( \frac{\sin(\theta_1 + \theta_2) - \cos(\theta_2) \sin(\theta_1)}{\sin(\theta_1)} \right)^2 + \sin^2(\theta_2) \\ &= \frac{\sin^2(\theta_2) \cos^2(\theta_1)}{\sin^2(\theta_1)} + \sin^2(\theta_2) \\ &= \frac{\sin^2(\theta_2) \cos^2(\theta_1) + \sin^2(\theta_2) \sin^2(\theta_1)}{\sin^2(\theta_1)} \\ &= \frac{\sin^2(\theta_2)}{\sin^2(\theta_1)},\end{aligned}$$

and consequently

$$\begin{aligned}f(\lambda_1) &= \frac{\sin(\theta_1 + \theta_2)}{\sin(\theta_1)} \cos(\theta_1) - \frac{\sin(\theta_2)}{\sin(\theta_1)} \\ &= \frac{\cos(\theta_1) \sin(\theta_2) + \sin(\theta_1) \cos(\theta_2)}{\sin(\theta_1)} \cos(\theta_1) - \frac{\sin(\theta_2)}{\sin(\theta_1)} \\ &= \frac{(\cos^2(\theta_1) - 1) \sin(\theta_2) + \cos(\theta_1) \sin(\theta_1) \cos(\theta_2)}{\sin(\theta_1)} \\ &= -\sin(\theta_1) \sin(\theta_2) + \cos(\theta_1) \cos(\theta_2) \\ &= \cos(\theta_1 + \theta_2)\end{aligned}$$

When  $\theta_1 = 0$  and  $\lambda > 0$  then  $f$  can be expressed as

$$\begin{aligned}f(\lambda) &= \lambda - \sqrt{1 - 2\lambda \cos \theta_2 + \lambda^2} \\ &= \frac{\lambda^2 - (1 - 2\lambda \cos \theta_2 + \lambda^2)}{\lambda + \sqrt{1 - 2\lambda \cos \theta_2 + \lambda^2}} \\ &= \frac{2\lambda \cos \theta_2 - 1}{\lambda + \sqrt{1 - 2\lambda \cos \theta_2 + \lambda^2}} \\ &= \frac{2 \cos \theta_2 - \frac{1}{\lambda}}{1 + \sqrt{1 - \frac{2}{\lambda} \cos \theta_2 + \frac{1}{\lambda^2}}}.\end{aligned}$$

Consequently, when  $\theta_1 = 0$ ,  $\lim_{\lambda \rightarrow +\infty} f(\lambda) = \cos \theta_2 = \cos(\theta_1 + \theta_2)$ . □

We now prove proposition 3.2

*Proof.* Let's assume first that  $|x| = |y| = |u| = 1$ , the general case can be easily deduced from this case.

For  $\lambda$  positive, we have

$$\begin{aligned} x^T y &= \lambda x^T u + x^T (y - \lambda u) \\ &\geq \lambda x^T u - |y - \lambda u| \\ &\geq \lambda \cos \theta_1 - \sqrt{1 - 2\lambda u^T y + \lambda^2} \\ &\geq \lambda \cos \theta_1 - \sqrt{1 - 2\lambda \cos \theta_2 + \lambda^2}. \end{aligned}$$

As  $\forall \lambda \geq 0$   $x^T y \geq f(\lambda)$  then  $x^T y \geq \sup_{\lambda} f(\lambda)$  and finally, using lemma A.1

$$x^T y \geq \cos(\theta_1 + \theta_2).$$

□

### APPENDIX B. PROOF OF PROPOSITION 4.3

*Proof.* (1) This property is a simple consequence of the convexity of the  $p$ -norm defining  $C_{U, \theta_u}^p$  when  $p \geq 1$ .

