Jacobi Sets of Multiple Morse Functions [*]

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Abstract

The Jacobi set of two Morse functions defined on a common d-manifold is the set of critical points of the restrictions of one function to the level sets of the other function. Equivalently, it is the set of points where the gradients of the functions are parallel. For a generic pair of Morse functions, the Jacobi set is a smoothly embedded 1-manifold. We give a polynomial-time algorithm that computes the piecewise linear analog of the Jacobi set for functions specified at the vertices of a triangulation, and we generalize all results to more than two but at most d Morse functions.

Keywords. Differential and computational topology, Morse functions, critical points, level sets, Betti numbers, algorithms.

1 Introduction

This paper is a mathematical and algorithmic study of multiple Morse functions, and in particular of their Jacobi sets. As we will see, this set is related to the Lagrange multiplier method in multi-variable calculus of which our algorithm may be viewed as a discrete analog.

Motivation. Natural phenomena are frequently modeled using continuous functions, and having two or more such functions defined on the same domain is a fairly common scenario in the sciences. Consider for example oceanography where researchers study the distribution of various attributes of water, with the goal to shed light on the ocean dynamics and gain insight into global climate changes [4]. One such attribute is temperature, another is salinity, an important indicator of water density. The temperature distribution is often studied within a layer of constant salinity, because water

tends to mix along but not between these layers. Mathematically, we may think of temperature and salinity as two continuous functions on a common portion of three-dimensional space. A layer is determined by a level surface of the salinity function, and we are interested in the temperature function restricted to that surface. This is a continuous function on a two-dimensional domain, whose critical points are generically minima, saddles, and maxima. In this paper, we study the paths these critical points take when the salinity value varies. As it turns out, these paths are also the paths the critical points of the salinity function take if we restrict it to the level surfaces of the temperature function. More generally, we study the relationship between continuous functions defined on a common manifold by analyzing the critical points within level set restrictions.

Sometimes it is useful to make up auxiliary functions to study the properties of given ones. Consider for example a function that varies with time, such as the gravitational potential generated by the sun, planets, and moons in our solar system [18]. At the critical points of that potential, the gravitational forces are at an equilibrium. The planets and moons move relative to each other and the sun, which implies that the critical points move, appear, and disappear. To study such a time-varying function, we introduce another, whose value at any point in space-time is the time. The paths of the critical points of the gravitational potential are then the Jacobi set of the two functions defined on a common portion of space-time.

Results. The main object of study in this paper is the Jacobi set $\mathbb{J} = \mathbb{J}(f_0, f_1, \ldots, f_k)$ of $k + 1 \leq d$ Morse functions on a common d-manifold. By definition, this is the set of critical points of f_0 restricted to the intersection of the level sets of f_1 to f_k. We observe that $\mathbb{J}$ is symmetric in the $k + 1$ functions because it is the set of points at which the $k + 1$ gradient vectors are linearly dependent. In the simplest non-trivial case, we have two Morse functions on a common 2-manifold. In this case, the Jacobi set $\mathbb{J} = \mathbb{J}(f, g) = \mathbb{J}(g, f)$ is generically a collection of pairwise disjoint smooth curves that are free of any self-intersections. Figure 1 illustrates the concept for two Morse functions on

the two-dimensional torus. The Jacobi set of a generic collection of $k + 1$ Morse functions is a submanifold of dimension k, provided $d > 2k - 2$. The first time this inequality fails is for $d = k + 1 = 4$. In this case, the Jacobi set is a 3-manifold except at a discrete set of points.
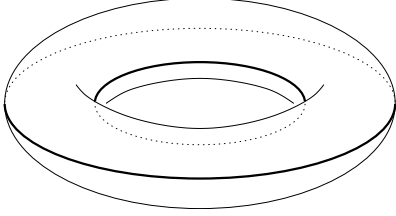

Figure 1: The two partially bold and partially dotted longitudinal circles form the Jacobi set of $f, g : \mathbb{M} \to \mathbb{R}$, where $\mathbb{M}$ is the torus and f and g map a point $x \in \mathbb{M}$ to the Cartesian coordinates of its orthogonal projection on a plane parallel to the longitudes.

We describe an algorithm that computes an approximation of the Jacobi set for $k + 1$ piecewise linear functions that are interpolated from values given at the vertices. In the absence of smoothness, it simulates genericity and differentiability and computes $\mathbb{J}$ as a subcomplex of the triangulation. The algorithm is combinatorial (as opposed to numerical) in nature and reduces the computations to testing the criticality of the k-simplices in the triangulation. Whether or not a simplex is considered critical depends on its local topology. By using Betti numbers to express that topology, we get an algorithm that works for triangulated manifolds and runs in time that is polynomial in the number of simplices. Assuming the links have sizes bounded from above by a constant, the running time is proportional to the number of simplices.

Related prior work. The work in this paper fits within the general area of singularities of smooth mappings, which was pioneered by Hassler Whitney about half a century ago; see eg. [19]. In this body of work, the *fold* of a mapping from a d-dimensional manifold $\mathbb{M}^d$ to a $(k + 1)$-dimensional manifold $\mathbb{N}^{k+1}$ is the image of the set of points at which the matrix of partial derivatives has less than full rank. In this paper, we consider $(k + 1)$-tuplets of Morse functions, which are special smooth mappings in which the range is the $(k + 1)$-dimensional Euclidean space, $\mathbb{R}^{k+1}$. The fold of such a special mapping is the image of the Jacobi set. Our restriction to Euclidean space is deliberate as it furnishes the framework needed for our algorithm.

