Certified Computation of Morse-Smale Complexes on Implicit Surfaces

A. Chattopadhyay * G. Vegter†

Abstract

The Morse-Smale complex is an important tool for global topological analysis in various problems of computational geometry and topology and data processing. A certified algorithm for computing Morse-Smale complexes has been presented in case of two-dimensional gradient vector field in a bounded planar domain [3]. In the current article we extend the approach to the computation of topologically correct Morse-Smale complexes on smooth implicit surfaces given by regular level sets of smooth functions. We present an outline of our method and some implementation results.

1 Introduction

Extracting global topological information of an implicit surface is an important problem in computational topology. One way to extract the global topological information of an implicit surface is by approximating the surface with a simplicial complex followed by a computation of its topological invariants, such as homology groups, Betti numbers, genus etc. There are many existing computational topology tools [4] for doing such an analysis. A second and more direct approach is to analyze the gradient field of a height function on an implicit surface. However, analyzing the gradient field of the height function can be done via computing its Morse-Smale (MS) complex, which is a configuration of singular points and separatrices of the corresponding gradient system. The MS-complex of a gradient system reveals the global topology of the underlying shape. Since it is known that almost all height functions are Morse functions, i.e., functions having only non-degenerate critical points, and by applying a small perturbation, a Morse function could be transformed into a MS function (defined in 2). Therefore, computation of the topologically correct MS-complex of a height function, or more generally, of a MS-function on an implicit surface is a worthwhile problem.

Existing algorithms for MS-complexes can compute the complex of a piecewise linear manifold or, in other words, of a discrete gradient-like vector field [6]. The topological correctness depends on how coarse the discretization is. On the other hand, we consider the problem of computing a *certified* approximation of the MS-complex of a smooth implicit MS-function. In other words we compute a configuration of piecewise-linear curves which is isotopic to the MS-complex on the implicit surface. Our algorithm uses interval arithmetic to bring the computation into the context of Exact Geometric Computation (EGC) paradigm [8].

Our contribution. In the current paper, we present an algorithm for computing a certified approximation of the MS-complex of a smooth implicit MS-function defined on an implicit surface. In particular, the algorithm determines the followings.

- isolated *certified boxes* each containing a unique saddle, source or sink, and each box has the local topological property of a saddle, source or sink;
- *certified initial and terminal intervals* (corresponding to a saddle), each of which is guaranteed to contain a unique point corresponding to a saddle-source or saddle-sink connector (separatrix);
- disjoint *certified strips*, lying on the implicit surface, around each separatrix, each of which containing exactly one separatrix and can be made as close to the separatrix as desired.

2 Preliminaries

Interval arithmetic (IA). Interval arithmetic is used to cope with rounding errors in finite precision computations. A *range function* $\Box F$ for a function $F : \mathbb{R}^m \to \mathbb{R}^n$ computes for each m-dimensional input interval I (i.e., an m-box) an n-dimensional output interval $\Box F(I)$, such that $F(I) \subset \Box F(I)$. A range function is said to be *convergent* if the diameter of the output interval converges to 0 when the diameter of the input interval shrinks to 0.

Morse function. A function $h : \mathcal{M} \subset \mathbb{R}^3 \to \mathbb{R}$, defined on an implicit manifold $\mathcal{M}$, is called a *Morse function* if all its critical points are non-degenerate. The *Morse lemma* [6] states that near a non-degenerate critical point a it is possible to choose local co-ordinates x, y in which h is expressed as $h(x, y) = h(a) \pm x^2 \pm y^2$. The number of minus signs is called the index $i_h(a)$ of h at a. Thus a two variable Morse function has three types of non-degenerate critical points: minima (index 0), saddles (index 1) and maxima (index 2).

*Department of Mathematics and Computing Science, University of Groningen, A.Chattopadhyay@rug.nl

†Department of Mathematics and Computing Science Science, University of Groningen, G.Vegter@rug.nl

Integral line. An integral line $x : I \subset \mathbb{R} \to \mathcal{M}$ passing through a point p_0 on $\mathcal{M}(\subset \mathbb{R}^3)$ is the unique maximal curve satisfying: $\dot{x}(t) = \mathbf{grad}\, h(x(t))$, $x(0) = p_0$, for all $t \in I$. Here the gradient is defined with respect to the metric inherited from $\mathbb{R}^3$. Integral lines corresponding to the gradient vector field of a smooth function $h : \mathcal{M} \to \mathbb{R}$ have many interesting properties, such as: (1) any two integral lines are either disjoint or coincide; (2) an integral line $x : I \to \mathcal{M}$ through a point p of h is injective and if $\lim_{t\to\pm\infty} x(t)$ exists, it is a critical point of h; (3) the function h is strictly increasing along the integral line of a regular point of h and integral; (4) regular integral lines are perpendicular to regular level sets of h.