(2) If we apply the Hölder inequality

$$\sum_{i>1} |a_i| |b_i| \leq \left( \sum_{i>1} |a_i|^r \right)^{\frac{1}{r}} \left( \sum_{i>1} |b_i|^{\frac{r}{r-1}} \right)^{1-\frac{1}{r}}$$

to  $a_i = |x_i|^p$ ,  $b_i = 1$  and  $r = \frac{q}{p}$ , we obtain

$$\sum_{i>1} |x_i|^p \leq \left( \sum_{i>1} |x_i|^q \right)^{\frac{p}{q}} (D-1)^{1-\frac{p}{q}}.$$

So if  $x \in C_{U, \theta_u}^q$ , we have

$$\begin{aligned} \left( \sum_{i>1} |x_i|^p \right)^{\frac{1}{p}} &\leq \left( \sum_{i>1} |x_i|^q \right)^{\frac{1}{q}} (D-1)^{\frac{1}{p}-\frac{1}{q}} \\ &\leq x_1 \tan(\theta_u) (D-1)^{\frac{1}{p}-\frac{1}{q}}, \end{aligned}$$

which implies that  $x \in C_{U, \theta'_u}^p$

(3) The case  $\theta_u = 0$  is obvious:  $C_{U,0}^p = C_{U,0}^q$ . If  $\theta_u > 0$ , let  $x \in C_{U, \theta_u}^p$ . By definition we have:

$$\sum_{i>1} \left( \frac{|x_i|}{x_1 \tan(\theta_u)} \right)^p \leq 1.$$

This implies that for  $i > 1$  we have  $\frac{|x_i|}{x_1 \tan(\theta_u)} \leq 1$ , consequently when  $p \leq q$

$$\left( \frac{|x_i|}{x_1 \tan(\theta_u)} \right)^q \leq \left( \frac{|x_i|}{x_1 \tan(\theta_u)} \right)^p,$$

which implies that  $x \in C_{U, \theta_u}^q$ .

(4) We consider only the case  $p = 2$  as the case  $p < 2$  can be easily deduced using the case  $p = 2$  and the property 3. To prove 4, we assume that  $\theta_u + \theta_v < \theta_{uv}$  and try to find the "closest" point from  $C_{V, \theta_v}^2$  in  $C_{U, \theta_u}^2$  by solving

$$\begin{aligned} \max & x^T v_1. \\ |x|^2 &= 1 \\ x^T u_1 &\geq \cos \theta_u \end{aligned}$$

As the domain of this problem is compact and the cost function is continuous, the supremum is also a local maximum. The global maximal value  $v_{\text{opt}}$  is reached at  $x_{\text{opt}}$  and satisfy Karush Kuhn Tucker conditions:

$$\begin{aligned} \text{(B.1)} \quad & v_1 + \lambda x - \mu u_1 = 0 \\ \text{(B.2)} \quad & x^2 = 1 \\ \text{(B.3)} \quad & \mu (\cos \theta_u - u_1^T x) = 0, \end{aligned}$$

with  $\mu \geq 0$ .

In the case  $\mu = 0$ , we have  $v_1 = -\lambda x$  which implies  $\lambda^2 = 1$  and consequently  $x_{\text{opt}} = v_1$ . But this means that  $v_1 \in C_{U, \theta_u}^2$  which contradicts  $\theta_u + \theta_v < \theta_{uv}$ .

In the case  $\mu > 0$ , we have  $x^T u_1 = \cos(\theta_u)$ . Considering the dot product of B.1 with successively  $u_1$ ,  $x$  and  $v_1$ , we obtain the system of equations:

$$\begin{aligned} \text{(B.4)} \quad & \cos(\theta_{uv}) + \lambda \cos(\theta_u) - \mu = 0 \\ \text{(B.5)} \quad & v_{\text{opt}} + \lambda - \mu \cos(\theta_u) = 0 \\ \text{(B.6)} \quad & 1 + \lambda v_{\text{opt}} - \mu \cos(\theta_{uv}) = 0. \end{aligned}$$

Using B.4 to substitute  $\mu$  in the equation B.5 and B.6, we obtain after simplification:

$$\begin{aligned} \text{(B.7)} \quad & v_{\text{opt}} + \lambda \sin^2(\theta_u) - \cos(\theta_u) \cos(\theta_{uv}) = 0 \\ \text{(B.8)} \quad & \sin^2(\theta_{uv}) + \lambda v_{\text{opt}} - \lambda \cos(\theta_u) \cos(\theta_{uv}) = 0. \end{aligned}$$