Whitney considered the case of a mapping between surfaces and studied mappings where d is small relative to k. A classic theorem in differential topology is the Whitney Embedding Theorem which states that a closed, orientable manifold of dimension n can always be embedded in $\mathbb{R}^{2n}$. Thom extended the work of Whitney, studying the spaces of jets (two functions have the same k-jet at p if their partial derivatives of order k or less are equal). The Thom Transversality

Theorem, together with the Thom-Boardman stratification of C^∞ functions on $\mathbb{M}$, give characterizations of the singularities of generic functions [11]. Mather studied singularities from a more algebro-geometric point of view and proved the equivalence of several definitions of stability for a map (a concept not used in this work). In particular he provided the appropriate framework to reconstruct a map from its restrictions to the strata of the Thom-Boardman stratification.

In a completely different context, Nicola Wolpert used Jacobi curves to develop exact and efficient algorithms for intersecting quadratic surfaces in $\mathbb{R}^3$ [20]. She does so by reducing the problem to computing the arrangement of the intersection curves projected to $\mathbb{R}^2$. Any such curve can be written as the zero set of a smooth function $\mathbb{R}^2 \to \mathbb{R}$, and any pair defines another curve, namely the Jacobi set of the two functions. Wolpert refers to them as *Jacobi curves* and uses them to resolve tangential and almost tangential intersections. To be consistent with her terminology, we decided to modify that name and to refer to our more general concept as Jacobi sets.

Outline. Section 2 reviews background material from differential and combinatorial topology. Section 3 introduces the Jacobi set of two Morse functions. Section 4 describes an algorithm that computes this set for piecewise linear data. Section 5 generalizes the results to three or more Morse functions. Section 6 discusses a small selection of applications. Section 7 concludes the paper.

2 Background

This paper contains results for smooth and for piecewise linear functions. We need background from Morse theory [15, 16] for smooth functions and from combinatorial and algebraic topology [1, 17] for designing an algorithm that works on piecewise linear data.

Morse functions. Let $\mathbb{M}$ be a smooth and compact d-manifold without boundary. The differential of a smooth map $f : \mathbb{M} \to \mathbb{R}$ at a point x of the manifold is a linear map $\mathrm{d}f_x : \mathrm{TM}_x \to \mathbb{R}$ mapping the tangent space at x to $\mathbb{R}$. A point $x \in \mathbb{M}$ is *critical* if $\mathrm{d}f_x$ is the zero map; otherwise, it is *regular*. Let $\langle , \rangle$ be a Riemannian metric, i.e. an inner product in the tangent spaces that varies smoothly on $\mathbb{M}$. Since each vector in TM_x is the tangent vector to a curve c in $\mathbb{M}$ through x, the *gradient* ∇f can be defined by the formula $\langle \partial c / \partial t, \nabla f \rangle = \partial (f \circ c) / \partial t$, for every c. It is always possible to choose coordinates x_i so that the tangent vectors $\frac{\partial}{\partial x_i}(x)$ are orthonormal with respect to the Riemannian metric. For such coordinates, the gradient is given by the familiar formula

$$\nabla f(x) = \left[\frac{\partial f}{\partial x_1}(x), \frac{\partial f}{\partial x_2}(x), \ldots, \frac{\partial f}{\partial x_d}(x) \right].$$

We compute in local coordinates the *Hessian* of f:

$$H_f(x) \quad = \quad \left[\begin{array}{ccc} \frac{\partial^2 f}{\partial x_1^2}(x) & \cdots & \frac{\partial^2 f}{\partial x_d \partial x_1}(x) \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_1 \partial x_d}(x) & \cdots & \frac{\partial^2 f}{\partial x_d^2}(x) \end{array} \right],$$

which is a symmetric bi-linear form on the tangent space $\mathrm{T}\mathbb{M}_x$. A critical point p is *non-degenerate* if the Hessian is non-singular at p. The Morse Lemma states that near a non-degenerate critical point p, it is possible to choose local coordinates so that the function takes the form

$$f(x_1, \ldots, x_d) \quad = \quad f(p) \pm x_1^2 \pm \ldots \pm x_d^2.$$

The number of minus signs is the *index* of p; it equals the number of negative eigenvalues of $H_f(p)$. The existence of these local coordinates implies that non-degenerate critical points are isolated. The function f is a called a *Morse function* if

(i) all its critical points are non-degenerate, and

(ii) $f(p) \neq f(q)$ for all critical points $p \neq q$.

Transversality and stratification. Let $F : \mathbb{X} \to \mathbb{Y}$ be a smooth map between two manifolds, and let $\mathbb{U} \subseteq \mathbb{Y}$ be a smooth submanifold. The map F is *transversal* to $\mathbb{U}$ if for every $y \in \mathbb{U}$ and every $x \in F^{-1}(y)$, we have $\mathrm{d}F_x(\mathrm{T}\mathbb{X}_x) + \mathrm{T}\mathbb{U}_y = \mathrm{T}\mathbb{Y}_y$. In words, the basis vectors of the image of the tangent space of $\mathbb{X}$ at x under the derivative together with the basis vectors of the tangent space of $\mathbb{U}$ at $y = F(x)$ span the tangent space of $\mathbb{Y}$ at y. The Transversality Theorem of differential topology asserts that if F is transversal to $\mathbb{U}$ then $F^{-1}(\mathbb{U})$ is a smooth submanifold of $\mathbb{X}$ and the co-dimension of $F^{-1}(\mathbb{U})$ in $\mathbb{X}$ is the same as that of $\mathbb{U}$ in $\mathbb{Y}$ [12].

A continuous family connecting two Morse functions necessarily goes through transitions at which the function violates conditions (i) and (ii) of a Morse function. We are interested in the minimum number of violations that cannot be avoided. For this purpose, consider the infinite-dimensional Hilbert space $C^\infty(\mathbb{M})$ of smooth functions $\mathbb{M} \to \mathbb{R}$. There is a stratification $C^\infty(\mathbb{M}) = C_0 \supset C_1 \supset C_2$, in which $C_0 - C_1$ is the set of Morse functions, $C_1 - C_2$ is the set of functions that violate either condition (i) or (ii) exactly once, and C_2 is the set of remaining functions. The set $C_0 - C_1$ is a submanifold of co-dimension 0, $C_1 - C_2$ is a submanifold of co-dimension 1, and C_2 has co-dimension 2. As an illustration of how we use the stratification, take two Morse functions f and g and consider the 1-parameter family of functions $h_\lambda = f + \lambda g : \mathbb{M} \to \mathbb{R}$. We can perturb one of the functions such that

- f and $f + g$ are both Morse,
- all h_λ belong to $C_0 - C_2$, and
- the 1-parameter family is transversal to $C_1 - C_2$.

