The topological correctness of the PL-approximation of isomanifolds

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Abstract

Isomanifolds are the generalization of isosurfaces to arbitrary dimension and codimension, i.e. manifolds defined as the zero set of some multivariate multivalued function $f : \mathbb{R}^d \to \mathbb{R}^{d-n}$. A natural (and efficient) way to approximate an isomanifold is to consider its Piecewise-Linear (PL) approximation based on a triangulation $\mathcal{T}$ of the ambient space $\mathbb{R}^d$. In this paper, we give conditions under which the PL-approximation of an isomanifold is topologically equivalent to the isomanifold. The conditions can always be met by taking a sufficiently fine triangulation $\mathcal{T}$.

1 Introduction

Isosurfacing especially in low dimensions is used in many fields of application, such as CT scans in medicine, biochemistry, biomedicine, deformable modeling, digital sculpting, environmental science, and mechanics and dynamics, see [29] and the references mentioned there. The marching cube approach [26] being the most popular approach taken. However the result of the marching cube algorithm is not necessarily topologically correct.

Some results on provable correctness were achieved within the computational geometry community [7, 30] in three dimensions. In case the isosurfacing is based on simplices instead of cubes, such as in the marching tetrahedra algorithm [19], some bounds can be given [1, 2], on for example the one-sided Hausdorff distance. In general homeomorphism proofs in higher dimensions rely on some perturbation scheme to prove that a triangulation is correct [34, 5, 8, 9, 12]. This is a major difference with one and two dimensional surfaces where no such requirements exist [21], [31, Section 10.2]. In this paper we shall see that no perturbations are necessary for isomanifolds as well.

The techniques used here are also different from many of the standard tools. Manifold triangulation/reconstruction algorithms use often Delaunay triangulations [32, 18, 14] and use the closed ball property [23], see for example [3, 13]. Others use Whitney's lemma [10] or are based on collapses [4]. While the current paper mainly relies on the non-smooth implicit function theorem [16] with some Morse theory.

We also emphasize that because we do not use a perturbation scheme, we cannot give lower bounds on the quality of the linear pieces in the Piecewise-Linear (PL) approximation. This is a clear difference with previous methods [34, 12, 11, 9] whose output is a thick triangulation. Although thickness is an appealing property, it complicates the analysis further and requires perturbation schemes that work fine in theory, but the constants are miserable and the methods do not work in practice in high dimension.

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This is an extended abstract of a presentation given at EuroCG'20. It has been made public for the benefit of the community and should be considered a preprint rather than a formally reviewed paper. Thus, this work is expected to appear eventually in more final form at a conference with formal proceedings and/or in a journal.

2 Isomanifolds without boundary

Let $f : \mathbb{R}^d \to \mathbb{R}^{d-n}$ be a smooth function and suppose that 0 is a regular value of f, meaning that at every point x such that $f(x) = 0$, the Jacobian of f is non-degenerate. Then the zero set of f is a manifold as a direct consequence of the implicit function theorem, see for example [20, Section 3.5]. We further assume that $f^{-1}(0)$ is compact. As in [1] we consider a triangulation $\mathcal{T}$ of $\mathbb{R}^d$. The function f_{PL} is a linear interpolation of the values of f at the vertices if restricted to a single simplex $\sigma \in \mathcal{T}$. *For any function* $g : \mathbb{R}^d \to \mathbb{R}^{d-n}$ *we write* g^i *for the components of* g.

We prove that under certain conditions there is an isotopy from the zero set of f to the zero set of f_{PL}. The proof will be using the Piecewise-Linear (PL) map $F_{PL}(x, \tau) = (1-\tau)f(x)+\tau f_{PL}(x)$, which interpolates between f and f_{PL} and is based on the generalized implicit function theorem. The isotopy is in fact stronger than just the existence of a homeomorphism from the zero set of f to that of f_{PL}.

Our result in particular implies that the zero set f_{PL} is a manifold. So this significantly improves on the result of Allgower and Georg [2, Theorem 15.4.1]. The conditions are also weaker, because we do not require that the zero set avoids simplices that have dimension less than the codimension, see [2, Definition 12.2.2] and the text above [2, Theorem 15.4.1]. The idea to avoid these low dimensional simplices originates with Whitney [34], with whom Allgower and George [2, 1] were apparently unfamiliar. Very heavy perturbation schemes for the vertices of the ambient triangulation $\mathcal{T}$ are required for the manifold to be sufficiently far from simplices in the ambient triangulations that have dimension less than the codimension of the manifold [34, 12]. Various techniques have been developed to compute such perturbations with guarantees. They typically consist in perturbing the position of the sample points or in assigning weights to the points. Complexity bounds are then obtained using volume arguments. See, for example [13, 11, 8, 6]. However, these techniques suffer from several drawbacks.

