# Simplicial Diffeomorphisms

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#### Abstract

In this paper we will develop a theory for simplicial diffeomorphims, that is, diffeomorphims that preserve the incidence relations of a simplicial complex, and analyze alternative schemes to construct them with different properties. In combining piecewise linear functions on complexes with simplicial diffeomorphisms, we propose a new representation of curves and surfaces (and hypersurfaces, in general) that is simultaneously implicit and parametric.

## 1 Introduction

Spatial transformations are basic operations for geometric modeling, visualization and computer vision. In geometric modeling, deformation techniques such as Free-Form Deformations (FFD) provide powerful tools for shape creation and editing. In visualization, warping and morphing techniques constitute the foundations of most image-based algorithms. In computer vision, projective transformations are at the heart of camera calibration and other fundamental problems.

Implicit surfaces turn out to be particularly suited to deformation based modeling and rendering techniques. In this setting, the surface S is defined as the inverse image  $f^{-1}(c)$  of a regular value c of a scalar function  $f : \mathbb{R}^3 \to \mathbb{R}$  in the ambient space. Therefore, warping the domain of f causes the surface S to be deformed.

In order to be able effectively work with implicit surfaces in the above context, it is necessary to use well behaved spatial transformations. More specifically, the warping must be 1-1 and smooth. In other words, a *diffeomorphism*. The main reason for this requirement is that the deformation should preserve the global topology of the level set.

A general and popular way to create implicit surfaces, and hypersurfaces, in general, is by resorting to a spatial decomposition that allows the construction of the function f in a piecewise manner. In particular, a simplicial space partition has all the required properties.

The definition of a simplicial implicit hypersurface is as follows: Let K be a simplicial complex in  $\mathbb{R}^m$  and  $f: V \to \mathbb{R} - \{0\}$  a function defined on the vertices of K. It is well known that f can be extended to a function  $\hat{f}$  defined on the set of points |K| in  $\mathbb{R}^m$  that belong to the simplexes of K by linear interpolation.

If  $p \in \sigma = \langle v_0, \ldots, v_m \rangle$ , do

$$\hat{f}(p) = \sum_{i=0}^{m} w^i f_{v_i},$$

where  $w^i$  are the baricentric coordinates of p relative to  $\sigma$ . The implicit hypersurface  $O = \hat{f}^{-1}(c)$  obtained in this way is clearly piecewise linear. Let's call them *linear isocomplexes*.

A linear isocomplex has various important properties that are intimately related with the linear structure of the simplexes which constitute its domain and the piecewise linear function  $\hat{f}$  itself. For example, it is easy to verify if a point  $p \in \mathbb{R}^m$  is inside or outside O. It is also easy to sample points in O. On the other hand, if we want to approximate a smooth hypersurface by an isocomplex O, probably we will have to take a mesh K with very small simplexes.

To overcome the limitations of the piecewise linear nature of f we can employ a simplicial diffeomorphism, that is, a diffeomorphism X attached to complex Kthat preserve its incidence relations. In this way, we are able to produce curved isocomplexes  $\mathcal{O} = (\hat{f} \circ X)^{-1}(c)$  while retaining the properties of the simplicial structure. Moreover, simplicial diffeomorphisms incorporate into the implicit hypersurface definition a very powerful deformation based modeling mechanism that can be exploited in many applications.

In this paper we will develop a theory for simplicial diffeomorphims and analyze alternative schemes to construct them with different properties. In section 2 we define K-invariant functions and prove that K-invariant functions locally injective are homeomorphisms. In order to apply the jacobian determinant criterion of local injectivity to functions defined on simplexes, we derive formulas to express the jacobian in barycentric coordinates in section 3. In section 4 we present the first non trivial example of simplicial diffeomorphisms, the monotonic ones. Section 5 is dedicated to the search of sufficient conditions for a polynomial function to be a simplicial diffeomorphism, and ditto for rational functions in section 6. In section 7, we show that simplicial diffeomorphisms combined with isocomplexes provide a new kind of hypersurface representation. Section 8 is devoted to the delicate question of smoothness conditions for curved isocomplexes. We present two simple applications in section 9 and finish the paper in a brief conclusion (section 10).

### 2 K-invariant functions

**Definition 2.1.** Let K be a simplicial complex and  $X: |K| \to |K|$  a continuous function. We say that X is K-invariant, if  $X(\sigma) \subset \sigma$  for all  $\sigma \in K$ .

In particular, the vertices of K are fixed points of X. The identity function on |K| is a trivial example of K-invariant function. Moreover, the composition of two K-invariant functions is clearly also K-invariant.

The first remarkable property exhibited by the K-invariant functions is that the " $\subset$ " symbol in definition 2.1 is, indeed, a equality. We'll prove this fact with the help of the following lemmas.

**Lemma 2.1** (Sperner). Let T be a triangulation of the standard m-dimensional simplex  $\Delta^m$ , and  $L:T_0 \to \{0, \ldots, m\}$  a mapping between the vertices of T and

the integers from 0 to m. We say that L labels the vertices of T. If, for each  $v = (v^0, \ldots, v^m) \in T_0$ ,

$$L(v) = i \Rightarrow v^i \neq 0,$$

then there is a m-simplex  $\sigma = \langle v_0, \ldots, v_m \rangle \in T$  which vertices are completely labeled, that is, such that

$$L(\{v_0,\ldots,v_m\}) = \{0,\ldots,m\}.$$

*Proof.* See [6] for a proof.

**Lemma 2.2.** Let  $X: \Delta^m \to \Delta^m$  be a  $\Delta^m$ -invariant function. Then there is a point  $x \in \Delta^m$  such that  $X(x) = \frac{1}{m+1}\mathbb{1}$ , where  $\mathbb{1} := (1, 1, \ldots, 1)$ . That is, X maps x to the barycenter of  $\Delta^m$ .

*Proof.* Let  $(T_n)_{n \in \mathbb{N}}$  be a sequence of triangulations of  $\Delta^m$  such that

$$\lim_{n \to \infty} \operatorname{mesh}(T_n) = 0,$$

where

$$mesh(T) = max\{diam(\sigma) | \sigma \in T\}.$$

Define the mapping  $L_n$  over the vertices of  $T_n$  as follows: if v is a vertex of  $T_n$ and  $X(v) = (w^0, \ldots, w^m)$ ,  $L_n(v) = i$ , where i is the smallest integer such that  $w^i = \max_j \{w^j\}$ . The hypothesis of X be  $\Delta^m$ -invariant means that, for each  $v = (v^0, \ldots, v^m) \in \Delta^m$ ,  $X(v) = (w^0, \ldots, w^m)$  satisfies

$$v^i = 0 \Rightarrow w^i = 0.$$

Therefore,

$$L_n(v) = i \Rightarrow w^i \neq 0 \Rightarrow v^i \neq 0,$$

that is, the hypothesis of Sperner Lemma holds for  $L_n$ , what ensure the existence of a sequence  $(\sigma_n)_{n\in\mathbb{N}}$  of completely labeled *m*-simplexes such that  $\lim_{n\to\infty} \operatorname{diam}(\sigma_n) = 0$ . As  $\Delta^m$  is a compact set, we can suppose, by taking a subsequence if necessary, that the sequence of barycenters of  $\sigma_n$  converges to a point *x*. It follows from *X* continuity and from  $L_n$  definition that  $X(x) = (w^0, \ldots, w^m)$ , with each  $w^i = \max_j \{w^j\}$ , that is,  $X(x) = \frac{1}{m+1} \mathbb{1}$ .

**Theorem 2.3.** Let  $X: \Delta^m \to \Delta^m$  be a  $\Delta^m$ -invariant function. Then  $X(\sigma) = \sigma$  for all  $\sigma \in \Delta^m$ . In particular, X is surjective.

*Proof.* By induction on m. The case m = 0 is trivial. Let be m > 0. By the induction hypothesis  $X(\sigma) = \sigma$  for each proper face  $\sigma$  in  $\Delta^m$ . We only need to prove that for all  $y \in int(\Delta^m)$ , that is, such that  $y \in \Delta^m$  and  $y^i > 0$ , there is a point  $x \in \Delta^m$  with X(x) = y. Consider the function  $Y_y: \Delta^m \to \Delta^m$  given by

$$Y_y(w^0, \dots, w^m) = \frac{1}{\sum \frac{w^i}{y^i}} (\frac{w^0}{y^0}, \dots, \frac{w^m}{y^m})$$

It is easy to see that  $Y_y$  is  $\Delta^m$ -invariant and invertible, with inverse

$$Y_y^{-1}(w^0, \dots, w^m) = \frac{1}{\sum w^i y^i} (w^0 y^0, \dots, w^m y^m).$$

Applying the preceding lemma to  $Y_y X$  we obtain a point x such that

$$Y_y X(x) = \frac{1}{m+1} \mathbb{1}.$$

It follows from the properties of  $Y_y$  that

$$X(x) = Y_y^{-1}(\frac{1}{m+1}1) = y_y^{-1}(\frac{1}{m+1}y_y^{-1}) = y_y^$$

**Corollary 2.4.** Let  $X: |K| \to |K|$  be a K-invariant function. Then  $X(\sigma) = \sigma$  for all  $\sigma \in K$ . In particular, X is surjective.

*Proof.* Write X in the barycentric coordinates of  $\sigma$  then apply the previous theorem.

Now that we know that K-invariant functions are surjective, we may ask when they are injective. It is hard, in general, to prove that a function is globally injective. On the other hand, it is easier to verify the local injectivity. In the case of a differentiable function F, for example, the local injectivity of Fin a neighborhood of x follows from the injectivity of DF(x).

In a classical paper [2], Meisters and Olech thoroughly described some conditions that a continuous locally injective function must satisfy to be globally injective. We present now an adaptation of their arguments to the case of Kinvariant functions. In order to make the exposition self-contained, we begin by demonstrating the following lemma.

**Lemma 2.5.** Let  $f: U \to \mathbb{R}^m$  be a continuous function defined on a open set  $U \subset \mathbb{R}^m$ . If f is locally injective, then f(U) is a open set.

*Proof.* If f(U) is empty, there is nothing to prove. If f(U) is not empty, let y = f(x) be a point of f(U). As U is open, there is a neighborhood N of x contained in U such that  $f|_N$  is injective. Moreover, there is a open set  $V \subset U$  with  $x \in V$ ,  $\overline{V}$  compact and  $\overline{V} \subset U$ . Therefore f restricted to  $\overline{V}$  is a homeomorphism. Because x is an interior point of  $\overline{V}$ , it follows from Brouwer invariance of domain theorem that f(x) is an interior point of  $f(\overline{V})$  and consequently is an interior point of f(U).

We are ready to present the main result of this section — K-invariant functions locally injective are injective.

**Theorem 2.6.** Let  $X: \Delta^m \to \Delta^m$  be a  $\Delta^m$ -invariant function. If X is locally injective, then X is injective.