If follows that h_λ belongs to $C_1 - C_2$ for only a discrete collection of values for λ. We use this later to prove the transversality of certain maps, which will then put us into the position to apply the Transversality Theorem.

Triangulations. A k-*simplex* is the convex hull of $k + 1$ affinely independent points. Given two simplices σ and τ, we write $\tau \leq \sigma$ if τ is a face of σ. A *simplicial complex* is a finite collection K of simplices that is closed under the face relation such that the intersection of any two simplices is either empty or a face of both. A *subcomplex* of K is a subset that itself is a simplicial complex. The *closure* of a subset $L \subseteq K$ is the smallest subcomplex $\mathrm{Cl}\, L \subseteq K$ that contains L. The *star* of a simplex $\tau \in K$ is the collection of simplices that contain τ, and the *link* is the collection of faces of simplices in the closure of the star that are disjoint from τ:

$$\begin{aligned} \mathrm{St}\, \tau &= \{\sigma \in K \mid \tau \leq \sigma\}, \\ \mathrm{Lk}\, \tau &= \{v \in \mathrm{Cl}\, \mathrm{St}\, \tau \mid v \cap \tau = \emptyset\}. \end{aligned}$$

The *vertex set* of K is denoted by $\mathrm{Vert}\, K$. The *underlying space* is the union of simplices: $\|K\| = \bigcup_{\sigma \in K} \sigma$. The *interior* of a simplex σ is the set of points that belong to σ but not to any proper face of σ. Note that each point of $\|K\|$ belongs to the interior of exactly one simplex in K. We specify a piecewise linear continuous function by its values at the vertices. To describe this construction, let $\varphi : \mathrm{Vert}\, K \to \mathbb{R}$ be a function defined on the vertex set. Each point $x \in \|K\|$ has barycentric coordinates $\alpha_u = \alpha_u(x) \in \mathbb{R}$ such that $\sum \alpha_u u = x$, $\sum \alpha_u = 1$, and $\alpha_u = 0$ unless u is a vertex of the simplex whose interior contains x. The *linear extension* of φ is the function $f : \|K\| \to \mathbb{R}$ defined by $f(x) = \sum_u \alpha_u(x)\varphi(x)$. It is continuous because the maps α_u are continuous.

The simplicial complex K is a *triangulation* of a manifold $\mathbb{M}$ if there is a a a homeomorphism $\|K\| \to \mathbb{M}$. In this case, the link of every k-simplex triangulates a sphere of dimension $d - k - 1$. We will extend the concept of a critical point from smooth to piecewise linear functions using subcomplexes of links. Assuming $f(u) \neq f(v)$ for any two vertices $u \neq v$ in K, the *lower star* of u consists of all simplices in the star that have u as their highest vertex, and the *lower link* is the portion of the link that bounds the lower star. Note that both the link and the lower link are always complexes.

Homology groups and Betti numbers. In the piecewise linear case, we use the topology of the lower link to define whether or not we consider a vertex critical, and we express that topology using ranks of homology groups for $\mathbb{Z}_2$ coefficients. To explain this, let K be a simplicial complex. A k-*chain* is a subset of the k-simplices, and *adding* two k-chains means taking their symmetric difference. The set of k-chains together with addition forms the group of k-chains, denoted as C_k. The *boundary* of a k-simplex is the set of its

$(k-1)$-simplices. This defines a *boundary homomorphism* $\partial_k : \mathsf{C}_k \to \mathsf{C}_{k-1}$ obtained by mapping a k-chain to the sum of boundaries of its k-simplices. Since we aim at reduced homology groups, we extend the list of non-trivial chain groups by adding $\mathsf{C}_{-1} = \mathbb{Z}_2$ and defining the boundary of a vertex as $\partial_0(u) = 1$. The boundary homomorphisms connect the chain groups as illustrated in Figure 2. A *k-cycle* is a k-
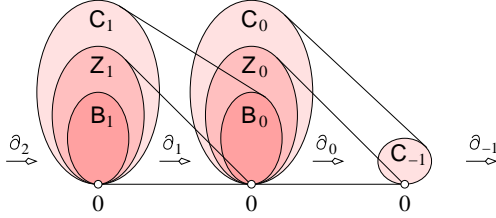

Figure 2: The chain complex formed by the chain groups and the connecting boundary homomorphisms.

chain with zero boundary, and a *k-boundary* is the boundary of a $(k+1)$-chain. The corresponding groups are nested subgroups of the group of k-chains: $\mathsf{B}_k \leq \mathsf{Z}_k \leq \mathsf{C}_k$. The *k-th reduced homology group* is the quotient defined by the k-cycles and the k-boundaries: $\tilde{\mathsf{H}}_k = \mathsf{Z}_k|\mathsf{B}_k$. The *k-th reduced Betti number* is the rank of the k-th reduced homology group: $\tilde{\beta}_k = \operatorname{rank} \tilde{\mathsf{H}}_k$. Since we add modulo 2, all groups are finite and $\tilde{\beta}_k$ is the binary logarithm of the size of $\tilde{\mathsf{H}}_k$. The reduced homology groups differ from the more common non-reduced versions only in dimensions 0 and -1. Specifically, $\tilde{\beta}_0$ is one less than the number of components, unless the complex is empty, in which case $\tilde{\beta}_0 = 0$, and $\tilde{\beta}_{-1} = 0$ unless the complex is empty, in which case $\tilde{\beta}_{-1} = 1$.