We are, by definition, only interested in $f^{-1}(0)$ so we can ignore points that are sufficiently far from this zero set. So,

▶ Remark. Write Σ_0 for the set of all $\sigma \in \mathcal{T}$, such that $(f^i)^{-1}(0) \cap \sigma \neq \emptyset$ for all i. Then for all τ, $\{x \mid F_{PL}(x, \tau) = 0\} \subset \Sigma_0$.

Now we define a few constants, depending only on f and the ambient triangulation $\mathcal{T}$, which will be useful in the statements of the main results.

▶ **Definition 2.1.** We define:

$$\gamma_0 = \inf_{x \in \Sigma_0} |\det(\mathrm{grad}(f^i) \cdot \mathrm{grad}(f^j))_{i,j}|,$$
$$\gamma_1 = \sup_{x \in \Sigma_0} \max_i |\mathrm{grad}(f^i)|,$$

where $|\cdot|$ denotes the Euclidean norm,

$$\alpha = \sup_{x \in \Sigma_0} \max_i \|\mathrm{Hes}(f^i)\|_2 = \sup_x \max_i \|(\partial_k \partial_l f^i)_{k,l}\|_2,$$

D is the longest edge length of a simplex in Σ_0, T is the smallest thickness of a simplex in Σ_0. Here $\mathrm{grad}(f^i) = (\partial_j f_i)_j$ denotes the gradient of component f^i, $\det(\mathrm{grad}(f^i) \cdot \mathrm{grad}(f^j))_{i,j}$ denotes the determinant of the matrix with entries $\mathrm{grad}(f^i) \cdot \mathrm{grad}(f^j)$, $\|\cdot\|_2$ the operator 2-norm, and $(\partial_k \partial_l f_i)_{k,l}$ the matrix of second order derivatives, that is the Hessian (Hes). The thickness is the ratio of the height over the longest edge length. We recall the definition of the operator norm: $\|A\|_p = \max_{x\in\mathbb{R}^n} \frac{|Ax|_p}{|x|_p}$, with $|\cdot|_p$ the p-norm on $\mathbb{R}^n$. We will assume that $\gamma_0, \gamma_1, \alpha, D, T \in (0,\infty)$.

A good choice for $\mathcal{T}$ is the Coxeter triangulation of type A_d, see [17, 15], or the related Freudenthal triangulations, see [24, 25, 22, 33], which can be defined for different values of D while keeping T constant. In this paper, we will thus think of all the above quantities as well as d and n as constants except D and our results will hold for D small enough.

The result

We are going to construct an ambient isotopy. The zero set of $F_{PL}(x,0)$ (or $f(x)$) gives the smooth isosurface, while the zero set of $F_{PL}(x,1)$ (or $f_{PL}(x)$) gives the PL approximation, that is the triangulation of the isosurface after possible barycentric subdivision. The map $\tau \mapsto \{x \mid F_{PL}(x,\tau) = 0\}$ in fact gives an isotopy.

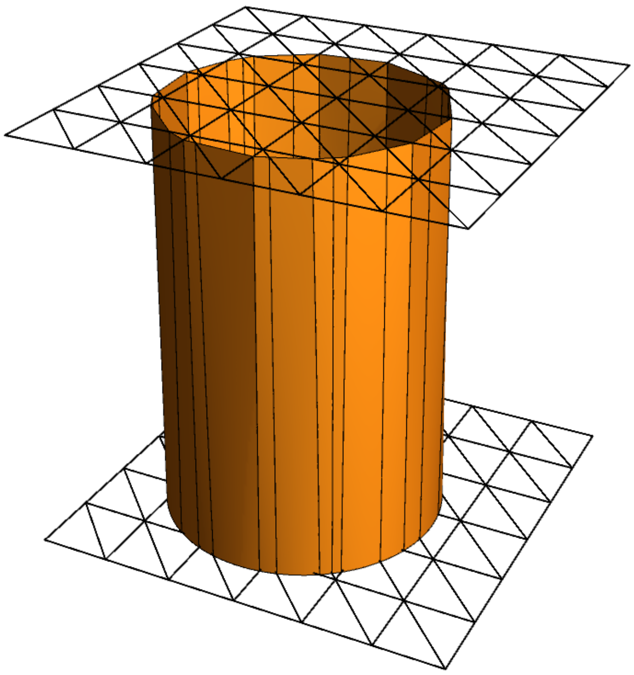

Figure 1 Similarly to Morse theory we find that $f_{PL}^{-1}(0)$ (top) and $f^{-1}(0)$ (bottom) are isotopic if the function τ restricted to $F_{PL}^{-1}(0)$ does not encounter a Morse critical point.