*Proof.* By induction on m. The case m = 0 is trivial. Let be m > 0. From lemma 2.5 combined to proposition 2.3 it results that

$$\begin{cases} X(\operatorname{bd}(\Delta^m)) = \operatorname{bd}(X(\Delta^m)) = \operatorname{bd}(\Delta^m) \\ X(\operatorname{int}(\Delta^m)) = \operatorname{int}(X(\Delta^m)) = \operatorname{int}(\Delta^m) \end{cases}$$
(1)

By theorem 2.3, for each point of  $y \in \Delta^m$  there is at least one point  $x \in \Delta^m$ such that X(x) = y. Let A be the set of  $y \in \Delta^m$  such that there is only one  $x \in \Delta^m$  with X(x) = y and  $B = \Delta^m \setminus A$ , that is, the points with more than one preimage. By the induction hypothesis, X restricted to  $bd(\Delta^m)$  is injective and by (1) there is no interior point of  $\Delta^m$  mapped on  $bd(\Delta^m)$ . It follows that  $bd(\Delta^m) \subset A$ , that is, A is not empty. Our objective is to show that B is empty. For that, we'll suppose that B is not empty, concluding from that supposition that  $A \cup B$  is a non trivial partition of  $\Delta^m$ , which is impossible because  $\Delta^m$  is a connected set. In order to derive this contradiction, we'll prove that  $\overline{A} \cap B = \emptyset$ and  $A \cap \overline{B} = \emptyset$ .

Let y be a point of B. Then there is two distinct points  $x_1$  and  $x_2$  in  $\Delta^m$  such that  $X(x_1) = X(x_2) = y$ . As  $X(\operatorname{bd}(\Delta^m)) = \operatorname{bd}(\Delta^m) \subset A$ , it follows from the induction hypothesis that  $x_1$  and  $x_2$  are not both in  $\operatorname{bd}(\Delta^m)$ . It's not possible also that  $x_1 \in \operatorname{bd}(\Delta^m)$  and  $x_2 \in \operatorname{int}(\Delta^m)$  (or vice-versa), by (1). Therefore  $x_1$  and  $x_2$  are in  $\operatorname{int}(\Delta^m)$ . Consequently, threre are open neighborhoods  $N_1$  and  $N_2$ , from  $x_1$  and  $x_2$  respectively, with  $N_1 \cap N_2 = \emptyset$ , such that

$$N_1 \subset \operatorname{int}(\Delta^m)$$
 and  $N_2 \subset \operatorname{int}(\Delta^m)$ .

By lemma 2.5,  $X(N_1)$  and  $X(N_2)$  are open sets. Thus,

$$N = X(N_1) \cap X(N_2)$$

is a open neighborhood of y entirely contained in B, because each point of N has at least two preimages. Hence  $\overline{A} \cap B = \emptyset$ .

Let  $(y_n)_{n \in \mathbb{N}}$  be a sequence of points in B that converges to a point  $y \in \Delta^m$ . Then there are sequences  $(x_n^1)_{n \in \mathbb{N}}$  and  $(x_n^2)_{n \in \mathbb{N}}$  in  $\Delta^m$  such that, for all n,

$$y_n = X(x_n^1) = X(x_n^2)$$
 and  $x_n^1 \neq x_n^2$ 

From the compactness of  $\Delta^m$ , passing to a subsequence if necessary, we can assume that  $(x_n^i)_{n\in\mathbb{N}}$  converges to a certain  $x^i \in \Delta^m$ , i = 1, 2. By the continuity of X, it results that

$$y = X(x^1) = X(x^2).$$

We have that  $x^1 \neq x^2$ , for otherwise X wouldn't be locally injective in  $x^1(=x^2)$ . Hence  $A \cap \overline{B} = A \cap B = \emptyset$ .

**Corollary 2.7.** Let  $X: |K| \to |K|$  be a K-invariant function. If X is locally injective, then  $X|_{\sigma}: \sigma \to \sigma$  is a homeomorphism, for all  $\sigma \in K$ .

In other words, every K-invariant function which is locally injective is a homeomorphism.

Until now, the continuity of X was sufficient to our purposes. But, in order to verify the local injectivity of X, the differentiability of X is more suitable, because the local injectivity of X follows from the injectivity of the linear transformation DX. In a nutshell, the idea is to pass from topology to analysis and from analysis to algebra. This justifies the following definition.

**Definition 2.2.** Let  $X: |K| \to |K|$  be a K-invariant function. We say that X is a simplicial diffeomorphism with respect to complex K or, more briefly, that X is a K-invariant diffeomorphism, if X restricted to  $int(\sigma)$  is a diffeomorphism for all  $\sigma \in K$ .

Let SD(K) be the set of all K-invariant diffeomorphisms. The following properties are easily verified:

- 1. Id  $\in$  SD(K);
- 2.  $X \in \mathrm{SD}(K) \Rightarrow X^{-1} \in \mathrm{SD}(K);$
- 3.  $X_1, X_2 \in \mathrm{SD}(K) \Rightarrow X_1 X_2 \in \mathrm{SD}(K).$

It's also clear that a K-invariant function X is a K-invariant diffeomorphism if  $X|_{int(\sigma)}$  is differentiable and  $D(X|_{int(\sigma)})(p)$  is injective for all  $\sigma \in K$  and for all  $p \in int(\sigma)$ .

# 3 Jacobian determinant in barycentric coordinates

In this section, our objective is to describe how to express the jacobian determinant of a differentiable function in barycentric coordinates, with respect to a simplex  $\sigma = \langle p_0, p_1, \ldots, p_m \rangle \subset \mathbb{R}^m$ . This result will help us to exhibit non trivial examples of simplicial diffeomorphisms.

The barycentric coordinates  $w := (w^0, \ldots, w^m)$  of a point  $x \in \mathbb{R}^m$ , with respect to a simplex  $\sigma$ , satisfy the relation

$$P_{\sigma} \begin{pmatrix} w^{0} \\ w^{1} \\ \vdots \\ w^{m} \end{pmatrix} = \begin{pmatrix} 1 \\ x^{1} \\ \vdots \\ x^{m} \end{pmatrix}$$
(2)

where

$$P_{\sigma} = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ p_0^1 & p_1^1 & \cdots & p_m^1 \\ \vdots & \vdots & \ddots & \vdots \\ p_0^m & p_1^m & \cdots & p_m^m \end{pmatrix}.$$

Let  $F := (F^1, \ldots, F^m) : \mathbb{R}^m \to \mathbb{R}^m$  and  $G := (G^0, \ldots, G^m) : \mathbb{R}^{m+1} \to \mathbb{R}^{m+1}$ be differentiable functions. We say that G is a *barycentric representation* of F if

$$P_{\sigma} \begin{pmatrix} G^{0}(w) \\ G^{1}(w) \\ \vdots \\ G^{m}(w) \end{pmatrix} = \begin{pmatrix} 1 \\ F^{1}(x) \\ \vdots \\ F^{m}(x) \end{pmatrix}$$
(3)

holds for all  $x \in \mathbb{R}^m$  and  $w \in \mathbb{R}^{m+1}$  related by (2). Moreover, we say that a barycentric representation G is *restricted* if there is a real function  $G_s: \mathbb{R} \to \mathbb{R}$  such that

$$\sum_{i=0}^{m} G^{i}(w^{0}, \dots, w^{m}) = G_{s}(\sum_{i=0}^{m} w^{i}),$$

for all  $(w^0, \ldots, w^m) \in \mathbb{R}^{m+1}$ . Note that  $G_s(1) = 1$  necessarily. Let  $F' := \det(JF)$  and  $G' := \det(JG)$  where

$$JF = \left(\frac{\partial F^i}{\partial x_j}\right)$$
 and  $JG = \left(\frac{\partial G^i}{\partial w_j}\right)$ .

are the jacobian matrices of F and G. By the inverse function theorem, if  $F'(x) \neq 0$ , then F is injective in a neighborhood of x. We may ask how this condition is translated in barycentric coordinates. Clearly, G can be locally injective in w even if G'(w) = 0, because the dependency between the barycentric coordinates can make JG(w) singular.

The following propositions show how to express F'(x) in barycentric coordinates, if a barycentric representation of F is restricted.

**Proposition 3.1.** Let G be a restricted barycentric representation of F. If  $G'_s(1) = \alpha \neq 0$ , then

$$F'(x) = \frac{G'(w)}{\alpha}.$$

*Proof.* By (2), (3) and the chain rule, the matrix

$$L = P_{\sigma} J G(w) P_{\sigma}^{-1}$$

has the following block decomposition:

$$\begin{pmatrix} u & v \\ q & JF(x) \end{pmatrix}.$$

By the hypothesis on  $G_s$ ,

$$\sum_{i} \partial_j G^i(w) = G'_s(1) = \alpha$$

for j = 0, ..., m. Therefore the product  $P_{\sigma}JG(w)$  can be written in blocks as

$$\begin{pmatrix} \alpha 1 \\ Q \end{pmatrix}$$

Thus, the first row of L satisfies

$$\begin{pmatrix} u & v \end{pmatrix} P_{\sigma} = \alpha \mathbb{1}.$$

Solving this system, we conclude that v = 0 and  $u = \alpha$ . Hence,

$$G'(w) = \det P_{\sigma}G'(w) \det P_{\sigma}^{-1} = \det L = u \det JF(x) = \alpha F'(x).$$

Proposition 3.2. Let G be a restricted barycentric representation of F. If

$$G'_s(1) = 0,$$

then

$$F'(p) = \sum_{i=0}^{m} JG^{ii}(w),$$

where  $JG^{ii}(w)$  are the diagonal cofactors of JG(w).

*Proof.* Applying the Cauchy-Binet formula to equation (3), we have that

$$F'(x) = \sum_{i=0}^{m} \sum_{j=0}^{m} (P_{\sigma})^{0j} J G^{ij}(w) (P_{\sigma}^{-1})^{i0}.$$

By the hypotheses on  $G_s$ ,

$$\sum_{i} \partial_j G^i(w) = G'_s(1) = 0.$$

for j = 0, ..., m. Therefore, lemma A.5 implies that  $JG^{ij} = JG^{ii}$ , hence

$$F'(x) = \sum_{i=0}^{m} JG^{ii}(w) \sum_{j=0}^{m} (P_{\sigma})^{0j} \frac{(P_{\sigma})_{0i}}{\det P_{\sigma}} = \sum_{i=0}^{m} JG^{ii}(w) \sum_{j=0}^{m} \frac{(P_{\sigma})^{0j}}{\det P_{\sigma}} = \sum_{i=0}^{m} JG^{ii}(w).$$

### 4 Monotonic simplicial diffeomorphisms

We'll show now the first non trivial example of simplicial diffeomorphisms. Let  $g:[0,1] \rightarrow [0,1]$  be a continuous function on the interval [0,1] such that g(0) = 0, g(1) = 1. As [0,1] is nothing more than a one dimensional simplex, the last condition on g means only that g is [0,1]-invariant function, in our terminology. It is well known that if g'(x) > 0 for all  $x \in [0,1]$ , then g is a diffeomorphism of [0,1], or a simplicial diffeomorphism. Let us generalize that result to higher dimensional simplexes.

Let  $g_i: [0,1] \to \mathbb{R}$  be functions such that  $g_i(0) = 0$  and  $g'_i(x) > 0$  for all  $x \in [0,1]$ , where  $i = 0, \ldots, m$ . As the derivative is positive,  $g_i$  is increasing and  $g_i(x) > 0$  if x > 0. Define

$$G := (G^0, \dots, G^m) : \Delta^m \subset \mathbb{R}^{m+1} \to \Delta^m$$

setting

$$G^{i}(w^{0},...,w^{m}) = \frac{g_{i}(w^{i})}{\sum_{j=0}^{m} g_{j}(w^{j})}$$

It's easy to see that  $G^i(w) = 0$  if  $w^i = 0$ , thus G is a  $\Delta^m$ -invariant function. Moreover, G is restricted because,

$$\sum_{i=0}^{m} G^{i}(w^{0}, \dots, w^{m}) = 1,$$

and  $G_s(t) = 1$ , therefore  $G'_s(1) = 0$ . Calculating its jacobian,

$$\partial_j G^i = \frac{\partial_j g_i(\sum_k g_k) - g_i \partial_j g_j}{(\sum_k g_k)^2} = \frac{\delta_{ij} g'_j(\sum_k g_k) - g_i g'_j}{(\sum_k g_k)^2}$$

$$=\frac{g_j'(\delta_{ij}(\sum_k g_k) - g_i)}{(\sum_k g_k)^2} = \frac{g_j'}{\sum_k g_k} \left(\delta_{ij} - \frac{g_i}{\sum_k g_k}\right).$$

Making  $u = \begin{bmatrix} g'_j \\ \sum_k g_k \end{bmatrix}$  and  $v = \begin{bmatrix} -\frac{g_j}{\sum_k g_k} \end{bmatrix}$ , where u and v are column vectors, we have that

$$JG = \operatorname{diag} u + uv^T$$
.