The main reason for preferring reduced over non-reduced homology groups is their simpler correspondence to spheres. The $(d-1)$-*sphere* is the set of points at unit distance from the origin of the d-dimensional Euclidean space: $\mathbb{S}^{d-1} = \{x \in \mathbb{R}^d \mid \|x\| = 1\}$. To triangulate $\mathbb{S}^{d-1}$ we may take the set of proper faces of a d-simplex. Note that $\mathbb{S}^{-1}$ is the empty set, which is triangulated by the empty complex. The $(d-1)$-sphere has only one non-zero reduced Betti number, namely $\tilde{\beta}_{d-1} = 1$, and this is true for all $d \geq 0$. In contrast, the reduced Betti numbers of a point all vanish.

3 Jacobi Sets of Two Functions

In this section, we consider the Jacobi set of a pair of Morse functions defined on the same manifold.

Definition of Jacobi sets. Let $\mathbb{M}$ be a smooth d-manifold and choose a Riemannian metric so that we can define gradients. We assume $d \geq 2$ and consider two generic Morse functions, $f, g : \mathbb{M} \to \mathbb{R}$. We are interested in the restrictions of f to the level sets of g. For a regular value $t \in \mathbb{R}$, the level set $\mathbb{M}_t = g^{-1}(t)$ is a smooth $(d-1)$-manifold, and the restriction of f to this level set is a Morse function

$f_t : \mathbb{M}_t \to \mathbb{R}$. The *Jacobi set* $\mathbb{J} = \mathbb{J}(f, g)$ is the closure of the set of critical points of such level set restrictions:

$$\mathbb{J} = \operatorname{cl}\{x \in \mathbb{M} \mid x \text{ is critical point of } f_t\}, \quad (1)$$

for some regular value $t \in \mathbb{R}$. The closure operation adds the critical points of f restricted to level sets at critical values t as well as the critical points of g, which form singularities in these level sets. Figure 3 illustrates the definition by showing $\mathbb{J}$ for two smooth functions defined on the two-dimensional plane. Think of the picture as a cone-like mountain indicated by the (dotted) level curves of f, and imagine an animation during which the (solid) level curves of g glide over that mountain. For example, on the left we see a circle expanding outwards on a slope, and we observe a maximum moving uphill and a minimum moving downhill from the starting point, which is a minimum of g.
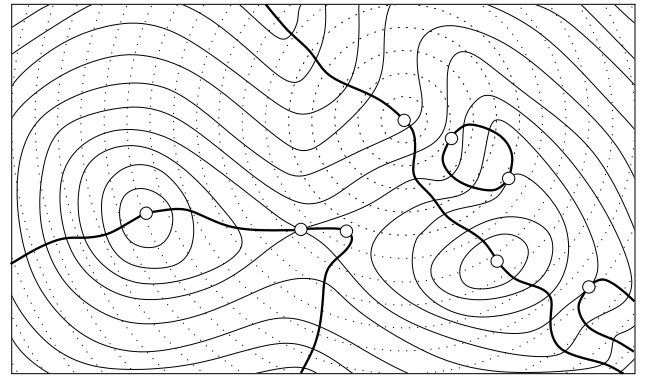

Figure 3: The functions f and g are represented by their dotted and solid level curves. The Jacobi set is drawn in bold solid lines. The birth-death points and the critical points of the two functions are marked.

Consider the gradient of the two functions at a point x: $\nabla f(x), \nabla g(x) \in \mathbb{R}^d$. Let $t = g(x)$. Then the gradient of f_t at $x \in \mathbb{M}_t = g^{-1}(t)$ is the projection of $\nabla f(x)$ onto the tangent space of $\mathbb{M}_t$ at x. It follows that $\nabla f_t(x) = 0$ iff the two gradient vectors are parallel. In other words,

$$\mathbb{J} = \{x \in \mathbb{M} \mid \nabla f(x) + \lambda \nabla g(x) = 0 \text{ or}$$
$$\lambda \nabla f(x) + \nabla g(x) = 0\}, \quad (2)$$

for some $\lambda \in \mathbb{R}$. The first relation in (2) misses the cases in which $\nabla g(x) = 0$ and $\nabla f(x) \neq 0$. The only reason for the second relation is to capture these cases. The description of $\mathbb{J}$ in Equation (2) is symmetric in f and g: $\mathbb{J}(f, g) = \mathbb{J}(g, f)$. We therefore call the points of $\mathbb{J}$ *simultaneous critical points* of f and g. Note that $\nabla f + \lambda \nabla g$ is the gradient of the function $f + \lambda g$. Equation (2) thus implies yet another characterization of the Jacobi set:

$$\mathbb{J} = \{x \in \mathbb{M} \mid x \text{ is critical point of}$$
$$f + \lambda g \text{ or of } \lambda f + g\}, \quad (3)$$

for some $\lambda \in \mathbb{R}$. This formulation should be compared with the Lagrange multiplier method in which λ is treated as an indeterminant.

Critical curves. Generically, f_t has a discrete collection of critical points, and these points sweep out $\mathbb{J}$ as t varies. It follows that $\mathbb{J}$ is a one-dimensional set. We strengthen this observation and prove that the Jacobi set is a smoothly embedded 1-manifold in $\mathbb{M}$. This follows form the stratification of the Jacobi set described in [11], which we will sketch in Section 5. For completeness, we give a direct proof that avoids the more advanced concepts needed to prove the more general result.

SMOOTH EMBEDDING THEOREM. Generically, the Jacobi set of two Morse functions $f, g : \mathbb{M} \to \mathbb{R}$ is a smoothly embedded 1-manifold in $\mathbb{M}$.