Stable and unstable manifolds. Consider the integral line $x(t)$ passing through a point p. If the limit $\lim_{t\to\infty} x(t)$ exists, it is called the ω-limit of p and is denoted by $\omega(p)$. Similarly, $\lim_{t\to-\infty} x(t)$ is called the α-limit of p and is denoted by $\alpha(p)$ – again provided this limit exists. The stable manifold of a singular point p is the set $W^s(p) = \{q \in \mathcal{M} \mid \omega(q) = p\}$. Similarly, the unstable manifold of a singular point p is the set $W^u(p) = \{q \in \mathcal{M} \mid \alpha(q) = p\}$ [7]. Here we note that both $W^s(p)$ and $W^u(p)$ contain the singular point p itself [7]. The components of $W^s(p) \setminus \{p\}$ ($W^u(p) \setminus \{p\}$) are called stable (unstable) separatrices. Each saddle has two stable and two unstable separatrices.

The Morse-Smale (MS) complex. A Morse function on $\mathcal{M}$ is called a MS-function if its stable and unstable manifolds intersect *transversally*. Since $\mathcal{M}$ is a 2-dimensional surface, this means that stable and unstable separatrices are disjoint. In particular, there are no saddle-saddle connections. The MS-complex associated with a MS-function h on $\mathcal{M}$ is the subdivision of $\mathcal{M}$ formed by the connected components of the intersections $W^s(p) \cap W^u(q)$, where p, q range over all singular points of h. According to the quadrangle lemma [6], each region of the MS-complex is a quadrangle with vertices of index $0, 1, 2, 1$, in this order on the boundary of the region.

Jacobi set. Let us consider two Morse functions $f, H : \mathbb{R}^3 \to \mathbb{R}$. Let c be a regular value of f and then by implicit function theorem $\mathcal{M}_c := f^{-1}(c)$ is a smooth 2-manifold. Then generically, the restriction h_c of H to the regular level set $\mathcal{M}_c$ of f is a Morse function [5]. The critical points of H restricted to a level set of the function f correspond to points where ∇f is a multiple of ∇H, i.e., the points where the Jacobian of the map $\mathcal{F} = (f, H) : \mathbb{R}^3 \to \mathbb{R}^2$ has rank < 2. The Jacobi set $\mathbb{J}(f, H)$ (or $\mathbb{J}$ for short) is the closure of the set of critical points of such level set restrictions $\mathbb{J}(f, H) = cl\{\mathbf{x} \in \mathcal{M}_c : \mathbf{x}$ is a critical point of $h_c\}$, for any regular value $c \in \mathbb{R}$. From the Smooth Embedding Theorem [5] we have, generically, that the Jacobi set of two Morse functions $f, H : \mathbb{R}^3 \to \mathbb{R}$ is a smoothly embedded 1-manifold in $\mathbb{R}^3$.

3 Method

Problem set-up. Let $f : \mathbb{R}^3 \to \mathbb{R}$ be a $\mathcal{C}^2$ function, and let zero be a regular value of f. Then the set $\mathcal{M} = \{\mathbf{x} \equiv (x, y, z) \in \mathbb{R}^3 : f(\mathbf{x}) = 0\}$ is a regular surface (Follows from the *implicit function theorem*). Let $H : \mathbb{R}^3 \to \mathbb{R}$ be a Morse function such that H has no critical point on $\mathcal{M}$. Then, generically, the function $h : \mathcal{M} \to R$, defined by $h = H|_{\mathcal{M}}$, is a Morse function. We assume h is a MS-function. Then the corresponding gradient field is a MS-system. We are interested in computing the MS-complex of $\mathbf{grad}\, h$.