From this especial structure, it follows that the submatrices of JG obtained by deleting the entries from the diagonal also have the same form, that is, denoting by  $v_i$  and  $u_i$  the vectors obtained from v and u by deleting the *i*-th row, we have that

$$JG^{ii} = \det(\operatorname{diag} u_i + u_i v_i^T).$$

From lemma A.4, it results that

$$\sum_{i=0}^{m} JG^{ii} = \sum_{i=0}^{m} \det(u_i v_i^T + \operatorname{diag} u_i) = \sum_{i=0}^{m} \prod_{j \neq i} \frac{g_j'}{\sum_k g_k} (1 - \sum_{j \neq i} \frac{g_j}{\sum_k g_k})$$
$$= \frac{1}{(\sum_k g_k)^{m+1}} (\sum_{i=0}^{m} (\prod_{j \neq i} g_j') g_i) > 0,$$

and G is a diffeomorphism  $\Delta^m$ -invariant.

This result can be extend to a simplicial complex K. Suppose that there is a function  $g_v: [0,1] \to \mathbb{R}$  with the properties above for each vertex  $v \in K$ . Let's define the function  $X: |K| \to |K|$  in the following way. Given  $x \in \sigma = \langle v_1, \ldots, v_n \rangle \subset K$ , let w be the barycentric coordinates of x with respect to  $\sigma$ . Set

$$X(x) = P_{\sigma} \frac{1}{\sum_{i=0}^{n} g_{v_i}(w_i)} (g_{v_1}(w_1), \dots, g_{v_n}(w_n)).$$

It's easy to see that X is K-invariant and a simplicial diffeomorphism, by the result above.

One feature of this kind of simplicial diffeomorphism, that we call *monotonic*, is that all the information about the warping produced by X is concentrated on vertices, so can be difficult to control what happens in the interior of higher dimensional simplexes. We want a more local control, so we must study other types of diffeomorphisms.

## 5 Polynomial simplicial diffeomorphisms

Let  $F := (F^1, \ldots, F^m) : \mathbb{R}^m \to \mathbb{R}^m$  be a polynomial mapping, that is, a mapping in the form

$$x := (x^1, \dots, x^m) \mapsto (F^1(x^1, \dots, x^m), \dots, F^m(x^1, \dots, x^m))$$

with each  $F^i \in \mathbb{R}[X] := \mathbb{R}[X_1, \dots, X_m]$ , the ring of polynomials in *m* indeterminates over  $\mathbb{R}$ . We set

$$\deg(F) = \max \deg F^i,$$

that is, the degree of F is equal to the highest degree among all  $F^i$ .

Let  $G := (G^0, \ldots, G^m) : \mathbb{R}^{m+1} \to \mathbb{R}^{m+1}$  be a polynomial barycentric representation of F, that is, each  $G^i$  is a polynomial of  $\mathbb{R}[W] := \mathbb{R}[W_0, \ldots, W_m]$ .

Note that F can have many representations because  $G^i$  assumes the same values that  $G^i + Q.(W_0 + \ldots + W_m - 1)$  when evaluated in w, where Q is any polynomial in  $\mathbb{R}[W]$ . In other words, if G and H are two barycentric representations of F, then

$$G^i = H^i \pmod{\mathcal{M}},$$

where  $\mathcal{M} = \langle W_0 + \ldots + W_m - 1 \rangle$  is the ideal of  $\mathbb{R}[W]$  generated by the polynomial  $W_0 + \ldots + W_m - 1$ .

We say that a barycentric representation H of F is homogeneous of degree nif each  $H^i$  is a homogeneous polynomial of degree n. There is a unique degree  $n = \deg(F)$  homogeneous barycentric representation of F. To see that, define polynomials  $G^i$  by relation (3), in such a way that

$$G^i = \sum_{|I| \le n} g^i_I W^I,$$

where I is a integer vector  $(I^0, \ldots, I^m)$ ,  $|I| = \sum_i I^i$  and  $W^I := W_0^{I^0} \ldots W_m^{I^m}$ . It is easy to see that  $H := (H^0, \ldots, H^m)$ , with

$$H^{i} = \sum_{|I| \le n} g_{I}^{i} W^{I} (W_{0} + \ldots + W_{m})^{n-|I|}$$

is the claimed representation.

Alternatively, H can be written in the form

$$H = \sum_{|I|=n} b_I B_I,\tag{4}$$

where the  $b_I$  are called *control points of* H and  $B_I := \binom{n}{I} W^I$  are thes *Bézier-Bernstein polynomials* [1]. To see that  $\sum_i b_I^i = 1$ , note that by (2) and (3)

$$\sum_{i} H^{i}(\frac{W_{0}}{W_{0} + \ldots + W_{m}}, \ldots, \frac{W_{m}}{W_{0} + \ldots + W_{m}}) = 1.$$

As  $H^i$  is homogeneous of degree n,

$$\sum_{i} H^{i} = (W_{0} + \ldots + W_{m})^{n}.$$
(5)

Therefore,

$$\sum_{i} \sum_{|I|=n} b_{I}^{i} B_{I} = (W_{0} + \ldots + W_{m})^{n}$$
$$\sum_{|I|=n} (\sum_{i} b_{I}^{i}) B_{I} = \sum_{|I|=n} B_{I}$$

hence

$$\sum_{i} b_{I}^{i} = 1.$$

We can define points  $c_I \in \mathbb{R}^m$ , related to  $b_I$  by equation

$$P_{\sigma}b_I = \begin{pmatrix} 1\\c_I^1\\\vdots\\c_I^m \end{pmatrix},$$

called *control points of* F with respect to simplex  $\sigma$ . Such points completely determine F and our objective is to find out sufficient conditions on  $c_I$  such that F be a  $\sigma$ -invariant diffeomorphism. In fact, the conditions will be given on the points  $b_I$ , turning then independent of the particular simplex  $\sigma$ .

Let's initially derive a sufficient condition for H be  $\Delta^m$ -invariant. Let  $\chi$  be a function that associates to each *n*-uple  $(x^1, \ldots, x^n)$  a *n*-uple  $(y^1, \ldots, y^n)$  such that

$$y^{i} = \begin{cases} -1, & \text{se } x^{i} < 0\\ 0, & \text{se } x^{i} = 0\\ 1, & \text{se } x^{i} > 0 \end{cases}$$

**Definition 5.1.** We say that a degree n homogeneous polynomial H is adjusted if  $\chi(b_I) = \chi(I)$  for all I with |I| = n.

The intuitive idea behind this definition can be resumed as follows: if p is a point of  $\Delta^m$ ,  $\chi(p)$  is a binary code that identifies the lower dimensional face of  $\Delta^m$  that contains p. Thus, the definition means that each control point  $b_I$ belongs to face of code  $\chi(I)$ .

#### **Proposition 5.1.** If H is adjusted, then H is $\Delta^m$ -invariant.

*Proof.* We must show that if  $w^i = 0$  then  $H^i(w) = 0$ . As H is adjusted,  $I^i = 0$  implies that  $b_I^i = 0$ . Therefore

$$w^{i} = 0 \Rightarrow H^{i}(w) = \sum_{|I|=n} b_{I}^{i} B_{I}(w) = \sum_{|I|=n, I^{i}=0} b_{I}^{i} B_{I}(w) = 0.$$

Equation (5) shows that H is a restricted barycentric representation of F, with  $H_s(t) = t^n$ . As  $H'_s(1) = n$ , it follows from proposition 3.1 that if H' is positive in  $\Delta^m$ , then F' is positive in  $\sigma$ . The following theorem, on the other hand, give us sufficient and necessary conditions for the positivity of H'.

**Theorem 5.2** (Pólya). Let  $H \in \mathbb{R}[W]$  be a homogeneous polynomial of degree n. Then H(w) > 0 for all  $w \in \Delta^m$  if and only if

$$H \cdot (W_0 + \ldots + W_m)^N$$

has, for some  $N \in \mathbb{N}$ , the form

$$\sum_{K|=n+N} a_K W^K$$

.

with  $a_K > 0$ .

*Proof.* A proof can be found in [5, Satz 3.6].

In order to apply it, we should write H' in a convenient form. Let us introduce some notation.

Given two matrices  $A = (a_{ij}), B = (b_{ij}) \in \mathbb{R}^{m \times m}$ , let  $A \odot B := (a_{ij}b_{ij})$ , that is, each entry of  $A \odot B$  is the product of the corresponding entries of Aand B. In general, there is no relation between the determinant of  $A \odot B$  and the determinants of A and B. But, if there is a constant  $c \in \mathbb{R}$  such that  $\prod_{i=1}^{m} b_{i\sigma(i)} = c$  for each permutation  $\sigma \in S_m$ , it is easy to see that  $\det(A \odot B) = c \det(A)$ .

Proposition 5.3.

$$H' = \sum_{|K| = (m+1)(n-1)} a_K W^K$$

where

$$a_{K} = \sum_{I_{0} > \dots > I_{m} \atop I_{0} + \dots + I_{m} = K+1} \det(b_{I_{0}}, \dots, b_{I_{m}}) \det(I_{0}, \dots, I_{m}) \prod_{i=0}^{m} \binom{n}{I_{i}}.$$

*Proof.* Writing H as the matrix product,

$$H = (b_I^i)_{(m+1) \times p} (B_I)_{p \times 1},$$

where  $p = \#\{I = (I^0, ..., I^m) \in \mathbb{N}^{m+1} | |I| = n\}$ , it follows that

$$JH = (b_I^i)(\nabla B_I) = (b_I^i)\left((I^j) \odot \left(\binom{n}{I}W^{I-e_j}\right)\right).$$

By the Cauchy-Binet formula and by the preceding observation,

$$H' = \sum_{I_0 > \ldots > I_m} \det(b_{I_0}, \ldots, b_{I_m}) \left( \det(I_0, \ldots, I_m) \prod_{i=0}^m \binom{n}{I_i} W^{\sum_{i=0}^m I_i - 1} \right),$$

therefore

$$H' = \sum_{|K| = (m+1)(n-1)} a_K W^K$$

with

$$a_{K} = \sum_{\substack{I_{0} > \ldots > I_{m} \\ I_{0} + \ldots + I_{m} = K + 1 \\ 1}} \det(b_{I_{0}}, \ldots, b_{I_{m}}) \det(I_{0}, \ldots, I_{m}) \prod_{i=0}^{m} \binom{n}{I_{i}}.$$

In the next subsections, we'll prove a set of sufficient conditions for a homogeneous application H of degree n be a  $\Delta^m$ -invariant diffeomorphism, for some combinations of n and m.