When  $\sin(\theta_u) = 0$ , the only admissible point is  $u_1$ , so  $v_{\text{opt}} = u_1 v_1 = \cos(\theta_{uv}) = \cos(\theta_{uv} - \theta_u)$ . Otherwise, solving for  $\lambda$  in equation B.7 and substituting in B.8, we obtain:

$$v_{\text{opt}}^2 - 2 \cos(\theta_u) \cos(\theta_{uv}) v_{\text{opt}} + \cos^2(\theta_u) \cos^2(\theta_{uv}) - \sin^2(\theta_{uv}) \sin^2(\theta_u) = 0$$

which is a quadratic equation in  $v_{\text{opt}}$  which is solved by:

$$v_{\text{opt}} = \cos(\theta_u) \cos(\theta_{uv}) \pm \sin(\theta_{uv}) \sin(\theta_u).$$

The maximal value is obtained with the plus sign and in this case we have:

$$v_{\text{opt}} = \cos(\theta_{uv} - \theta_u).$$

But when  $\theta_u + \theta_v < \theta_{uv}$  we have  $\cos(\theta_v) > \cos(\theta_{uv} - \theta_u)$  so  $\forall x \in C_{U, \theta_u}^2$  we have  $x^T v_1 < \cos(\theta_v)$  and consequently  $C_{U, \theta_u}^2 \cap C_{V, \theta_v}^2 = \emptyset$ .

- (5) As  $-C_{V, \theta_v}^p = C_{-V, \theta_v}^p$  and the angle between  $u_1$  and  $-v_1$  is  $\pi - \theta_{uv}$ , the property 5 is a simple consequence of the property 4.  $\square$

#### APPENDIX C. PROOF OF PROPOSITION 4.8

*Proof.* Let's have a closer look to the second term in the  $M_X$  expression. If  $\xi \in \{-1, 1\}$ , we have

$$\begin{aligned} \frac{t_u t_v}{s_{uv}(s_{uv} - \xi t_v c_{uv})} &= \frac{t_u s_v}{s_{uv}(c_v s_{uv} - \xi s_v c_{uv})} \\ &= \frac{t_u s_v}{s_{uv} \sin(\theta_{uv} - \xi \theta_v)}. \end{aligned}$$

We also have:

$$(C.1) \quad \begin{aligned} \theta_u + \theta_v &< \theta_{uv} &< \pi - (\theta_u + \theta_v) \\ \theta_u &< \theta_{uv} - \theta_v &< \pi - (\theta_u + 2\theta_v) < \pi - \theta_u \\ s_u &< \sin(\theta_{uv} - \theta_v) & . \end{aligned}$$

and

$$(C.2) \quad \begin{aligned} \theta_u + \theta_v &< \theta_{uv} &< \pi - (\theta_u + \theta_v) \\ \theta_u < \theta_u + 2\theta_v &< \theta_{uv} + \theta_v &< \pi - \theta_u \\ s_u &< \sin(\theta_{uv} + \theta_v) & . \end{aligned}$$

Consequently, when  $\theta_u = \theta_v$ , we have

$$\begin{aligned} \frac{t_u t_v}{s_{uv}(s_{uv} - \xi t_v c_{uv})} &= \frac{t_u}{s_{uv}} \frac{s_u}{\sin(\theta_{uv} - \xi \theta_v)} \\ &\leq \frac{t_u}{s_{uv}}, \end{aligned}$$

which implies that  $M_X = \frac{t_u}{s_{uv}}$ .