Gradients on surfaces. First we analyze the vector field $\mathbf{grad}\, h$ by finding its singularities and their types. We have assumptions: (1) zero is a regular value of f and (2) H has no critical point on $\mathcal{M} = f^{-1}(0)$. For a $\mathcal{C}^2$ function h on a compact manifold $\mathcal{M}$ the gradient vector field $\mathbf{grad}\, h$ on $\mathcal{M}$ is characterized as follows: for $p \in \mathcal{M}$ and $\mathbf{grad}\, h(p) \in T_p\mathcal{M}$, $\langle \mathbf{grad}\, h(p), v\rangle = d_v h(p), \quad \forall v \in T_p\mathcal{M}$. Here, $d_v h$ is called the directional derivative of h along v. Again from figure 1, we note that

$$\begin{aligned}\mathbf{grad}\, h(p) &= proj_{\mathcal{M}} \nabla H(p) = \nabla H(p) - (\nabla H(p).\hat{n})\hat{n} \\ &= \nabla H(p) - \frac{\nabla f(p) \cdot \nabla H(p)}{\|\nabla f(p)\|^2} \nabla f(p).\end{aligned}$$

Here $\hat{n}$ is the unit normal vector at point p of the implicit surface $\mathcal{M}$.

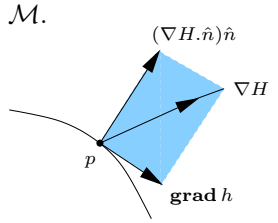


Figure 1: Tangential and normal components of ∇H.

Local expression in a parametric domain. Let $f_z(p) \neq 0$ at $p \in \mathcal{M}$. Then locally near p the manifold $\mathcal{M}$ can be parametrized by a map $\tau : U \to \mathbb{R}^3$ of the form $\tau(x, y) = (x, y, g(x, y))$, where U is an open subset of $\mathbb{R}^2$. Let $q \in U$ be the point in U corresponding to p, i.e., $\tau(q) = p$. Let us consider $\tilde{h}(x, y) = H(x, y, g(x, y))$, locally in U. Then we denote the local gradient field as $\nabla\tilde{h}$ where $\tilde{h}_x = H_x - \frac{f_x}{f_z} H_z$ and $\tilde{h}_y = H_y - \frac{f_y}{f_z} H_z$. Similarly, one can derive local expressions of the gradient field on the yz and zx-plane, by assuming $f_x \neq 0$ and $f_y \neq 0$ respectively.

Again the integral curves of $\mathbf{grad}\, h$ (on $\mathcal{M}$) are projected onto integral curves of the vector field $\mathrm{grad}_{\tau^* G}\tilde{h}$ on $U \subseteq \mathbb{R}^2$ given by,

$$X = \frac{1}{f_x^2 + f_y^2 + f_z^2} \begin{pmatrix} (f_y^2 + f_z^2)\, H_x - f_x f_y\, H_y - f_x f_z\, H_z \\ -f_x f_y\, H_x + (f_y^2 + f_z^2)\, H_y - f_y f_z\, H_z \end{pmatrix}.$$

In particular, the integral curves of $\mathbf{grad}\, h$ are mapped onto those of $\mathrm{grad}_{\tau^* G}\tilde{h}$ by the projection τ^{-1} of the neighborhood $\tau(U)$ of p in $\mathcal{M}$ onto the xy-plane.

Note that a singular point $(x_0, y_0, z_0) \in \mathcal{M}$ of $\mathbf{grad}\, h$ has the same type (saddle, sink or source) as the point (x_0, y_0), considered as a singular point of $\nabla\tilde{h}$ (even though the integral curves of the latter gradient are different from the projections of the integral curves of $\mathbf{grad}\, h$). We use this observation in the following analysis of saddles, sinks and sources.

To determine the type (minima, maxima or saddle) and nature (degenerate or non-degenerate) of the critical points we consider the bordered Hessian matrix, which is expressed as:

$$\mathcal{H}L = \begin{pmatrix} 0 & -f_x & -f_y & -f_z \\ -f_x & L^{xx} & L^{xy} & L^{xz} \\ -f_y & L^{xy} & L^{yy} & L^{yz} \\ -f_z & L^{xz} & L^{yz} & L^{zz} \end{pmatrix}.$$

where $L^{xx} = H_{xx} - \frac{H_z}{f_z} f_{xx}$ etc. Let $\det \mathcal{H}L$ be the corresponding determinant. The following theorem [9] gives a necessary and sufficient condition for h to have a critical point.