#### 5.1 Unidimensional case (m = 1)

The simplest case is the unidimensional one. Initially, we note that the lexicografical order applied to the points of  $\Delta^1$  provides the same information that the usual order in the interval [0, 1], that is, if  $b_I >_{\text{lex}} b_J$ , with  $b_I, b_J \in \Delta^1$ , then  $b_I$  is "at right" of  $b_J$ . The following proposition shows that if the control points keep its relative positions, then H is a simplicial diffeomorphism (figure 1).

**Proposition 5.4.** Let  $H = \sum_{|I|=n} b_I B_I$  be an adjusted polynomial application in  $\Delta^1$ . If the control points are ordered, that is, if  $I >_{lex} J \Rightarrow b_I >_{lex} b_J$ , then  $H|_{\Delta^1}$  is a  $\Delta^1$ -invariant diffeomorphism.

Proof. Note that

$$b_I >_{\text{lex}} b_J \Leftrightarrow \det(b_I, b_J) > 0.$$

The result follows from Pólya theorem and from proposition (5.3).



Figure 1: A degree 6  $\Delta^1$ -invariant diffeomorfism. Note that the control points are ordered.

The above proposition holds for unidimensional applications of any degree, but it's possible to achieve better results in particular cases. For n = 2, it's easy to see that if H is adjusted then the control points are ordered. The case n = 3is more interesting, where it's sufficient that H be adjusted, because suppose that  $b_{21} < b_{12}$ . Replacing relations

$$det(b_{12}, b_{03}) = det(b_{21}, b_{03}) + det(b_{12}, b_{21})$$
$$det(b_{30}, b_{03}) = det(b_{21}, b_{03}) + det(b_{12}, b_{21}) + det(b_{30}, b_{12})$$
$$det(b_{30}, b_{21}) = det(b_{12}, b_{21}) + det(b_{30}, b_{12})$$

in the expression of H', we obtain

$$H' = 9(\det(b_{21}, b_{03})(W^{22} + 2W^{13} + W^{04}) + \det(b_{12}, b_{21})(W^{40} - 2W^{22} + W^{04}) + \det(b_{30}, b_{12})(W^{40} + 2W^{31} + W^{22})).$$

It is not difficult to see that H' is positive in  $\Delta^1$ , because

$$(W^{40} - 2W^{22} + W^{04})$$

is positive in  $\Delta^1$ , except in the point  $(\frac{1}{2}, \frac{1}{2})$ , where is zero. But in this point the other terms are positive.

In the case n = 4, the counterexample of figure 2 shows that H be adjusted is not sufficient. An analogous counterexample holds for dimensions greater than 1.

### 5.2 Quadratic case (n = 2)

In order to show that every adjusted polynomial application of degree two is a  $\Delta^m$ -invariant diffeomorfism, for all m > 0, we'll prove a combinatorial lemma.



Figure 2: An adjusted polynomial application of degree 4 that is not injective. Note that control points  $b_{13}$  and  $b_{31}$  are exchanged.

**Lemma 5.5.** Given a vector  $K = (K^0, \ldots, K^m) \in \mathbb{N}^{m+1}$ , with |K| = m + 1, it's always possible to find vectors  $I_0, \ldots, I_m \in \mathbb{N}^{m+1}$ , with  $|I_i| = 2$ , such that

$$I_0 + \ldots + I_m = K + 1$$

and  $\det(I_0,\ldots,I_m) \neq 0$ .

*Proof.* By induction on *m*. The case m = 0 is trivial. We can suppose without loss of generality that  $K^i \ge K^j$  if i < j. There are two possible cases: or  $K^m = 0$  or  $K^m = 1$ . If  $K^m = 1$ , we set  $I_j^i = 2\delta_{ij}$ , and  $\det(I_0, \ldots, I_m) = 2^{m+1} > 0$ . If  $K^m = 0$ , we define  $K' = (K^0 - 1, \ldots, K^{m-1})$  and, applying the induction step, we obtain vectors  $I'_j \in \mathbb{N}^m$ , with  $|I'_j| = 2$  and  $\det(I'_0, \ldots, I'_{m-1}) > 0$ . It's enough now to set  $I_j = (I'_j, 0)$  for  $j = 0, \ldots, m-1$  and  $I_m$  satisfying  $I^i_m = [i = 0 \text{ or } i = m]$ . Applying the Laplace expansion, we conclude that  $\det(I_0, \ldots, I_m) = \det(I'_0, \ldots, I'_{m-1}) > 0$ . □

**Proposition 5.6.** Let  $H = \sum_{|I|=2} b_I B_I$  be an adjusted aplication of degree 2. Then  $H|_{\Delta^m}$  is a  $\Delta^m$ -invariant diffeomorphism.

*Proof.* The idea is to show that the  $a_K$  coefficient of proposition 5.3 is positive. Initially, we'll prove that  $a_K \ge 0$ . Note that

$$\det(I_0, \dots, I_m) \prod_{i=0}^m \binom{2}{I_i} = \det(\binom{2}{I_0} I_0, \dots, \binom{2}{I_m} I_m) = 2^{m+1} \det(A).$$

where A is a 0-1 matrix with at most two ones per row. It follows from corollary A.2 that  $a_K \ge 0$ . But lemma 5.5 implies that at least one term of  $a_K$  is not zero. Hence,  $a_K > 0$  and  $H|_{\Delta^m}$  is a  $\Delta^m$ -invariant diffeomorphism.



Figure 3: The action of a quadratic simplicial diffeomorphism: in (a), the control points are in their natural positions, hence the diffeo is the identity; in (b), the control points were moved.

#### 5.3 One free control point

Let us study a very interesting and useful case. What happens when, intuitively, there is only one free control point ?

**Proposition 5.7.** Let  $H = \sum_{|I|=n} b_I B_I$  be an adjusted application of degree nand  $J = (J^0, \ldots, J^m) \in \mathbb{N}^{m+1}$  with |J| = n and  $J^i \in \{0, 1\}$ . If  $b_I = I/n$  for  $I \neq J$ , then  $H|_{\Delta^m}$  is a  $\Delta^m$ -invariant diffeomorphism.

*Proof.* We have that

$$H = \sum_{|I|=n} \frac{I}{n} B_I + b_J B_J - \frac{J}{n} B_J =$$
$$(W_0 + \ldots + W_m)^{n-1} \begin{pmatrix} W_0 \\ \vdots \\ W_m \end{pmatrix} + (b_J - \frac{J}{n}) B_J.$$

It follows that

$$UH = (W_0 + \ldots + W_m)^{n-1} (\mathrm{Id} + uv^T + ab^T),$$

with

$$u = \frac{n-1}{W_0 + \ldots + W_m} \begin{pmatrix} W_0 \\ \vdots \\ W_m \end{pmatrix},$$
$$v^T = \begin{pmatrix} 1 & \cdots & 1 \end{pmatrix},$$
$$a = \frac{n}{(W_0 + \ldots + W_m)^{n-1}} (b_J - J/n) \text{ and}$$
$$b^T = \begin{pmatrix} J^0 B_{J-e_0} & \cdots & J^m B_{J-e_m} \end{pmatrix}.$$

Applying lemma A.3,

$$H' = n(W_0 + \ldots + W_m)^{(m+1)(n-1)} (1 + b^T \frac{n}{(W_0 + \ldots + W_m)^{n-1}} (b_J - J/n)) =$$
$$n(W_0 + \ldots + W_m)^{m(n-1)-1} ((W_0 + \ldots + W_m)^n + n(W_0 + \ldots + W_m) b^T (b_J - J/n)) =$$
$$n(W_0 + \ldots + W_m)^{m(n-1)-1} E,$$

where

$$E = \sum_{|I|=n} B_I + D(b_J - J/n) \text{ and}$$

 $D = \left(\sum_{i} J^{0} (1 - \delta_{i0} + J^{i}) B_{J-e_{0}+e_{i}} \cdots \sum_{i} J^{m} (1 - \delta_{im} + J^{i}) B_{J-e_{m}+e_{i}}\right).$ That is,

$$E = \sum_{|I|=n} B_I + \sum_j \sum_i J^j (1 - \delta_{ij} + J^i) B_{J-e_j+e_i} (b_J^j - J^j/n) =$$

$$\sum_{|I|=n} B_I + \sum_j \sum_{i \neq j} J^j (1 + J^i) B_{J-e_j+e_i} (b_J^j - J^j/n) + \sum_j (J^j)^2 B_J (b_J^j - J^j/n) =$$

$$\sum_{|I|=n} B_I + \sum_j \sum_{i \neq j} J^j (1 + J^i) B_{J-e_j+e_i} (b_J^j - J^j/n) + B_J \sum_j (b_J^j - J^j/n) =$$

$$\sum_{|I|=n} B_I + \sum_j \sum_{i \neq j} J^j (1 + J^i) B_{J-e_j+e_i} (b_J^j - J^j/n) =$$

Analyzing the coefficients of E, we verify that, for  $i \neq j$ ,

$$\operatorname{Coeff}(E, B_{J-e_j+e_i}) = 1 + J^j (1 + J^i) (b_J^j - J^j/n) =$$
$$(1 - J^j (1 + J^i)/n) + J^j (1 + J^i) b_J^j =$$
$$(1 - J^j (1 + J^i)/n) + (1 + J^i) b_J^j > 0,$$

because n > 1,  $J^i \in \{0, 1\}$  and  $b^j_j = 0 \Leftrightarrow J^j = 0$ . As  $\operatorname{Coeff}(E, B_I) = 1$  for the remaining coefficients, it follows from Pólya theorem that H' is positive in  $\Delta^m$ , therefore  $H|_{\Delta^m}$  is a  $\Delta^m$ -invariant diffeomorphism.

Let us detail the meaning of that proposition. As previously mentioned, each face of  $\Delta^m$  can be identified by a binary code, accordingly the number of non zero coordinates of its points. Thus, for m = 3, we have the following correspondence:

$$(1111) \rightarrow 3\text{-simplex}$$
  
 $(1110), (1101), (1011), (0111) \rightarrow 2\text{-simplexes}$   
 $(1000), (1001), (0110), (0101), (0011) \rightarrow 1\text{-simplexes}$   
 $(1000), (0100), (0010), (0001) \rightarrow 0\text{-simplexes}$   
 $(0000) \rightarrow \text{empty simplex}$ 

Let  $G_J$  be a polynomial application such that

(

$$G_J^i = W_i + (b_J^i - J^i / |J|) B_J,$$

where  $J^i \in \{0, 1\}$ . Examining the proposition, we see that

$$G^i_J = H^i \pmod{\mathcal{M}},$$

therefore  $G_J$  and H define the same application in  $\Delta^m$  and, as proved above,  $G_J$  is a  $\Delta^m$ -invariant diffeomorphism.

Moreover, by definition,  $G_J$  only affects those points in face  $\delta_J$ , as well the points in incident faces to  $\delta_J$  with greater dimensions. That is, the control point  $b_J$  effectively controls the action of  $G_J$  over  $\delta_J$ .

Now, we can compose the diffeomorfisms  $G_J$  and define a diffeomorfism G that depends on parameters associated to each face of  $\Delta^m$ . In the case m = 3, we can define, for instance,

$$G = G_{0011}G_{0101}G_{0110}G_{1001}G_{1010}G_{1100}G_{0111}G_{1011}G_{1101}G_{1110}G_{1111}.$$

We see that G depends on 17 independent parameters, 1 for each 1-simplex, 2 for each 2-simplex and 3 for the 3-simplex. That scheme is perfectly general but, as the applications  $G_J$  do not commute in general, the resulting application G depends on the composition order, causing an assimetry with respect to the action of the control points, what can be a problem in certain applications.