We prove similarly that when  $\theta_u = \theta_v$ ,  $M_Y = \frac{t_u}{s_{uv}} = M_X$

□

#### APPENDIX D. PROOF OF LEMMA 4.10

*Proof.* First note that  $B_{u,v,\theta_u,\theta_v}$  is in the half space delimited by the plane orthogonal to  $u \wedge v$ . Thus, it is enclosed in a cone of axis  $u \wedge v$ :

$$B_{u,v,\theta_u,\theta_v} \subset C_{u \wedge v, \frac{\pi}{2}}.$$

Let's now find the minimal enclosing circular cone of axis  $u \wedge v$ . The semi-angle of this cone is the maximal angle between  $u \wedge v$  and  $x \in B_{u,v,\theta_u,\theta_v}$ . Using the parameterization of  $B_{u,v,\theta_u,\theta_v}$ ,  $x = a'u_2 + b'u_3 + c'v_3 \in B_{u,v,\theta_u,\theta_v}$  with  $|b'| \leq M_X a'$  and  $|c'| \leq M_Y a'$ , we will minimize the cosine between  $x$  and  $u \wedge v$  which is given by

$$\begin{aligned} \frac{u_2^T x}{|x|} &= \frac{a'}{\sqrt{a'^2 + b'^2 + c'^2 + 2b'c'u_3^T v_3}} \\ &= \frac{1}{\sqrt{1 + \frac{b'^2}{a'^2} + \frac{c'^2}{a'^2} + 2c_{uv} \frac{b'c'}{a'^2}}}. \end{aligned}$$

If we set  $b = \frac{b'}{a'}$  and  $c = \frac{c'}{a'}$ , this cosine is minimized over  $|b'| \leq M_X a'$  and  $|c'| \leq M_Y a'$  when

$$b^2 + c^2 + 2bcc_{uv}$$

is maximal over  $|b| \leq M_X$  and  $|c| \leq M_Y$ . For any fixed  $c$ , this second order polynomial in  $b$  is maximal at one of the bounds of  $|b| \leq M_X$ , that is to say  $b = \xi_b M_X$  with  $\xi_b \in \{-1, 1\}$ . The same reasoning on  $c$  when  $b = \xi_b M_X$  gives  $c = \xi_c M_Y$  with  $\xi_c \in \{-1, 1\}$ .  $\xi_b$  and  $\xi_c$  are then chosen such that  $\xi_b \xi_c c_{uv}$  is positive.

So the optimal angle is

$$\bar{\theta}_{uv} = \arccos \left( \frac{1}{\sqrt{1 + M_X^2 + M_Y^2 + 2M_X M_Y |c_{uv}|}} \right)$$

But as

$$\arccos\left(\frac{1}{\sqrt{1+x^2}}\right) = \arctan(|x|),$$

we have

$$\bar{\theta}_{uv} = \arctan\left(\sqrt{M_X^2 + M_Y^2 + 2M_X M_Y |c_{uv}|}\right)$$

□

#### APPENDIX E. PROOF OF PROPOSITION 4.12

*Proof.* As a function of  $\theta_{uv}$ ,  $\bar{\theta}$  varies jointly to  $E = M_X^2 + M_Y^2 + 2M_X M_Y |c_{uv}|$ : we can restrict the analysis to the study of  $E$ . One can also see that  $M_X(\theta_{uv})$  and  $M_Y(\theta_{uv})$  are symmetric about  $\theta_{uv} = \frac{\pi}{2}$ . So we can restrict the analysis to the case  $\theta_{uv} \in ]\theta_u + \theta_v, \frac{\pi}{2}]$ . As  $M_X$  and  $M_Y$  are both defined as the maximum of two smooth functions of  $\theta_{uv}$ ,  $] \theta_u + \theta_v, \frac{\pi}{2} ]$  can be partitionned into a finite number of intervals on which  $M_X$  and  $M_Y$  are smooth. We will show below that on each of these intervals  $E$  is always decreasing. The continuity of  $M_X$  and  $M_Y$  with respect to  $\theta_{uv}$  (and consequently of  $E$  and  $\bar{\theta}$ ) allows concluding on the decrease of  $\bar{\theta}$  over the whole interval  $] \theta_u + \theta_v, \frac{\pi}{2} ]$ . We split the analysis in four case depending on the value of  $M_X$  and  $M_Y$ .

case  $M_X = \frac{t_v}{s_{uv}}, M_Y = \frac{t_u}{s_{uv}}$ . In this case we have:

$$\begin{aligned} E &= \frac{t_u^2 + t_v^2 + 2t_u t_v c_{uv}}{s_{uv}^2} \\ &= \frac{(t_u + t_v c_{uv})^2}{s_{uv}^2} + t_v^2. \end{aligned}$$