Proving isotopy consists of two technical steps, as well as the use of a standard observation from Morse theory/gradient flow in the third step. The technical steps are 1) Let $\sigma \in \mathcal{T}$. In Corollary 2.6 we show that $\{(x,\tau) \mid F_{PL}(x,\tau) = 0\} \cap (\sigma \times [0,1])$ is a smooth manifold. 2) In Corollary 2.15 we prove that $F_{PL}^{-1}(0)$ is a manifold using nonsmooth analysis.
In Proposition 2.7 we also see that $F_{PL}^{-1}(0)$ is never tangent to the $\tau = c$ planes, where c is a constant. So we find that the gradient field of τ restricted to $F_{PL}^{-1}(0)$, is piecewise smooth and never vanishes.

Now we arrive at the third step, where we use gradient flows to find an isotopy. This is similar to a standard observation in Morse theory [27, 28], with the exception that we now consider piecewise-smooth instead of smooth vector fields. We refer to Milnor [27] for an excellent introduction, see Lemma 2.4 and Theorem 3.1 in particular.

▶ **Lemma 2.2** (Gradient flow induced isotopies). *The flow of a non-vanishing piecewise-smooth gradient vector field of a function τ on a compact manifold generates a isotopy from $\tau = c_1$ to $\tau = c_2$, where c_1 and c_2 are constants.*

2.1 Estimates for a single simplex

We now first concentrate on a single simplex σ and write f_L for the linear function whose values on the vertices of σ coincide with f.

2.1.1 Preliminaries and variations of know results

We need simple estimates similar to Propositions 2.1 and 2.2 of Allgower and Georg [1].

▶ **Lemma 2.3.** *Let $\sigma \subset \Sigma_0$ and let f_L be as described above. Then $|f_L^i(x) - f^i(x)| \leq 2D^2\alpha$ for all $x \in \sigma$.*

▶ **Proposition 2.4.** *Let $\sigma \subset \Sigma_0$ and let f_L be as described above. Then, for all $x \in \sigma = \{v_k\}$,*

$$|\mathrm{grad} f_L^i - \mathrm{grad} f^i| = \sqrt{\sum_j (\partial_j f_L^i(x) - \partial_j f^i(x))^2} \leq \frac{4dD\alpha}{T}.$$

2.1.2 Estimates on the gradient inside a single simplex

We write $F_L(x, \tau) = (1 - \tau)f(x) + \tau f_L(x)$. We note that F_L extends smoothly outside σ. Here and throughout we restrict ourselves to the setting where $\tau \in [0, 1]$. The function F_L has $\mathbb{R}^{d-n}$ as image.

We can now state the following

▶ **Lemma 2.5.** *If we write* $\mathrm{grad}_{(x,\tau)}$ *for the gradient that includes the τ component, we have*

$$|\det(\mathrm{grad}_{(x,\tau)}(F_L^i) \cdot \mathrm{grad}_{(x,\tau)}(F_L^j))_{i,j}| > \gamma_0 - g_1(D), \tag{1}$$

with $g_1(D) = \mathcal{O}(D)$. See (2) *in Appendix 3 for the exact expression of g_1.*

From the previous statement we immediately have that

▶ **Corollary 2.6** ($F_L^{-1}(0)$ is a manifold in a neighbourhood of $\sigma \times [0, 1]$). *If $\gamma_0 > g_1(D)$ the implicit function theorem applies to $F_L(x, \tau)$ inside $\sigma \times [0, 1]$. (In fact it applies to an open neighbourhood of this set). In particular, we have proven the first of our two technical steps, $\{(x, \tau) \mid F_{PL}(x, \tau) = 0\} \cap (\sigma \times [0, 1])$ is a smooth manifold.*

2.1.3 Transversality with regard to the τ-direction

We will also prove the main result which we need for the third step, that is the gradient of τ restricted to $F_{PL}(x, \tau) = 0$, is piecewise smooth and never vanishes. We now prove inside each $\sigma \times [0, 1]$ the gradient of τ on $F_L = 0$ is smooth and does not vanish.