Figure 4: The action of a cubic simplicial diffeomorphism: in (a), the control points are in their natural positions; in (b), the central control point  $b_{111}$  was moved.

#### 5.4 Stratified scheme

In order to overcome that problem, let us present a *stratified scheme* where G can be written as a composition of m applications  $G_j$ ,

$$G = G_1 G_2 \dots G_m,$$

with,

$$G_j^i = W_i + \sum_{|J|=j+1, J^k \in \{0,1\}} (b_J^i - J^i/|J|) B_J.$$

The idea is that  $G_j$  summarizes the combined effect of the control points associated to the *j*-simplexes of  $\Delta^m$ . But what can be said about the applications  $G_j$ ?

Note that  $G_j$  defines the same application in  $\Delta^m$  that the homogeneous application of degree j + 1  $H_j$ , with

$$H_j^i = W_i (W_0 + \ldots + W_m)^j + \sum_{|J|=j+1, J^k \in \{0,1\}} (b_J^i - J^i/|J|) B_J.$$

Thus, by propositions 5.6 and 5.7, it turns out that  $G_j$  is a  $\Delta^m$ -invariant diffeomorfism for j = 1 and j = m. But what happens for other values of j?

A possible approach is regard the jacobian determinant  $H'_j$  as a function of the control points  $b_J$  too. As each  $b_J$  is limited to a *j* dimensional face of  $\Delta^m$ , it turns out that  $H'_j$  can be regarded as a function defined in the product of simplexes

$$\Delta^m \times \underbrace{\Delta^j \times \ldots \times \Delta^j}_{r \text{ times}},$$

where r is the number of j dimensional simplexes of  $\Delta^m$ . Before taking this approach, let us consider some facts about the positivity of polynomial functions defined on products of simplexes.

Let  $P: \Delta^{m_1} \times \Delta^{m_2} \ldots \times \Delta^{m_r} \to \mathbb{R}$  be a polynomial function defined on a product of r simplexes of dimensions  $m_1, \ldots, m_r$ , given by

$$(u_1,\ldots,u_r)\mapsto P(u_1^0,\ldots,u_1^{m_1},u_2^0,\ldots,u_2^{m_2},\ldots,u_r^0,\ldots,u_r^{m_r}),$$

with  $P \in \mathbb{R}[U] := \mathbb{R}[U_{10}, \dots, U_{1m_1}, U_{20}, \dots, U_{2m_2}, \dots, U_{r0}, \dots, U_{rm_r}].$ Letting  $\mathcal{U} := \langle \sum_{l=0}^{m_i} U_{il} - 1; i = 1, \dots, r \rangle$ , we see that if two polynomials

Letting  $\mathcal{U} := \langle \sum_{i=0}^{n} U_{ii} - 1; i = 1, ..., r \rangle$ , we see that if two polynomials  $P, Q \in \mathbb{R}[U]$  are such that

$$P = Q \pmod{\mathcal{U}},$$

then they define the same application on  $\Delta^{m_1} \times \Delta^{m_2} \dots \times \Delta^{m_r}$ , because  $\sum_l u_i^l = 1$ .

Given a r-uple  $N = (n^1, \ldots, n^r) \in \mathbb{N}^r$ , he say that  $P \in \mathbb{R}[U]$  is N-homogeneous if

$$P = \sum_{|I_1|=n^1} \dots \sum_{|I_r|=n^r} a_{I_1 \dots I_r} U_1^{I_1} \dots U_r^{I_r}.$$

with  $U_i^I := (U_{i0})^{I^0} \dots (U_{im_i})^{I^{m_i}}$ .

We state now the generalization of Pólya theorem to polynomial application defined on a product of simplexes.

**Theorem 5.8.** Let  $H \in \mathbb{R}[U]$  be N-homogeneous polynomial application with  $N = (n^1, \ldots, n^r)$ . Then  $H(u_1, \ldots, u_r) > 0$  for all  $(u_1, \ldots, u_r) \in \Delta^{m_1} \times \Delta^{m_2} \ldots \times \Delta^{m_r}$  if and only if

$$H \cdot (U_{10} + \ldots + U_{1m_1})^{R_1} \ldots (U_{r0} + \ldots + U_{rm_r})^{R_r}$$

has, for some  $R = (R_1, \ldots, R_r) \in \mathbb{N}^r$ , the form

$$\sum_{|K_1|=n^1+R_1} \dots \sum_{|K_r|=n^r+R_r} a_{K_1\dots K_r} U_1^{K_1} \dots U_r^{K_r},$$

with  $a_{K_1...K_r} > 0$ .

Proof. See [5, Satz 3.54].

Let  $C_{m,n} = \{C \in \mathbb{N}^n | 0 \leq C^0 < C^1 < \ldots < C^{n-1} < m\}$ , that is,  $C_{m,n}$  represents the combinations of m objects  $\{0, 1, \ldots, m-1\}$  taken n at a time. This set can be linearly ordered by the lexicographic order in  $\mathbb{N}^n$ , therefore we denote the *i*-nth element of  $C_{m,n}$  by  $C_{m,n,i}$ , where *i* runs from 1 to  $\binom{m}{n}$ .

There is also a clear bijection between the set of  $J \in \mathbb{N}^m$  such that  $J^k \in \{0, 1\}$ with |J| = n and  $C_{m,n}$ . Let's denote by J(C) the image of  $C \in C_{m,n}$  by such bijection, that is,  $J(C) = (J^0, \ldots, J^{m-1})$ , with  $J^i = [\exists l, C^l = i]$ .

Returning to the stratified scheme, let's parametrize control points  $b_J$  in  $G_j$  in terms of indeterminates U. Initially, we set  $r = \binom{m+1}{j+1}$  and  $m_1 = m_2 = \ldots = m_r = j$ , that is, r counts the j dimensional faces of  $\Delta^m$ . The parametrization goes as follows:

$$b_{J(C_{m+1,j+1,i})}^{k} = \begin{cases} U_{il} & , \text{ if } C_{m+1,j+1,i}^{l} = k \\ 0 & , \text{ otherwise.} \end{cases}$$

Replacing  $b_J$  in  $H_j$  and applying proposition 5.3, we have that the coefficients  $a_K$  of  $H'_j$  are polynomials in  $\mathbb{R}[U]$  now. The idea is apply the generalized Pólya theorem to show that  $a_K > 0$ , resulting that  $G_j$  is a  $\Delta^m$ -invariant diffeomorphism. Let's firstly write  $a_K$  as a homogeneous polynomial.

Define

$$d(I_0, \dots, I_m) = \prod_{i=1}^r (\sum_{l=0}^j U_{il})^{t(i, I_0, \dots, I_m)} \det(b_{I_0}, \dots, b_{I_m}),$$

where  $t(i, I_0, \ldots, I_m)$  is a predicate that only says if

$$J(C_{m+1,j+1,i}) = I_k$$

for some k, that is,

$$t(i, I_0, \dots, I_m) = \begin{cases} 0 & \text{, if } \exists k, J(C_{m+1,j+1,i}) = I_k \\ 1 & \text{, otherwise.} \end{cases}$$

By the determinant properties, we conclude that  $d(I_0, \ldots, I_m)$  is 11-homogeneous. Moreover,

$$d(I_0,\ldots,I_m) = \det(b_{I_0},\ldots,b_{I_m}) \pmod{\mathcal{U}}$$

Therefore, if we define

$$u_{K} = \sum_{\substack{I_{0} > \dots > I_{m} \\ I_{0} + \dots + I_{m} = K + 1}} d(I_{0}, \dots, I_{m}) \det(I_{0}, \dots, I_{m}) \prod_{i=0}^{m} \binom{n}{I_{i}}$$

then  $u_K$  is 11-homogeneous too and

$$u_K = a_K \pmod{\mathcal{U}}.$$

Note that  $u_K$  has  $(j+1)^r$  terms in general.

Let's apply these ideas to the tridimensional case, that is, to m = 3. We already know that  $G_1$  and  $G_3$  are  $\Delta^3$ -invariant diffeomorphisms, so it remains to prove this for  $G_2$ . Following the parametrization recipe, we have that

$$b_{1110} = (U_{10}, U_{11}, U_{12}, 0), b_{1101} = (U_{20}, U_{21}, 0, U_{22}),$$

$$b_{1011} = (U_{30}, 0, U_{31}, U_{32})$$
 and  $b_{0111} = (0, U_{40}, U_{41}, U_{42}).$ 

Then, using the symbolic computation package ASIR[3], we compute  $u_K$  for every  $K \in \mathbb{N}^4$  with |K| = 8. We verify that these 165 polynomials have exactly  $3^{\binom{4}{3}} = 81$  terms with positive coefficients. Thus, we prove the following fact:

## **Proposition 5.9.** $G_1$ , $G_2$ and $G_3$ are $\Delta^3$ -invariant diffeomorphisms.

We belive that this result extends for m > 3, but the computations are increasingly complex. For example, for m = 4 the  $u_K$  polynomials corresponding to  $G^2$  have  $3^{\binom{5}{3}} = 59\ 049$  terms.

The natural question posed now is what can be said about rational functions. That is the theme of next section.

# 6 Rational simplicial diffeomorphisms

Let Q be a degree n rational application

$$Q = \frac{1}{\sum_{|I|=n} q_I B_I} \sum_{|I|=n} q_I b_I B_I,$$

where  $q_I > 0$  are weights associated to control points  $b_I$ . We say that Q is adjusted if  $\chi(b_I) = \chi(I)$ . It's easy to see that Q is  $\Delta^m$ -invariant if Q is adjusted. On what conditions is Q a  $\Delta^m$ -invariant diffeomorphism? Surprisingly, there is a simple, yet powerful, sufficient condition: set the control points fixed ( $b_I = I/n$ ) and let the weights  $q_I$  free.

Using the properties of Bézier-Bernstein polynomials, we see that

$$\sum_{i} Q^{i}(W_0, \dots, W_m) = 1,$$

therefore a sufficient condition for Q be a  $\Delta^m$ -invariant diffeomorphism is that

$$\sum_{i} JQ^{ii}(w) > 0,$$

for all  $w \in \Delta^m$ . Let's compute the jacobian of Q.