PROOF. Assume $\mathbb{M}$ is a d-manifold, for $d \geq 2$, and consider the functions $F, G : \mathbb{M} \times \mathbb{R} \to \mathbb{R}^d$ that map a point $x \in \mathbb{M}$ and a parameter $\lambda \in \mathbb{R}$ to the gradients of $f + \lambda g$ and $\lambda f + g$:

$$
\begin{aligned}
F(x, \lambda) &= \nabla f(x) + \lambda \nabla g(x), \\
G(x, \lambda) &= \lambda \nabla f(x) + \nabla g(x).
\end{aligned}
$$

By Equation (2), a point x belongs to $\mathbb{J}$ iff there is a $\lambda \in \mathbb{R}$ such that $F(x, \lambda) = 0$ or $G(x, \lambda) = 0$. Letting $\Gamma_F = F^{-1}(0)$ and $\Gamma_G = G^{-1}(0)$, we get $\mathbb{J}$ by projecting onto $\mathbb{M}$:

$$
\begin{array}{ccccccc}
\Gamma_F & \subseteq & \mathbb{M} \times \mathbb{R} & & \Gamma_G & \subseteq & \mathbb{M} \times \mathbb{R} \\
\downarrow & & \downarrow & \text{and} & \downarrow & & \downarrow \\
\mathbb{J}_F & \subseteq & \mathbb{M} & & \mathbb{J}_G & \subseteq & \mathbb{M}.
\end{array}
$$

We have $\mathbb{J} = \mathbb{J}_F \cup \mathbb{J}_G$, where $\mathbb{J}_F$ is $\mathbb{J}$ minus the discrete set of points where $\nabla g(p) = 0$, and $\mathbb{J}_G$ is $\mathbb{J}$ minus the points where $\nabla f(p) = 0$. We prove that F is transversal to 0 or, equivalently, that for every $(p, \lambda) \in F^{-1}(0)$, the derivative of F at (p, λ) has rank d. We compute $\mathrm{d}F_{(p,\lambda)} = [H_{f+\lambda g}(p), \nabla g(p)]$, where the Hessian is a d-by-d matrix. As mentioned in Section 2, we can assume that all functions $h_\lambda = f + \lambda g$ are in $C_0 - C_1$, except for a discrete number, which are in $C_1 - C_2$. The former have only non-degenerate critical points, so the Hessian itself already has rank d. Let λ_0 be a value for which h_{λ_0} is not Morse. If there are two critical points sharing the same function value, then the Hessian is still invertible and there is nothing else to show. Otherwise, there is a single birth-death point p_0, and we write $c_0 = h_{\lambda_0}(p_0)$. There exist local coordinates such that $p_0 = (0, 0, \ldots, 0)$, $\lambda_0 = 0$, and

$$
\begin{aligned}
h_\lambda(p) &= c_0 + x_1^3 - \lambda x_1 \pm x_2^2 \pm \ldots \pm x_d^2 \\
&= \lambda(-x_1) + (c_0 + x_1^3 \pm x_2^2 \pm \ldots \pm x_d^2)
\end{aligned}
$$

in a neighborhood of (p_0, λ_0). Note that this implies $g(p) = -x_1$. We can write the Hessian and the gradient explicitly and get

$$
\mathrm{d}F_{(p_0, \lambda_0)} = \begin{bmatrix}
0 & 0 & \ldots & 0 & -1 \\
0 & \pm 2 & \ldots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \ldots & \pm 2 & 0
\end{bmatrix}.
$$

This matrix has rank d. Since $0 \in \mathbb{R}^d$ has co-dimension d, the Transversality Theorem now implies that $\Gamma_F = F^{-1}(0)$ is a smooth 1-manifold in $\mathbb{M} \times \mathbb{R}$. We still need to prove that the projection of this 1-manifold is smoothly embedded in $\mathbb{M}$. Let $\pi : \Gamma_F \to \mathbb{J}$ be defined by $\pi(p, \lambda) = p$. We show that π is one-to-one and $\mathrm{d}\pi_{(p,\lambda)} \neq 0$ for all $(p, \lambda) \in \Gamma_F$. If $\pi(p, \lambda) = \pi(p', \lambda')$ then $p = p'$ and $\nabla f(p) + \lambda \nabla g(p) = \nabla f(p) + \lambda' \nabla g(p) = 0$. Since $\nabla g(p) \neq 0$ on Γ_F, $\lambda = \lambda'$ so the projection is injective. To prove that the derivative $\mathrm{d}\pi$ of π is non-zero, note that the tangent line to Γ_F at (p, λ) is the kernel of $\mathrm{d}F_{(p,\lambda)} = [H_{f+\lambda g}(p), \nabla g(p)]$. If $\mathrm{d}\pi$ is zero at (p, λ), then this tangent line must be vertical, spanned by the vector $v = (0, \ldots, 0, 1)$. But since $\nabla g(p) \neq 0$, v cannot be in the kernel of $\mathrm{d}F_{(p,\lambda)}$.

By symmetry, everything we proved for F also holds for G. This concludes our proof that generically, $\mathbb{J}$ is a smoothly embedded 1-manifold in $\mathbb{M}$. $\square$

4 Algorithm

In this section, we describe an algorithm that computes an approximation of the Jacobi set of two Morse functions from approximations of these functions. We begin by laying out our general philosophy and follow up by describing the details of the algorithm.

General approach. In applications, we never have smooth functions but usually non-smooth functions that approximate smooth functions. We choose not to think of the non-smooth functions as approximations of smooth functions. Quite the opposite, we think of the non-smooth functions as being approximated by smooth functions. The relatively simple smooth case then becomes the guiding intuition in designing the algorithm that constructs what one may call the Jacobi set of the non-smooth functions. To be more specific, let K be a triangulation of a d-manifold $\mathbb{M}$ and let $\varphi, \psi : \mathrm{Vert}\, K \to \mathbb{R}$ be two functions defined at the vertices. We obtain $f, g : \|K\| \to \mathbb{R}$ as piecewise linear extensions of φ and ψ. We imagine that both piecewise linear functions are limits of series of smooth functions: $\lim_{n \to \infty} f_n = f$ and $\lim_{n \to \infty} g_n = g$. For each n, the Jacobi set $\mathbb{J}_n = \mathbb{J}(f_n, g_n)$ is perfectly well defined, and we aim at constructing the Jacobi set of f and g as the limit of the $\mathbb{J}_n$. Along the way, we will take some liberties in resolving the ambiguities in what this means exactly. As a guiding principle, we resolve ambiguities in a way consistent with the corresponding smooth concepts that arise in the imagined smooth approximations of f and g. We call this principle the *simulation of differentiability* and combine it with the simulation of simplicity [9] to put ourselves within the realm of generic smooth functions.