Theorem 1 *Let X be open in $\mathbb{R}^3$ and let $f, H : X \to \mathbb{R}$ be functions of class C^2 such that 0 is a regular value of f. Let $\mathcal{M}$ be the manifold $\{\mathbf{x} \in X : f(\mathbf{x}) = 0\}$ and let $\mathbf{x}_0$ be a point on $\mathcal{M}$. Then h (the restriction of H to $\mathcal{M}$) has a critical point at $\mathbf{x}_0$ iff there exists some scalar λ such that $\nabla H(\mathbf{x}_0) = \lambda \nabla f(\mathbf{x}_0)$.*

Monotonicity of f on $\mathbb{J}$. Finally, for certified isolation of a critical point of h inside a box I we first prove that along each component of the Jacobi set $\mathbb{J}$, inside I, function f is monotonic in the following theorem:

Theorem 2 *Consider a box I, in the domain of the function f, satisfying (i) $I \cap \mathcal{M} \neq \emptyset$, (ii) $\nabla f \neq 0$, (iii) $\nabla H \neq 0$, (iv) $\det \mathcal{H}L \neq 0$. Then if $I \cap \mathbb{J} \neq \emptyset$, 1. $\mathbb{J}$ is regular, 2. $\mathbb{J}$ can have at most finitely many components inside I, 3. Each component of $\mathbb{J}$ is transversal to $\mathcal{M}$ inside I, 4. f is monotonic along each component of $I \cap \mathbb{J}$.*

Isolating and detecting critical points of h. Here we describe the first step of our MS-complex computation method. Let us consider a three-dimensional bounding box, say B, that contains the implicit surface $\mathcal{M}$. Now the subdivision algorithm subdivides the box B until for each subinterval, I say, it is possible to determine whether h has a unique critical point inside I or not. The subdivision process is driven by the following set of conditions:

(i) $C_1 : 0 \in \Box f(I)$

(ii) $C_2 : o \in \Box\nabla H(I) \times \Box\nabla f(I)$

(iii) $C_3 : \langle \Box\nabla f(I), \Box\nabla f(I)\rangle > 0$

(iv) $C_4 : 0 \notin \Box\nabla H(I)$

(v) $C_5 : 0 \notin \det \Box\mathcal{H}L(I)$

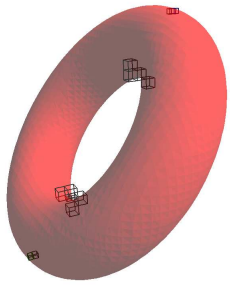


Figure 2: Finding Critical Boxes by domain subdivision

In the subdivision process, if $\neg C_1$ holds for an interval I then I does not contain a zero of f and we stop further subdivision of I. In the subdivision process, if $\neg C_2$ holds, then we stop further subdividing that interval I, since by Theorem 1, in that case I is not a possible candidate for containing a critical point of h. C_3 is a *small normal variaton* condition ensuring parametrizability of $\mathcal{M} \cap I$. C_4 ensures the non-singularity of function H in I. Finally, C_5 ensures that the number of critical points of h in I is at most one. The following subdivision algorithm isolates the critical points of a MS-function h in a bounding box B

Algorithm. SearchCritical(h, B)

1. Initialize an octree $\mathcal{T}$ to the bounding box B.
2. Subdivide $\mathcal{T}$ until for all the leaves I we have:

$$\neg C_1 \vee \neg C_2 \vee (C_3 \wedge C_4 \wedge C_5).$$

3. For each leaf I_l
4. Do if C_1, C_2, C_3, C_4 and C_5 hold then
5. Check if $\mathbb{J}(f, H) \cap \mathcal{M} \neq \emptyset$ inside I_l.
6. If intersection found, the leaf contains a critical point of h. Denote this leaf as I_c.
7. Else, the leaf does not contain a critical point of h.

Now the following corollary of theorem 2 gives a strategy to determine whether inside I_l $\mathbb{J}(f, H) \cap \mathcal{M}$ is $\emptyset$ or not.

Corollary 3 *Let I_l be a leaf interval, obtained by* SearchCritical *(I_l can contain at most one critical point of h). Assume that (i) the Jacobi set $\mathbb{J}(f, H)$ intersects the faces of I_l transversally, and (ii) there is no critical point of h lying on a face of I_l. Let n_{pos} be the number of intersection points of $\mathbb{J}(f, H)$ with the six faces of I_l, where f is positive. Again let n_{neg} be*

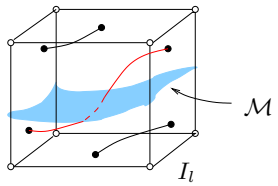


Figure 3: Components of the Jacobi set inside I_l.

the number of intersection points of $\mathbb{J}(f, H)$ with six faces of I_l, where f is negative. If both n_{pos} and n_{neg} are odd numbers, then there is exactly one critical point of h inside I_l. Otherwise, there is no critical point of h inside I_l.