**Proposition 6.1.**  $JQ = [q_{ij}]$ , with

$$q_{ij} = \frac{1}{(\sum_{I} q_{I} B_{I})^{2}} \sum_{I>J} q_{I} q_{J} (b_{I}^{i} - b_{J}^{i}) \frac{(I^{j} - J^{j})}{W^{j}} B_{I} B_{J}.$$

Proof.

$$\begin{split} q_{ij} &= \partial_j Q^i = \frac{n(\sum_I q_I b_I^i B_{I-e_j} \sum_J q_J B_J - \sum_J q_J b_J^i B_J \sum_I q_I B_{I-e_j})}{(\sum_I q_I B_I)^2} = \\ &\frac{n}{(\sum_I q_I B_I)^2} (\sum_{I,J} q_I q_J (b_I^i - b_J^i) B_J B_{I-e_j}) = \\ &\frac{n}{(\sum_I q_I B_I)^2} (\sum_{I,J} q_I q_J (b_I^i - b_J^i) \frac{I^j}{nW^j} B_J B_I) = \end{split}$$

$$\frac{1}{(\sum_{I} q_{I}B_{I})^{2}} ((\sum_{I < J} + \sum_{I > J})q_{I}q_{J}(b_{I}^{i} - b_{J}^{i})\frac{I^{j}}{W^{j}}B_{J}B_{I}) = \frac{1}{(\sum_{I} q_{I}B_{I})^{2}} \sum_{I > J} q_{I}q_{J}(b_{I}^{i} - b_{J}^{i})\frac{(I^{j} - J^{j})}{W^{j}}B_{J}B_{I}.$$

In order to make the computations more manageable, let's express JQ as a product of matrices. Let

$$U = \begin{bmatrix} b_I - b_J \end{bmatrix}$$
 and  $V = \begin{bmatrix} I - J \end{bmatrix}$ 

two  $(m+1) \times \#(N)$ , where the columns are indexed by the set N of pairs (I, J), with I > J, lexicographly ordered. Thus, analysing the expression of JQ, we have that

$$JQ = \frac{1}{(\sum_{I} q_{I} B_{I})^{2}} U \operatorname{diag}(q_{I} q_{J} B_{I} B_{J})_{(I,J) \in N} V^{T} \operatorname{diag}(1/W^{0}, \dots, 1/W^{m}).$$

Given a integer k = 0, ..., m and a sequence  $L = (I_1, J_1) > ... > (I_m, J_m)$  of elements of N, we'll denote by  $U^{k,L}$  the matrix obtained from U by deleting the k-th row and the columns not in  $\{(I_1, J_1), ..., (I_m, J_m)\}$ . Depending on the context,  $U^{k,L}$  also will mean the determinant of such matrix.

#### Proposition 6.2.

$$\sum_{i=0}^{k} JQ^{kk} = \frac{1}{(\sum_{I} q_{I}B_{I})^{2m}} \sum_{|K|=m(2n-1)} a_{K}W^{K},$$

where

$$a_K = \sum_{K=\sum L-1 + e_k} q_L U^{k,L} V^{k,L}$$

and  $q_L = \prod_{l=1}^m q_{I_l} q_{J_l} {n \choose I_l} {n \choose J_l}$ , with  $L = (I_1, J_1) > \ldots > (I_m, J_m)$  ranging over the ordered sequences of lenght m of N.

Proof. Applying the Cauchy-Binet formula,

$$\sum_{k=0}^{m} JQ^{kk} =$$

$$\sum_{k=0}^{m} \frac{1}{(\sum_{I} q_{I}B_{I})^{2m}} \sum_{L} U^{k,L} (\prod_{l} q_{I_{l}}q_{J_{l}}B_{I_{l}}B_{J_{l}})V^{k,L}W^{-1+e_{k}} =$$

$$\frac{1}{(\sum_{I} q_{I}B_{I})^{2m}} \sum_{L} \sum_{k=0}^{m} q_{L}U^{k,L}V^{k,L}W^{\sum L-1+e_{k}} =$$

$$\frac{1}{(\sum_{I} q_{I}B_{I})^{2m}} \sum_{|K|=m(2n-1)} \left(\sum_{K=\sum L-1+e_{k}} q_{L}U^{k,L}V^{k,L}\right) W^{K}.$$

In order to show that every adjusted rational application with fixed control points is a  $\Delta^m$ -invariant diffeomorfism, for all m > 0, we'll prove a combinatorial lemma.

**Lemma 6.3.** Given a vector  $K = (K^0, \ldots, K^m) \in \mathbb{N}^{m+1}$ , with |K| = m(2n-1), it's always possible to find a decreasing sequence L of pairs of vectors  $(I_1, J_1) > (I_2, J_2) > \ldots > (I_m, J_m)$ , with  $I_i > J_i$  and  $|I_i| = |J_i| = n$ , and a integer  $k = 0, \ldots, m$  such that

$$I_1 + J_1 + \ldots + I_m + J_m - 1 + e_k = K$$

and  $V^{k,L} \neq 0$ , where

$$V = \left[ I - J \right]_{(m+1) \times \#(I > J)}.$$

Proof. Without loss of generality, we can suppose that  $K^0 \ge K^1 \ge \cdots \ge K^m$ , because otherwise we can order the entries of K and permute suitablely the sequence L obtained, what cause possibily just a change in the signal of  $V^{k,L}$ . The proof is by induction in n. If n=1, we have that |K| = m. Take  $I_i$  such that  $|I_i| = 1$ ,  $I_i \ge I_{i+1}$ ,  $\sum_{i=1}^m I_i = K$ ,  $J_i = e_{i+1}$  and k = 0. It's easy to see that there is only one sequence  $I_i$  satisfying this properties and that  $I_i > J_i$ . Therefore, the matrix  $V^{k,L}$  is higher triangular, with each diagonal entries equals to -1. Hence  $D^{k,L} \ne 0$ .

If n > 1, we have that |K| = m(2n - 1). We can write K in the form K = K' + 2K'', where |K'| = m(2(n - 1) - 1), |K''| = m and  $K'_0 \ge \ldots \ge K'_m$ . This can be done in the following way: set initially K' := K and K'' := 0. Repeat m times the operation  $K' := K' - 2e_l$  and  $K'' := K'' + e_l$ , where l is the larger index such that  $K_l \ge 2$ . Clearly this procedure works, because suppose that after m' steps, with m' < m, there were no entries  $K_l \ge 2$ . This implies that  $|K| \le 2m' + m + 1$ . But

$$m' < m \Rightarrow 2m' + 1 < 2m \Rightarrow$$
$$|K| \le 2m' + m + 1 < 3m \le m(2n - 1) = |K|,$$

and we have a contradiction.

Now we can apply the induction step to K', obtaining the sequence  $L' = (I'_1, J'_1) > \ldots > (I'_m, J'_m)$  and k = 0. Take  $I_i = I'_i + K''_i$  and  $J_i = J'_i + K''_i$ , where  $|K''_i| = 1$ ,  $K''_i \ge K''_{i+1}$  and  $\sum_{i=1}^m K''_i = K''$ . Thus

$$I_1 + J_1 + \ldots + I_m + J_m - 1 + e_0 =$$
$$I'_1 + K''_1 + J'_1 + K''_1 + \ldots + I'_m + K''_m + J'_m + K''_m - 1 + e_0 =$$
$$K' + 2K'' = K,$$

and  $V^{k,L} = V^{k,L'}$ , because  $I_i - J_i = I'_i - J'_i$ .

Theorem 6.4. Let

$$Q = \frac{1}{\sum_{|I|=n} q_I B_I} \sum_{|I|=n} q_I b_I B_I,$$

be a rational application. If  $b_I = I/n$  and  $q_I > 0$ , then Q is a  $\Delta^m$ -invariant diffeomorphism.

*Proof.* The idea is to show that the  $a_K$  coefficient of proposition 6.2 is positive. Initially, we'll prove that  $a_K \ge 0$ . Note that

$$U^{k,L}V^{k,L} = \frac{1}{n^m} (V^{k,L})^2,$$

therefore  $a_K \ge 0$ . But lemma 6.3 implies that at least one term of  $a_K$  is not zero. Hence,  $a_K > 0$  and  $Q|_{\Delta^m}$  is a  $\Delta^m$ -invariant diffeomorphism.



Figure 5: The action of a rational degree 5 simplicial diffeomorphism: in (a), the control points are in their natural positions and the weights are equal; in (b), the control points are unchanged, but some weights were changed. Note that control points with greater weights are more attractive.

We have an additional result if Q has degree 2. In this case, the matrices  $U^{k,L}$  and  $V^{k,L}$  have at most two non zero entries per row. Applying corollary A.2, we obtain the following theorem.

Theorem 6.5. Let

$$Q = \frac{1}{\sum_{|I|=2} q_I B_I} \sum_{|I|=2} q_I b_I B_I,$$

be a degree 2 adjusted rational application. If  $q_I > 0$ , then Q is a  $\Delta^m$ -invariant diffeomorphism.

### 7 Curved isocomplexes

In section 1, we define a linear isocomplex as the piecewise linear hypersurface  $O = \hat{f}^{-1}(c)$ , where  $\hat{f}$  is the piecewise linear function obtained by linear interpolation of a real function f defined in the vertices of complex a K. If X is a K-invariant diffeomorphism, we can use it to deform the set |K|, obtaining a curved isocomplex  $\mathcal{O} = (\hat{f} \circ X)^{-1}(c)$ . As this deformation is bijective, continuous and preserve the incidence relations of K, it results that  $\mathcal{O}$  has the same topology of O. Moreover, the topological and geometrical information of  $\mathcal{O}$  are clearly separated: the topology is codified in the complex K and in the signal of f in the vertices, and the geometry is given by X.



Figure 6: The zero set of function  $f(x, y) = x^2 + y^2 - 0.28^2$  in four versions: in (a), the linear interpolation over complex K is far from the real curve (b). Composition with the identity changes nothing (c), but a suitable diffeo X deforms the linear interpolation closer to the real curve.

Let's relate this representation with two other representations of hypersurfaces. In the implicit representation, the hypersurface is represented as a zero set of a given equation. In the parametric representation, the hypersurface is represented by a collection of patches that covers the hypersurface and are glued each other in a precise way. We can write the expression of  $\mathcal{O}$  above in two ways:

$$\mathcal{O} = (\hat{f} \circ X)^{-1}(c) = X^{-1}(\hat{f}^{-1}(c)),$$

The two equalities above have sligthly different interpretations. In the first case,

$$\mathcal{O} = (\hat{f} \circ X)^{-1}(c),$$

is clearly a implicit hypersurface, being the set of points  $p \in \mathbb{R}^n$  that satisfies equation  $\hat{f}(X(p)) = c$ . In the second case,

$$\mathcal{O} = X^{-1}(\hat{f}^{-1}(c)),$$

says that the set  $\mathcal{O}$  is covered by parametrizations in the form  $X^{-1}(\theta)$ , where  $\theta$  is linear patch of O, being therefore a parametric hypersurface. That is why we call this a *implicit-parametric* representation.

Let's consider how the implicit-representation performs in two typical problems: (1) determine if a point  $p \in \mathbb{R}^n$  is inside or outside  $\mathcal{O}$  and (2) sample points  $q \in \mathcal{O}$ . To solve (1), we find which cell  $\sigma \in K$  contains p, compute  $q = X|_{\sigma}(p)$  and evaluate the signal of  $\hat{f}_{\sigma}(q)$ . For problem (2), we sample a point  $p \in O$ , what is a easy task because O has a simple parametrization for each linear patch  $\theta \subset \sigma \in K$ , and compute  $q = X|_{\sigma}^{-1}(p)$ .

In general, the simplicial diffeomorphism X depends on a set of *intrinsic parameters*  $\beta$ , therefore we will denote the diffeomorphism by  $X_{\beta}$  when necessary. In the case of polynomial diffeomorphisms, for example,  $\beta$  could be represented by a vector of control points. As we will see in section 9, the main task of the applications is to fit the intrinsic parameters to the data.

### 8 Smoothness conditions for curved isocomplexes

By our definition, a simplicial diffeomorphism X is a diffeomorphism in the interior of each simplex of K, but there are no guarantees that X is a global diffeomorphism and, in fact, in the applications we focus, namely the representation of curved isocomplexes, X cannot be a global diffeomorphism. Let's understand why this happens.