▶ **Proposition 2.7.** *Let $v^1, \ldots, v^{d-n} \in \mathbb{R}^d$, $|v^i| \leq \gamma_1$, for all i, and assume that $\det(v^i \cdot v^j)_{i,j} > \gamma_0$. If $\gamma_0 > g_1(D)$, and $\sqrt{\gamma_0}/\gamma_1^{d-n-1} > \frac{4dD\alpha}{T}$, then inside each $\sigma \times [0, 1]$ the gradient of τ on $F_L^{-1}(0)$ is smooth and does not vanish.*

2.2 Global result

We are now going to prove the global result. For this, we need to recall some definitions and results from non-smooth analysis. We refer to [16] for an extensive introduction.

▶ **Definition 2.8** (Generalized Jacobian, Definition 2.6.1 of [16]). Let $F : \mathbb{R}^{d+1} \to \mathbb{R}^{d-n}$, where F is assumed to be just Lipschitz. The generalized Jacobian of F at x_0 denoted by $J_F(x_0)$, is the convex hull of all $(d-n) \times (d+1)$-matrices B obtained as the limit of a sequence of the form $J_F(x_i)$, where $x_i \to x_0$ and F is differentiable at x_i.

▶ **Definition 2.9** ([16, page 253]). The generalized Jacobian $J_F(x_0)$ is said to be of maximal rank provided every matrix in $J_F(x_0)$ is of maximal rank.

Write $\mathbb{R}^{d+1} = \mathbb{R}^{n+1} \times \mathbb{R}^{d-n}$ and denote the coordinates of $\mathbb{R}^{d+1}$ by (x, y) accordingly. Fix a point (a, b), with $F(a, b) = 0 \in \mathbb{R}^{d-n}$. We now write:

▶ **Notation 2.10** ([16, page 256]). *$J_F(x_0, y_0)|_y$ is the set of all $(n+1)\times(n+1)$-matrices M such that, for some $(n+1) \times (d-n)$-matrix N, the $(n+1) \times (d+1)$-matrix $[N, M]$ belongs to $J_F(x_0, y_0)$.*

▶ **Theorem 2.11** (The generalized implicit function theorem [16, page 256]). *Suppose that $J_F(a, b)|_y$ is of maximal rank. Then there exists an open set $U \subset \mathbb{R}^{n+1}$ containing a such that there exists a Lipschitz function $g : U \to \mathbb{R}^{d-n}$, such that $g(a) = b$ and $F(x, g(x)) = 0$ for all $x \in U$.*

Because of the definition of α, see Definition 2.1, and Proposition 2.4, we have that $\mathrm{grad}_{(x,\tau)} F_{PL}(x, \tau)$ and $\mathrm{grad}_{(x,\tau)} F_{PL}(\tilde{x}, \tau)$ are close if x and $\tilde{x}$ are. In particular,

▶ **Lemma 2.12.** *Let v be a vertex in $\mathcal{T}$, $x_1, x_2 \in star(v)$, and $\tau_1, \tau_2 \in [0, 1]$, such that $\mathrm{grad}_{(x,\tau)} F^i_{PL}(x_1, \tau_1)$ and $\mathrm{grad}_{(x,\tau)} F^i_{PL}(x_2, \tau_2)$ are well defined, then*

$$|\mathrm{grad}_{(x,\tau)} F^i_{PL}(x_1, \tau_1) - \mathrm{grad}_{(x,\tau)} F^i_{PL}(x_2, \tau_2)| \leq \frac{10d^2 D\alpha}{T} + 4\gamma_1 D + 4D^2\alpha.$$

We now immediately have the same bound on points in the convex hull of a number of such vectors:

▶ **Corollary 2.13.** *Suppose we are in the setting of Lemma 2.12 and $x_0, x_1, \ldots, x_m \in star(v)$, $\tau_0, \ldots, \tau_m \in [0, 1]$, and suppose that $\mu_1, \ldots, \mu_m$ are positive weights such that $\mu_1 + \cdots + \mu_m = 1$ then,* $\left|\mathrm{grad}_{(x,\tau)} F^i_{PL}(x_0, \tau_0) - \sum_{k=1}^m \mu_k \mathrm{grad}_{(x,\tau)} F^i_{PL}(x_k, \tau_k)\right| \leq \frac{10d^2 D\alpha}{T} + 4\gamma_1 D + 4D^2\alpha.$