After constructing the Jacobi set of f and g, we may need to resolve the result into something whose structure is consistent with that of its smooth counterpart. Most importantly,

the algorithm will generally construct a one-dimensional subcomplex J of K in which edges have positive integer multiplicities. We will prove that J can be unfolded into a union of disjoint closed curves in which all edges have multiplicity one. In other words, we can indeed think of $\mathbb{J} = |J|$ as the limit of a series of smoothly embedded 1-manifolds.

Edge selection. We compute $\mathbb{J}$ by tracing the critical points of the 1-parameter family of functions $h_\lambda = f + \lambda g$. In the piecewise linear limit, the set of critical points is generically a collection of vertices. With varying λ, the critical points move to other vertices and, in the limit, that movement happens along the edges of K and at infinite speed. Instead of keeping track of the critical points and their movements, we construct $\mathbb{J}$ as the union of edges along which the critical points move. In other words, we decide for each edge how many critical points move from one endpoint to the other, and we let J be the collection of edges for which this number is positive. We then make J a subcomplex by adding the endpoints of the edges to the set. Note that we do not have to repeat the construction for the family $\lambda f + g$. By definition, the *Jacobi set* is the underlying space of this subcomplex: $\mathbb{J} = |J|$.

Let uv be an edge of K, and let $\lambda = \lambda_{uv}$ be the moment at which the function values at u and v are the same. At this moment, we have $h_\lambda(u) = h_\lambda(v)$ and therefore $\lambda_{uv} = [f(v) - f(u)]/[g(u) - g(v)]$. In order for a critical point to travel along the edge from u to v or vice versa, the entire edge must be critical for $\lambda = \lambda_{uv}$. We express this condition by considering the link of u, which is a triangulation of the $(d-1)$-sphere. Let l be the restriction of $h_{\lambda_{uv}}$ to that link.

CRITICAL EDGE LEMMA. The edge uv belongs to J iff v is a critical point of l. Moreover, the multiplicity of uv in J is the multiplicity of v as a critical point of l.

We describe shortly how we decide whether or not a vertex is critical and, if it is critical, how we compute its multiplicity. For both operations, it suffices to look at the lower link of v in the link of u. Note that the link of v in the link of u is the same as the link of uv in K, and that l is defined at all vertices of this link as well as at v. We can therefore construct the lower link of uv as the subcomplex induced by the vertices w whose function values are smaller than that of v. We denote this lower link as $\underline{\mathrm{Lk}}\, uv$ and note that it is the same as the lower link of v in the link of u. This formulation makes it obvious that the test of the edge uv is symmetric in u and v. We implement the Critical Edge Lemma as follows:

```
integer ISJACOBI(Edge uv)
   λ = [f(v) − f(u)]/[g(u) − g(v)];
   Lk uv = {τ ∈ Lk uv | w ≤ τ ⟹ h_λ(w) < h_λ(v)};
   return ISCRITICAL(Lk uv).
```

As described shortly, Function ISCRITICAL returns 0 if the lower link of uv is that of a regular point, and it returns the multiplicity of the criticality otherwise.

Criticality and multiplicity. The smooth analogue of a vertex link is a sufficiently small sphere drawn around a point x of the manifold $\mathbb{M}$. If $\mathbb{M}$ is a d-manifold the dimension of that sphere is $d - 1$. The analogue of the lower link is the portion of that sphere where the value of the function is less than or equal to the value at x. assuming smoothness, the topology of this portion is the same for all sufficiently small spheres, and assuming a Morse function, it has either the homotopy type of a point or that of a sphere. In the former case, x is regular, and in the latter case, x is critical. The dimension of the sphere is one less than the index of x. This suggests we use the reduced Betti numbers of the lower link to classify vertices in a triangulation as shown in Table 1. The

	$\tilde{\beta}_{-1}$	$\tilde{\beta}_0$	$\tilde{\beta}_1$	$\tilde{\beta}_2$	$\ldots$
regular	0	0	0	0	$\ldots$
0	1	0	0	0	$\ldots$
1	0	1	0	0	$\ldots$
2	0	0	1	0	$\ldots$
3	0	0	0	1	$\ldots$
$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$

Table 1: Classification of vertices into regular points and simple critical points (identified by their index) using the reduced Betti numbers of the lower link.

multiplicity of a vertex u is the sum of reduced Betti numbers of its lower link: $\mu(u) = \sum_{k \geq 0} \tilde{\beta}_{k-1}$. Table 1 shows only the regular point, which has multiplicity 0, and the simple critical points, which have multiplicity 1. All other points may be thought of as accumulations of $\mu \geq 2$ simple critical points. In small dimensions, it is easy to effectively unfold such a point into μ simple critical points. We illustrate this for a vertex u in the triangulation of a 3-manifold. Its link is a 2-sphere. We refer to the components of the lower link as *oceans* and to the components of the complement as *continents*. Because the multiplicity is at least 2, we have $\mu(u) = \tilde{\beta}_0 + \tilde{\beta}_1 \geq 2$. There are $\tilde{\beta}_0 + 1$ oceans and $\tilde{\beta}_1 + 1$ continents. As illustrated in Figure 4, we cut the link along a circle that passes through exactly one ocean and one continent and meets each in a single interval. Next we replace u
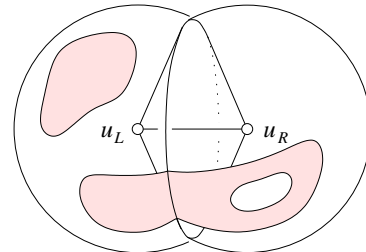