Let's consider the case of complex  $K = \sigma \cup \sigma'$ , where  $\sigma = \langle p_0, p_1, \ldots, p_n \rangle$  and  $\sigma' = \langle p'_0, p_1, \ldots, p_n \rangle$ . Note that  $\sigma$  and  $\sigma'$  share a common facet  $\delta = \langle p_1, \ldots, p_n \rangle$ . Let X be a K-invariant diffeomorphism and f a real function defined on the vertices of K. If p is a point in  $\delta \cap \mathcal{O}$ , the hypersurface normal  $\mathcal{O}$  is proportional to the gradient

$$\nabla(\hat{f} \circ X)(p) = \nabla\hat{f}(X(p)).DX(p).$$

But  $\nabla \hat{f}$  is not well defined in  $\delta$ , because  $\hat{f}$  is only piecewise linear. Let  $n = \nabla \hat{f}|_{\sigma}$ and  $n' = \nabla \hat{f}|_{\sigma'}$ . For  $\mathcal{O}$  to be smooth in p is necessary that

$$n.DX(p) = n'.DX(p).$$

If X were smooth at the point p, then DX(p) would be not-singular and therefore we would have that n = n'. In other words,  $\mathcal{O}$  would be smooth in  $\delta$ only if O were also smooth. Thus, in order for  $\mathcal{O}$  to be smooth, the simplicial diffeomorphism X must have a discontinuous derivative in  $\delta$ .

We have to admit that the above fact poses a small difficulty to the analysis, since we are used to continuity conditions and not to discontinuity conditions. Among the various types of simplicial diffeomorphisms that we studied in the previous sections, only in the rational case we were able to derive simple conditions such that  $\mathcal{O}$  be smooth. To simplify the notation, we are going to define  $c_I$  as the control point in cartesian coordinates corresponding to the points  $\frac{I}{n}$ , in the following way.

$$P_{\sigma} \frac{I}{n} = \begin{pmatrix} 1\\ c_I^1\\ \vdots\\ c_I^m \end{pmatrix}.$$

Now, we can state the result:

**Theorem 8.1.** Let X be a rational diffeomorphism K-invariant of degree n, with

$$X|_{\sigma} = \frac{1}{\sum_{|I|=n} q_I B_I} \sum_{|I|=n} q_I c_I B_I \text{ and,}$$
$$X|_{\sigma'} = \frac{1}{\sum_{|I|=n} q'_I B_I} \sum_{|I|=n} q'_I c'_I B_I,$$

where K is like described above. Then  $\mathcal{O}$  is  $C^1$ -continuous in  $\delta$  if

$$q_{J+e_0}\hat{f}|_{\sigma}(c_{J+e_0}) = \sum_i w_i q'_{J+e_i} \hat{f}|_{\sigma'}(c'_{J+e_i}),$$

where |J| = m - 1,  $J^0 = 0$  and  $(w_0, \ldots, w_n)$  are the barycentric coordinates of  $p_0$  in relation to  $\sigma'$ .

*Proof.* Note initially, that if  $p \in \delta \cap \mathcal{O}$  then  $\hat{f}(X(p)) = 0$ , by definition. Moreover, it follows from the linearity of  $\hat{f}$  that

$$\hat{f}(X(p)) = \frac{\sum_{|I|=n} q_I \hat{f}(c_I) B_I(X(p))}{\sum_{|I|=n} q_I B_I(X(p))}.$$

Computing the gradient of  $\hat{f} \circ X$  in p, with relation to the simplex  $\sigma$ , we have that

$$\nabla(\hat{f} \circ X)(p) = \frac{u'v - uv'}{v^2},$$

where

$$u = \sum_{|I|=n} q_I \hat{f}(c_I) B_I(X(p)),$$
$$u' = \sum_{|I|=n} q_I \hat{f}(c_I) \nabla B_I(X(p)),$$
$$v = \sum_{|I|=n} q_I B_I(X(p)),$$
$$v' = \sum_{|I|=n} q_I \nabla B_I(X(p)).$$

But u = 0 because  $u = \hat{f}(X(p)).v$  and v > 0. The gradient at a point  $p \in \delta \cap \mathcal{O}$  is equal to

$$\nabla(\hat{f} \circ X)(p) = \frac{\sum_{|I|=n} q_I \hat{f}(c_I) \nabla B_I(X(p))}{\sum_{|I|=n} q_I B_I(X(p))}$$

The function in the denominator is continuous in  $\delta$ , and the numerator is the gradient of the function  $g(q) = \sum_{|I|=n} q_I \hat{f}(c_I) B_I(q)$  in q = X(p), which is  $C^1$ -continuous in  $\delta$  if

$$q_{J+e_0}\hat{f}|_{\sigma}(c_{J+e_0}) = \sum_i w_i q'_{J+e_i} \hat{f}|_{\sigma'}(c'_{J+e_i}), \tag{6}$$

from the usual  $C^1$ -continuity conditions.

We can apply the condition (6) to all faces of the complex K, what originates a system of linear equations in  $q_I$ , in general underdetermined, whose solutions represent the simplicial diffeomorphisms which make the isocomplex O smooth. However, we have an additional problem: we are interested in the *positive* solutions, since the weights  $q_I$  should be positive. The investigation of existence conditions of such positive solutions is a very interesting topic which we hope to develop in a future paper. Presently, we can attack this problem using optimization. The idea is to consider the error function

$$\operatorname{err}(\delta,\beta) = \sum_{J} \|q_{J+e_0}\hat{f}|_{\sigma}(c_{J+e_0}) - \sum_{i} w_i q'_{J+e_i} \hat{f}|_{\sigma'}(c'_{J+e_i})\|^2,$$

which associates to each face  $\delta$  a value that measures the  $C^1$  discontinuity of the isocomplex in  $\delta$ , where  $\beta$  is a vector containing all the weights  $q_I$ , and then we optimize

$$\min_{\beta>0}\sum_{\delta\in K}\operatorname{err}(\delta,\beta).$$

We tested this method in an aplication with very good results, even though some numerical problems might eventually arise due to small values (near zero) in the denominator.

In any case, the smoothness criterion discussed above is valid only for rational mappings. In the case of polynomial mappings, such analysis becomes difficult because the need to reconcile smoothness criteria with injectivity criteria. Furthermore, in the polynomial models that we proposed, we made extensive use of function composition, what makes the analysis even harder. In those cases, the most viable approach is, once again, to deal with the problem through optimization, now considering the error function

$$\operatorname{err}(\delta,\beta) = \sum_{p_i \in \delta} \|n_{\delta,\beta}(p_i) - n'_{\delta,\beta}(p_i)\|^2,$$

which measures the deviation between the normals with respect to the cells  $\sigma$ and  $\sigma'$  incident at a face  $\delta$  in some number of sample points  $p_i$ , where  $\beta$  denote the intrinsic parameters of the diffeomorphism. We have also implemented this other method with good results. Although we cannot guarantee that the surfaces generated in this way will be smooth at all points, we have a more compact representation than a piecewise linear approximation with the added benefits of a simultaneous parametric and implicit representation. As an example, we are going to discuss briefly in the next section some applications of simplicial diffeomorphisms.

## 9 Applications

In this section we are going to present two applications of using the simplicial diffeomorphisms proposed in this paper. The applications are free-form modeling of implicit shapes and adapted polygonization of implicit objects. In both applications, we use the polynomial diffeomorphisms described in section 5.4.

#### 9.1 Free-Form Modeling of Implict Objects

To present the application of free-form modeling of implicit shapes, first we will briefly describe how the user interacts with the program and subsequently we are going to discuss the implementation.

The basic idea is that the user starts the interaction by visualizing an initial coarse grid  $K_0$ . The user can refine the triangulation using restricted stellar subdivision, obtained a finer simplicial complex K. At the same time, the user can alter some parameters associated with the vertices and edges of K, which are going to determine a curved isocomplex  $\mathcal{O}$  with suport in K.

In each vertex v, the user can make three operations: 1) drag the vertex, moving it to a new position; 2) change the sign s(v), making v to belong either to the interior of the object if s(v) = -1, or to the exterior of the object if s(v) = +1; and change the scalar value r(v). These operations allows one to build a linear isocomplex  $O = \hat{f}^{-1}(0)$ , where f(v) = s(v)r(v), which gives a piecewise linear approximation of the object that we wish to model.

In each edge  $\epsilon$  of K that is intercepted by O, the user has access to two controls, which are responsible for controlling the K-invariant diffeomorphism X. There is a control handle that can be moved along the edge, indicating the point  $p(\epsilon)$  where  $\mathcal{O}$  should intercept the edge. The other control is a unit vector  $n(\epsilon)$ , represented by an arrow, that indicates the direction of the normal of  $\mathcal{O}$ should have at  $p(\epsilon)$ .

These modeling parameters are intuitive for the user, but we need to compute the intrinsic parameters  $\beta$ . For this purpose, we observe that when interpreted mathematically the modeling parameters should satisfy

$$\hat{f} \circ X_{\beta}(p(\epsilon)) = 0 \text{ and } \frac{\nabla(\hat{f} \circ X_{\beta})(p(\epsilon))}{\|\nabla(\hat{f} \circ X_{\beta})(p(\epsilon))\|} = n(\epsilon).$$

such that all edges  $\epsilon$  that are intecepted by  $\mathcal{O}$ , that are the ones with vertices with opposite signs. Let's define the error function

$$\operatorname{err}(\sigma,\beta) = \sum_{\substack{\epsilon = \{v_0, v_1\} \in \sigma \\ s(v_0)s(v_1) < 0}} \left( \frac{F_{\sigma,\beta}^2(p(\epsilon))}{\|\nabla F_{\sigma,\beta}(p(\epsilon))\|^2} + \alpha \| \frac{\nabla F_{\sigma,\beta}(p(\epsilon))}{\|\nabla F_{\sigma,\beta}(p(\epsilon))\|} - n(\epsilon) \|^2 \right),$$

where  $F_{\sigma,\beta} = \hat{f}_{\sigma} \circ X_{\beta}$ , that associates to each cell  $\sigma$ , an error  $\operatorname{err}(\sigma,\beta)$  that measures how much the parameters  $\beta$  satisfy the geometric requisites in each cell  $\sigma$ . The parameter  $\alpha$  is a weight that controls how much emphasis is given to the position or direction of the intersection point.

Thus, to determine the parameters  $\beta$ , we simply minimize the error over all cells of K:

$$\min_{\beta} \sum_{\sigma \in K} \operatorname{err}(\sigma,\beta).$$

Some iterations of this optimization program are performed every time the user updates the modeling parameters. It is possible also to run the optimization program with more interactions in order to obtain a beter result. In Figure 7 we show an example of user interaction.



Figure 7: Example of interaction in the free-form modeling application.

#### 9.2 Polygonization of Implicit Objects

The input to the program for polygonization of implicit objects is a function  $g: [0,1]^n \to \mathbb{R}$ , which we assume continuous and differentiable. We want to determine a curved isocomplex  $\mathcal{O}$  such that

$$\mathcal{O} \subset g^{-1}((-a,a)),$$

for a small, in other words, we would like that  $\mathcal{O}$  lies on a neighborhood of  $g^{-1}(0)$ .

The idea is to build a sequence of isocomplexes  $\mathcal{O}_i = (\hat{f}_i \circ X_{\beta_i})^{-1}(0)$  that approximates  $g^{-1}(0)$ . We set initially  $K_0$  equal to the canonical triangulation of  $[0, 1]^n$ ,  $f_0(v) = g(v)$ , for all  $v \in K_0$ , and  $X_{\beta_0}$  equal to identity. In order to describe the inductive step that computes  $\mathcal{O}_{i+1}$  from  $\mathcal{O}_i$ , we need to define a function  $\operatorname{err}(\sigma_i, \beta_i)$  which associates to each cell  $\sigma_i \in K_i$  an error that measures how close  $\mathcal{O}$ , restricted to  $\sigma_i$ , is from  $g^{-1}(0)$ .