So  $E$  varies jointly to  $\frac{(t_u + t_v c_{uv})}{s_{uv}}$ . The derivative of this last expression with respect to  $\theta_{uv}$  is

$$-\frac{t_v + t_u c_{uv}}{s_{uv}^2}$$

which is negative, so  $\bar{\theta}$  is decreasing in this case.

case  $M_X = \frac{t_v}{s_{uv}}, M_Y = \frac{t_u t_v}{s_{uv}(s_{uv} - t_u c_{uv})}$ . In this case, we have:

$$\begin{aligned} E &= \frac{t_v^2}{s_{uv}^2} \left( 1 + \frac{t_u^2}{(s_{uv} - t_u c_{uv})^2} + \frac{2t_u c_{uv}}{s_{uv} - t_u c_{uv}} \right) \\ &= \frac{t_v^2}{s_{uv}^2 (s_{uv} - t_u c_{uv})^2} (s_{uv}^2 - 2t_u c_{uv} s_{uv} + t_u^2 c_{uv}^2 + t_u^2 + 2t_u c_{uv} s_{uv} - 2t_u^2 c_{uv}^2) \\ &= \frac{t_v^2}{s_{uv}^2 (s_{uv} - t_u c_{uv})^2} (s_{uv}^2 + t_u^2 s_{uv}^2) \\ &= \frac{t_v^2 (1 + t_u^2)}{(s_{uv} - t_u c_{uv})^2} \\ &= \frac{c_u^2 t_v^2 (1 + t_u^2)}{\sin^2(\theta_{uv} - \theta_u)}. \end{aligned}$$

In this case also,  $E$  is a decreasing function of  $\theta_{uv}$

case  $M_X = \frac{t_u t_v}{s_{uv}(s_{uv} - t_v c_{uv})}, M_Y = \frac{t_u}{s_{uv}}$ . This case is similar to the previous one and here again,  $\bar{\theta}$  is decreasing.

case  $M_X = \frac{t_u t_v}{s_{uv}(s_{uv} - t_v c_{uv})}$ ,  $M_Y = \frac{t_u t_v}{s_{uv}(s_{uv} - t_u c_{uv})}$ . In this case we have

$$\begin{aligned} M_X &= \frac{t_u t_v}{s_{uv}(s_{uv} - t_v c_{uv})} \geq \frac{t_v}{s_{uv}} \\ \implies & t_u \geq s_{uv} - t_v c_{uv} \\ \implies & c_v t_u \geq \sin(\theta_{uv} - \theta_v). \end{aligned}$$

But as  $\theta_{uv} \in ]\theta_u + \theta_v, \frac{\pi}{2}]$ , we have  $\sin(\theta_{uv} - \theta_v) > s_u$  and consequently we must have  $c_v > c_u$ . With the same reasoning on  $M_Y$ , we also prove that  $c_u > c_v$ . Consequently, this case never happen when  $\theta_{uv} \in ]\theta_u + \theta_v, \frac{\pi}{2}]$ .

To conclude,  $\bar{\theta}$  is a decreasing function of  $\theta_{uv}$  on the interval  $]\theta_u + \theta_v, \frac{\pi}{2}]$ . Using the symmetry of  $\bar{\theta}$ , it is an increasing function of  $\theta_{uv}$  on the interval  $[\frac{\pi}{2}, \pi - (\theta_u + \theta_v)[$ .  $\square$

#### APPENDIX F. PROOF OF PROPOSITION 4.13

*Proof.* When  $\theta_u = \theta_v$ ,  $M_X = M_Y = \frac{t_u}{s_{uv}}$  and we have

$$\begin{aligned} \bar{\theta}_{uv} &= \arctan \left( \sqrt{M_X^2 + M_Y^2 + 2M_X M_Y |c_{uv}|} \right) \\ &= \arctan \left( \sqrt{2 \frac{t_u^2}{s_{uv}^2} (1 + |c_{uv}|)} \right) \\ &= \arctan \left( \frac{\sqrt{2} t_u}{\sqrt{1 - |c_{uv}|}} \right) \end{aligned}$$

$\square$

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