Figure 4: A 2-sphere with two (shaded) oceans and two continents is cut to form two 2-spheres, whose structures are those of a simple index-1 critical point on the left and a simple index-2 critical point on the right.

by two vertices u_L and u_R and connect them to the respective

side of the link and to each other. We have $\tilde{\beta}_{0L} + \tilde{\beta}_{0R} = \tilde{\beta}_0$ and $\tilde{\beta}_{1L} + \tilde{\beta}_{1R} = \tilde{\beta}_1$. To guarantee progress, we cut such that $\tilde{\beta}_{0L} + \tilde{\beta}_{1L}$ and $\tilde{\beta}_{0R} + \tilde{\beta}_{1R}$ are both less than μ. This implies that both are at least one, which is equivalent to avoiding the creation of regular points and of minima and maxima. We repeat the process until all vertices are simple critical points. This happens after $\tilde{\beta}_0 + \tilde{\beta}_1 - 1$ splits, which generate $\tilde{\beta}_0$ simple critical points of index 1 and $\tilde{\beta}_1$ simple critical points of index 2. In summary, we compute the multiplicity of a vertex by summing the reduced Betti numbers of its lower link:

```
integer ISCRITICAL(Complex L)
    foreach k ≥ 0 do compute β̃_{k-1} of L endfor;
    return ∑_{k≥0} β̃_{k-1}.
```

To compute the reduced Betti numbers, we may use the Smith normal form algorithm described in [17]. For coefficients modulo 2, this amounts to doing Gaussian elimination on the incidence matrices, which takes a time cubic in the number of simplices in L. Even for integer coefficients, the worst-case running time is polynomial in the number of simplices [13]. For manifolds of dimension $d \leq 5$, we get the lower links as subcomplexes of spheres of dimension $d - 2 \leq 3$. For these we can use the significantly faster incremental algorithm of [7], whose running time is ever so slightly larger than proportional to the number of simplices in the link.

Post-processing. The second step amounts to unfolding the union of edges to a 1-manifold. Define the *degree* of a vertex u as the number of edges in J that share u, where we count each edge with its multiplicity. We use the fact that every vertex has even degree. This is suggested by our analysis of $\mathbb{J}$ in the smooth case but needs a direct proof, which is given below using an elementary parity argument. For good piecewise linear approximations of smooth functions, most vertices will have degree zero. If u has degree 2 or higher, we glue the incident selected edges in pairs. For $d = 2$, this is done so that glued pairs do not cross at u.

EVEN DEGREE LEMMA. The degree of every vertex in J is even.

PROOF. We consider a vertex u and the family of functions $h_\lambda = f + \lambda g$. For $\lambda = \pm\infty$, $\mu(u)$ is independent of f and the same at both extremes. We increase λ continuously from $-\infty$ to $+\infty$. Each time we pass a value $\lambda = \lambda_{uv}$, the status of the neighbor v changes from inside to outside the lower link of u, or vice versa. The effect of this change on the type of u depends on the type of v in the restriction of h_λ to Lk u. Specifically, the multiplicity of u either increases or decreases by the multiplicity of v in the lower link of u. For example, if v is regular then the change has no effect, and if v is a simple critical point then it either increases or decreases $\mu(u)$ by one. The number of operations, each counted with multiplicity of v, is equal to the degree of u. Since we start

and end with the same multiplicity of u, we add and subtract equally often, which implies that the degree is even. □

5 Jacobi Sets of $k + 1$ Functions

We generalize the results of Sections 3 and 4 from two to three or more functions defined on the same manifold.

Smooth case. Let $\mathbb{M}$ be a smooth d-manifold and choose a Riemannian metric. Consider $k + 1 \leq d$ Morse functions $f_0, f_1, \ldots, f_k$ on $\mathbb{M}$, and write $\Phi = (f_0, f_1, \ldots, f_k) : \mathbb{M} \to \mathbb{R}^{k+1}$. The generic intersection of the level sets of $j \leq d$ of the f_i is a $(d - j)$-dimensional smooth manifold. Let $t = (t_0, \ldots, \hat{t}_\ell, \ldots, t_k)$ be a k-vector of image values, where the hat indicates that t_ℓ is not in the vector. Generically, the intersection of the corresponding level sets is a smooth $(d - k)$-manifold: $\mathbb{M}_t = \bigcap_{i \neq \ell} f_i^{-1}(t_i)$, and the restriction $f_{\ell t}$ of f_ℓ to $\mathbb{M}_t$ is a Morse function. We call a critical point of this restriction a *simultaneous critical point* of Φ. The *Jacobi set* $\mathbb{J} = \mathbb{J}(\Phi)$ is the closure of the set of simultaneous critical points:

$$\mathbb{J} = \text{cl}\,\{x \in \mathbb{M} \mid x \text{ is critical point of } f_{\ell t}\}, \quad (4)$$

for some index ℓ and some k-vector t. Generically, the k gradients ∇f_i at a point $x \in \mathbb{M}_t$ span the k-dimensional linear subspace of vectors normal to $\mathbb{M}_t$ at x, and x is a critical point of $f_{\ell t}$ iff $\nabla f_\ell(x)$ belongs to this linear subspace. This means that a direct definition of the Jacobi set is:

$$\mathbb{J} = \{x \in \mathbb{M} \mid \text{rank}\, d\Phi_x \leq k\}, \quad (5)$$

where $d\Phi_x$ is the d-by-$(k + 1)$ matrix whose columns are the gradients of f_0 to f_k at x. Equation (5) is symmetric in the components of Φ, which implies that $\mathbb{J}$ is independent of the ordering of the f_i. The linear dependence of the $k + 1$ gradient vectors implies that for each $x \in \mathbb{J}$ there is a gradient that can be written as a linear combination of the others: $\nabla f_\ell(x) + \sum_{i \neq \ell} \lambda_i \nabla f_i(x) = 0$. Since the combination of gradients is the gradient of the corresponding combination of functions, this implies