Let  $\theta_i$  be the linear patch of O in  $\sigma_i$ . We compute the m sample points  $p_1, \ldots, p_m$  over  $\theta_i$  and define

$$\operatorname{err}(\sigma_i, \beta_i) = \sum_{p_j \in \theta_i} |g(X_{\beta_i}(p_j))|^2,$$

that is,  $\operatorname{err}(\sigma_i, \beta_i)$  measures how well  $\theta_i$  is taken to  $g^{-1}(0)$  by  $X_{\beta_i}$ .

The inductive step is done in the following way: we choose the cell  $\sigma_i \in K_i$ with the largest error. Subsequently we perform

$$K_{i+1} = \text{SUBDIVIDE}(K_i, \sigma_i),$$

where SUBDIVIDE( $K, \sigma$ ) represents the subdivision of  $\sigma$  with adaptive propagation.

After such subdivision, k new vertices  $v_1, \ldots, v_k$  are inserted, in that order. For each vertex  $v_k$ , we make  $f_{i+1}(v_k) = g(v_k)$ ,  $f_{i+1}$  being equal to  $f_i$  in the other vertices, and we execute the optimization program.

$$\min_{\beta_{i+1}} \sum_{\sigma_{i+1} \in \operatorname{st}(v_k, K_{i+1})} \operatorname{err}(\sigma_{i+1}, \beta_{i+1}),$$

in order to compute  $X_{\beta_{i+1}}$ . Notice that in this way we are computing  $X_{\beta_{i+1}}$  only in the regions of the mesh that were modified by the subdivision.

The stopping criterion is based on the one described in [4]. Let  $I_{\sigma}$  be the smallest *n*-dimensional box which contains a cell  $\sigma$ . The inclusion function  $\Box g$  for a function g computes for each *n*-dimensional box  $I_{\sigma}$  an interval  $\Box g(I_{\sigma})$  such that

$$x \in I_{\sigma} \Rightarrow g(x) \in \Box g(I_{\sigma}).$$

Such an inclusion function for g can be computed by the usual methods of interval arithmetic. Before evaluating the subdivision in a cell  $\sigma$ , we evaluate the condition

$$0 \notin \Box g(I_{\sigma}) \lor \langle \Box \nabla g(I_{\sigma}), \Box \nabla g(I_{\sigma}) \rangle > 0.$$

If the condition is true, the subdivision is not done, that is, if  $\sigma$  does not contains a zero of g or if g is parametrizable along one direction, then it is not necessary to perform the subdivision.

In Figures 8, 9 and 10 we show the polygonization algorithm applied to Taubin's curve,

$$0.004 + 0.110x - 0.177y - 0.174x^{2} + 0.224xy - 0.303y^{2} - 0.168x^{3} + 0.327x^{2}y - 0.087xy^{2} - 0.013y^{3} + 0.235x^{4} - 0.667x^{3}y + 0.745x^{2}y^{2} - 0.029xy^{3} + 0.072y^{4} = 0,$$

in three distinct stages. Note how the geometry is well captured, even with a small number of subdivisions.



Figure 8: Polygonization of Taubin's curve (1).



Figure 9: Polygonization of Taubin's curve (2).



Figure 10: Polygonization of Taubin's curve (3).

# 10 Conclusion

We have developed a theory of simplicial diffeomorphisms. This type of spatial mapping is very powerful and can be used in several applications. In particular, it can be applied to the pieciewise description of shapes through curved isocomplexes. Simplicial diffeomorphisms can also be employed as a general warping mechnism with intuitive controls.

We have shown how to define simplicial diffeomorphisms using the notion of simplicial invariant functions and three alternative ways to construct them with different properties: using monotonic functions; using polynomial basis; and rational polynomials.

We have also discussed conditions to enforce smoothness fo curved isocomplexes generated with simplicial diffeomorphism, and demonstrated examples of applications to free-form modeling and implicit surface approximation.

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### A Linear algebra lemmas

**Lemma A.1.** Let  $A = (a_{ij}) \in \mathbb{R}^{m \times m}$  be a 0-1 matrix where rows and columns have exactly two ones and such that  $\det(A) \neq 0$ . Then there are permutations  $\pi, \gamma \in S_m$ , that are related to permutation matrices  $P = (p_{ij}) e C = (c_{ij})$ , with  $p_{ij} = \delta_{\pi(i),j}$  and  $c_{ij} = \delta_{\gamma(i),j}$ , such that

- 1. PA = Id + C;
- 2.  $\gamma$  is a derangement;
- 3. If  $\gamma = \gamma_1 \gamma_2 \dots \gamma_k$ , where  $\gamma_i$  are disjoint cycles, then each  $\gamma_i$  is even and  $\det(\mathrm{Id} + C) = 2^k$ ;
- 4. If  $B = (b_{ij}) \in \mathbb{R}^{m \times m}$  is a matrix such that  $b_{ij} \ge 0$  and  $b_{ij} = 0 \Leftrightarrow a_{ij} = 0$ , then  $\det(A) \det(B) > 0$ .
- *Proof.* 1. There is a matrix P such that PA has only ones in its diagonal, because otherwise, by the very definition of determinant, det(A) would be zero. Define, therefore, C = PA Id. As A has exactly two ones in each row and column, C has exactly one one in each row and column, hence is a permutation matrix;
  - 2. As C diagonal has only zeros,  $\gamma$  is a derangement;
  - 3. Let D = Id + C. We have that

$$d_{ij} = [i = j] + [\gamma(i) = j].$$

By the definition of determinant,

$$\det(D) = \sum_{\sigma \in S_m} \operatorname{sgn}(\sigma) \Pi_i([i = \sigma(i)] + [\gamma(i) = \sigma(i)]).$$

But

$$\forall i, [i = \sigma(i)] + [\gamma(i) = \sigma(i)] = 1 \Leftrightarrow \sigma = \gamma_{k_1} \dots \gamma_{k_j},$$

where  $\{k_1, \ldots, k_j\} \subset \{1, \ldots, k\}$ . It follows that

$$\det(D) = \sum_{\{k_1, \dots, k_j\} \subset \{1, \dots, k\}} \operatorname{sgn}(\gamma_{k_1} \dots \gamma_{k_j}) = \prod_{i=1}^k (1 + \operatorname{sgn}(\gamma_i)).$$

Therefore each  $\gamma_i$  is a even permutation, because otherwise det(D) would be zero, and det $(D) = 2^k$ .

4.

$$\det(A)\det(B) = \det(P)\det(A)\det(P)\det(B) = \det(D)\det(E)$$

where E = PB is such that  $e_{ij} > 0 \Leftrightarrow d_{ij} > 0$ . Thus the permutations  $\sigma$  such that  $\prod_{i=1}^{m} e_{i\sigma(i)} \neq 0$  are exactly equal to  $\gamma_{k_1} \dots \gamma_{k_j}$ . As each  $\gamma_i$  is even,  $\det(E) > 0$ , and  $\det(A) \det(B) > 0$ .

**Corollary A.2.** Let  $A = (a_{ij}) \in \mathbb{R}^{m \times m}$  be a 0-1 matrix having at most two ones per row and such that  $\det(A) \neq 0$ . If  $B = (b_{ij}) \in \mathbb{R}^{m \times m}$  is a matrix with  $b_{ij} \geq 0$  and  $b_{ij} = 0 \Leftrightarrow a_{ij} = 0$ , then  $\det(A) \det(B) > 0$ .

*Proof.* If A has exactly two ones per row and column, we can apply the previous lemma. Otherwise, we can exchange rows and columns in such a way that

$$P_1AQ_1 = \begin{pmatrix} 1 & 0 \\ q & A_1 \end{pmatrix}$$
 or  $P_1AQ_1 = \begin{pmatrix} 1 & q \\ 0 & A_1 \end{pmatrix}$ 

for permutation matrices  $P_1$  and  $Q_1$ . Note that  $\det(A) = s_1 \det(A_1)$ , with  $s_1 \in \{-1, 1\}$ . Proceeding inductively, we obtain a matrix  $A_n$  that has exactly two ones per row and column, such that

$$\det(A) = s_n \det(A_n).$$

Applying the same procedure to matrix B, we conclude that

$$\det(A) \det(B) = (s_n \det(A_n))(s_n b_1 \dots b_k \det(B_n)) =$$
$$s_n^2(b_1 \dots b_k)(\det(A_n) \det(B_n)) > 0$$

where  $b_i$  are certain elements of B.

**Lemma A.3.** If  $M = \text{Id} + uv^T + ab^T$ , with  $v^T a = 0$ , then

$$\det M = (1 + v^T u)(1 + b^T a).$$

Proof. The identity

$$\det(\mathrm{Id} + uv^T) = 1 + v^T u$$

holds in general, therefore we conclude that

$$\begin{split} \det(N+ab^T) &= \det(N^{-1})\det(N+ab^T)\det(N) = \\ \det(\operatorname{Id}+N^{-1}ab^T)\det(N) &= \det(N) + b^T(\det(N)N^{-1})a, \end{split}$$

for an invertible N. Letting  $N = \mathrm{Id} + uv^T$ , gives

$$N^{-1} = \operatorname{Id} - \frac{1}{1 + v^T u} u v^T,$$

and

$$det(M) = det(N + ab^{T}) = (1 + v^{T}u) + b^{T}((1 + v^{T}u) \operatorname{Id} - uv^{T})a =$$
$$= (1 + v^{T}u)(1 + b^{T}a).$$

**Lemma A.4.** If  $M = \operatorname{diag}(u) + uv^T$ , then

$$\det M = (\prod_i u_i)(1 + \sum_i v_i)$$

Proof.

$$\det(\operatorname{diag}(u) + uv^T) = \det(\operatorname{diag}(u)(\operatorname{Id} + \mathbb{1}v^T)) = (\prod_i u_i)(1 + \sum_i v_i).$$

**Lemma A.5.** Let  $A = [a_{ij}]$  be a  $n \times n$  matrix such that  $\sum_i a_{ij} = 0$ , for all  $j = 1, \ldots, n$ . Then  $A^{ij} = A^{kj}$ , for all  $i, j, k = 1, \ldots, n$ , where  $A^{ij}$  denotes the cofator of A obtained by deleting row i and column j.

*Proof.* We'll show that  $A^{21} = A^{11}$  and the general result follows after a suitable permutation of rows and columns. We have that

$$A^{21} = - \begin{vmatrix} a_{12} & a_{13} & \cdots & a_{1n} \\ a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n2} & a_{n3} & \cdots & a_{nn} \end{vmatrix} = \\ - \begin{vmatrix} -\sum_{i=2}^{n} a_{i2} & -\sum_{i=2}^{n} a_{i3} & \cdots & -\sum_{i=2}^{n} a_{in} \\ a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n2} & a_{n3} & \cdots & a_{nn} \end{vmatrix} = \begin{vmatrix} a_{22} & a_{23} & \cdots & a_{2n} \\ a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n2} & a_{n3} & \cdots & a_{nn} \end{vmatrix} = \begin{vmatrix} a_{22} & a_{23} & \cdots & a_{2n} \\ a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n2} & a_{n3} & \cdots & a_{nn} \end{vmatrix} = \begin{vmatrix} a_{22} & a_{23} & \cdots & a_{2n} \\ a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n2} & a_{n3} & \cdots & a_{nn} \end{vmatrix} = A^{11}.$$