Using Lemma 2.5 we see

▶ **Lemma 2.14.** *Let v be a vertex in $\mathcal{T}$, $x_1, \ldots, x_m \in star(v)$, and $\tau_1, \ldots, \tau_m \in [0, 1]$, such that $\mathrm{grad}_{(x,\tau)} F^i_{PL}(x_k, \tau_k)$, $k = 0, \ldots, m$ are well defined. If we moreover assume $D \leq 1$, and $\frac{6dD\alpha}{T} \leq \gamma_1$ we have that*

$$\left|\det\left(\left(\sum_{k=1}^m \mu_k \,\mathrm{grad}_{(x,\tau)} F^i_{PL}(x_k, \tau_k)\right) \cdot \left(\sum_{k=1}^m \mu_k \,\mathrm{grad}_{(x,\tau)} F_{PL}(x_k, \tau_k)\right)\right)_{i,j}\right| \geq \gamma_0 - g_2(D),$$

with $g_2(D) = \mathcal{O}(D)$. See (3) in Appendix 3 for the exact expression of g_2.

▶ **Corollary 2.15** ($\{x \mid F_{PL}(x, \tau) = 0\}$ is a manifold). *If $D \leq 1$, $\frac{6dD\alpha}{T} \leq \gamma_1$, and $\gamma_0 > g_2(D)$ the generalized implicit function theorem, Theorem 2.11, applies to $F_{PL}(x, \tau) = 0$. In particular, $\{x \mid F_{PL}(x, \tau) = 0\}$ is a manifold.*

This bound is stronger than the one in Corollary 2.6. So, $\{x \mid F_{PL}(x,\tau) = 0\}$ is a Piecewise-Smooth manifold if the conditions of Corollary 2.15 hold. The fact that $F_L(x,\tau) = 0$ is a Piecewise-Smooth manifold and Proposition 2.7 give that the gradient of τ is a Piecewise-Smooth vector field whose flow we can integrate to give an isotopy from the zero set of f to that of f_{PL}. Thus,

▶ **Theorem 2.16.** *If, $D \leq 1$, $\frac{6dD\alpha}{T} \leq \gamma_1$, $\sqrt{\gamma_0}/\gamma_1^{d-n-1} > \frac{4dD\alpha}{T}$, and $\gamma_0 > g_2(D)$ then the zero set of f is isotopic to the zero set of f_{PL}.*

We stress that one can satisfy all conditions by choosing D sufficiently small.

3 Overview of constants

We give an overview. We write Σ_0 for the set of all $\sigma \in \mathcal{T}$, such that $(f^i)^{-1}(0) \cap \sigma \neq$ for all i. We write

$$\begin{aligned}
\gamma_0 &= \inf_{x\in\Sigma_0} |\det(\mathrm{grad}(f^i)\cdot \mathrm{grad}(f^j))_{i,j}| \\
\gamma_1 &= \sup_{x\in\Sigma_0} \max_i |\mathrm{grad}(f^i)| \\
\alpha &= \sup_{x\in\Sigma_0} \max_i \|\mathrm{Hes}(f^i)\|_2 = \sup_x \max_i \|(\partial_k\partial_l f^i)_{k,l}\|_2 \\
D &: \text{ the longest edge length of a simplex in } \Sigma_0 \\
T &: \text{ the smallest thickness of a simplex in } \Sigma_0.
\end{aligned}$$

$\Xi = \mathbb{R}^d \subset \mathbb{R}^{d+1}$ is the space spanned by the d basis vectors corresponding to the x-directions. The precise expressions for the $g_i(D)$ are:

$$g_1(D) = n^{n+1}\left(\gamma_1 + \frac{6dD\alpha}{T}\right)^{2n-1}\left(2\gamma_1\frac{4dD\alpha}{T} + \left(\frac{6dD\alpha}{T}\right)^2\right) \tag{2}$$

$$g_2(D) = n^{n+1}\left(2^{2n-1}\gamma_1^{2n}\left(\frac{14dD\alpha}{T}\right) + 5^{n-1}\gamma_1^{2n-1}(2d+5)\left(\frac{24d^2D\alpha}{T} + 9\gamma_1 D\right)\right) \tag{3}$$

If $\frac{4dD\alpha}{T} \leq \gamma_1$, $g_1(D)$ can be replaced by the simpler $34 \cdot \left(\frac{5}{2}\right)^{2n-1} n^{n+1}\gamma_1^{2n}\frac{dD\alpha}{T}$.

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