Here we note that the assumptions in the corollary 3 ensure only the non-degenerate cases. In the full article, cf [2], we describe how to handle degenerate cases with small perturbation of interval I.

Refinement of intervals containing critical points. Next we further refine the boxes I_c as in the planar vector field situation, see [3, 2]. In the current situation we use the vector field X projected onto one of the faces of I_c, and after refinement use the corresponding pull-back vector field on $\mathcal{M}$.

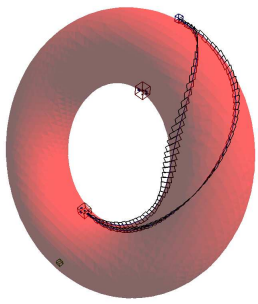
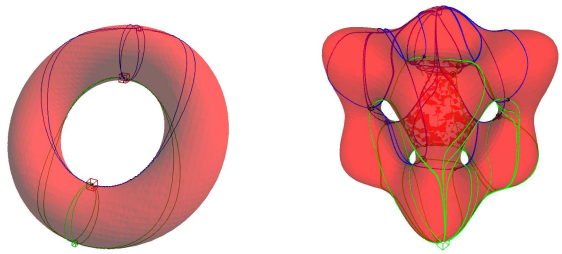


Figure 4: Representing a curve on the implicit surface by the intersection of plane-segments and the surface.

Algorithm for computing separatrices. We compute small rectangular plane-segments, transversal to the implicit surface, such that the intersections of these pieces of planes and the implicit surface together represent a boundary curve of the strip (Figure 4) which contains a separatrix. The gradient vector field **grad** h must satisfy an orientation property which is along the left (for the right boundary curve) and along the right (for the left boundary curve). This will ensure that each separatrix lies in the corresponding strip. The details of this method are discussed in the full version of the article, cf [2].

Implementation results. We implemented of our algorithm using `Boost` library [1] for IA. All experiments have been performed on a 3GHz Intel Pentium 4 machine under Linux with 1 GB RAM using the `g++` compiler, version 3.3.5. Figure 5 show MS-complexes consisting of saddles (red boxes), minima (green boxes) and maxima (blue boxes). Moreover, a pair of blue boundary curves contains a certified unstable separatrix (saddle-maximum connection) and a pair of green boundary curves contains a stable separatrix (saddle-minimum connection).



(a) (b)

Figure 5: Certified MS-complexes on implicit functions given by $f_1(x, y, z) \equiv (x^2 + y^2 + z^2 - R^2 - r^2)^2 - 4R^2(r^2 - x^2) = 0$ and $f_2(x, y, z) \equiv x^4 - 5x^2 + y^4 - 5y^2 + z^4 - 5z^2 + 10 = 0$ where we consider $H(x, y, z) = z$.

Conclusion. We give a novel approach for computing the certified MS-complex on implicit surfaces. In the end some implementation results are given to give a proof of concept and to justify those algorithms.

References

[1] `Boost` interval arithmetic library. `http://www.boost.org`.

[2] A. Chattopadhyay. *Certified Geometric Computation: Radial Basis Function based Isosurfaces and Morse-Smale Complexes.* PhD thesis, University of Groningen, 2010.

[3] A. Chattopadhyay, S.J. Holtman, and G. Vegter. Certified computation of planar Morse-Smale complexes. In *Abstracts of the 26th European Workshop on Computational Geometry*, pages 105–108, Dortmund, Germany, March 22-24 2010.

[4] H. Edelsbrunner and J. Harer. *Computational Topology. An Introduction.* Amer. Math. Soc., Providence, Rhode Island, 2010.

[5] H. Edelsbrunner and J. Harer. Jacobi Sets of Multiple Morse Functions. In *In Foundations of Computational Mathematics*, pages 37–57, Minneapolis 2002, eds.

[6] H. Edelsbrunner, J. Harer, and A. Zomorodian. Hierarchical Morse-Smale complexes for piecewise linear 2-manifolds. *Discrete Comput. Geom*, 30:87–107, 2003.

[7] M. W. Hirsch and S. Smale. *Differential Equations, Dynamical Systems, and Linear Algebra.* Academic Press, 1974.

[8] C. Li, S. Pion, and C. Yap. Recent progress in Exact Geometric Computation. *J. of Logic and Algebraic Programming*, 64(1):85–111, 2004. Special issue on "Practical Development of Exact Real Number Computation".

[9] S. Plantinga and G. Vegter. Computing contour generators of evolving implicit surfaces. *ACM Transactions on Graphics.*, 25:1243–1280., 2006.