$$\mathbb{J} = \{x \in \mathbb{M} \mid x \text{ is crit. pt. of } f_\ell + \sum_{i \neq \ell} \lambda_i f_i\}, \quad (6)$$

for some index ℓ and some parameters λ_i. Generically, $\mathbb{J}$ is swept out by a k-parameter family of discrete points. It follows that $\mathbb{J}$ is a set of dimension k. Unfortunately, $\mathbb{J}$ is not always a submanifold of $\mathbb{M}$. Following [11], we define $S_r = \{x \in \mathbb{M} \mid \text{rank}\, d\Phi_x = k + 1 - r\}$. Clearly, $\mathbb{J}$ is the disjoint union of the S_r for $r \geq 1$. The Transversality Theorem explained in Section 2 and the Thom Transversality Theorem [11, page 54] imply that S_r is a submanifold of $\mathbb{M}$ of co-dimension $r(r + d - k - 1)$ for each r, not necessarily a closed submanifold, however. Furthermore the closure

of each S_r is the union $S_r \cup S_{r+1} \cup \ldots$, however it is not necessarily a manifold. In particular, $\mathbb{J} = \text{cl } S_1$ is a manifold whenever S_2 (and therefore every S_r for $r \geq 2$) is empty. This happens as long as $d < r(r + d - k - 1)$, for $r = 2$, since a negative co-dimension implies it is empty. This inequality is equivalent to $d > 2k - 2$, and the first time it fails is for a map from a 4-manifold to $\mathbb{R}^4$.

Algorithm. Let K be a triangulation of the d-manifold $\mathbb{M}$ and let $\varphi_i : \text{Vert } K \to \mathbb{R}$ be a function defined at the vertices, for $0 \leq i \leq k$. We obtain $f_i : \|K\| \to \mathbb{R}$ as the piecewise linear extension of φ_i, for each i. As in the case of $k + 1 = 2$ functions, we think of the f_i as limits of smooth functions and construct a k-dimensional subcomplex $J \subseteq K$ as the limit of the Jacobi sets of these smooth functions. Specifically, we compute the multiplicity of every k-simplex in K and define J as the collection of k-simplices with positive multiplicity plus the collection of faces of these k-simplices. By definition, the *Jacobi set* is the underlying space of this subcomplex: $\mathbb{J} = |J|$.

As suggested by Equation (6), we introduce a k-parameter family of functions $h_\lambda = f_\ell + \sum_{i \neq \ell} \lambda_i f_i$, where $\lambda = [\lambda_0, \ldots, \hat{\lambda}_\ell, \ldots, \lambda_k]$. Next, we consider a k-simplex σ with vertices $u_0, u_1, \ldots, u_k$ in K and let λ_σ be the k-vector such that $h_{\lambda_\sigma}(u_0) = h_{\lambda_\sigma}(u_1) = \ldots = h_{\lambda_\sigma}(u_k)$. The link of σ is a triangulated $(d - k - 1)$-sphere, and as before we construct the lower link as the subcomplex induced by the vertices w with function values smaller than those of the vertices of σ. Whether or not σ belongs to J depends on the topology or, more precisely, the reduced Betti numbers of the lower link:

```
integer ISJACOBI(k-Simplex σ)
  compute λ = λσ;
  Lkσ = {τ ∈ Lkσ | w ≤ τ ⟹ hλ(w) < hλ(u0)};
  return ISCRITICAL(Lkσ).
```

Function ISCRITICAL is the same as in Section 4. It is possibly surprising that the criticality test gets easier the more functions we have, simply because the dimension of the link decreases with increasing k.

6 Towards Applications

Different applications provide data in different ways and require different adaptations of the algorithm. To illustrate the broad potential of the results presented in this paper, we discuss a few applications while emphasizing the diversity of questions they raise.

Contours. Let $\mathbb{M}$ be a smoothly embedded 2-manifold in $\mathbb{R}^3$ and $a \in \mathbb{S}^2$ an arbitrary but fixed viewing direction. The *contour* is the set of points $x \in \mathbb{M}$ for which the viewing direction belongs to the tangent plane: $a \in T\mathbb{M}_x$. We introduce two functions, $f, g : \mathbb{M} \to \mathbb{R}$, defined by $f(x) = \langle x, b \rangle$

and $g(x) = \langle x, c \rangle$, where $b, c \in \mathbb{S}^2$ are directions orthogonal to a. Assuming $c \neq \pm b$, $f(x)$ and $g(x)$ are coordinates of the projection of x along the viewing direction. As illustrated in Figure 1, the Jacobi set of f and g is exactly the contour of $\mathbb{M}$, and the projection of the contour is the fold of the two maps. Note that $\mathbb{J} = \mathbb{J}(f, g)$ is a smoothly embedded 1-manifold in $\mathbb{M}$, whereas the fold can have singularities such as cusps and self-intersections.

Suppose $\mathbb{M}$ is given by an approximating simplicial complex K in $\mathbb{R}^3$. The algorithm described in Section 4 amounts to selecting the edges in K for which the plane parallel to a that passes through the edge has both incident triangles on one side. It has been observed experimentally that $\mathbb{J}$ approximates the contour geometrically but not necessarily topologically. Specifically, we can improve the geometric accuracy of the approximation by subdividing K. In the process, spurious cycles of the Jacobi set get smaller but they may not disappear, not even in the limit [5]. This 'topological noise' is an artifact of the piecewise linear approximation and particularly common in hyperbolic regions, such as around the inner longitudinal circle of the torus in Figure 1. We pose the extension of the methods in [8] for measuring topological noise to Jacobi sets as an open problem.

Protein interaction. An energy potential is a type of smooth function common in the sciences. The corresponding force relates to the potential like the gradient relates to the smooth function. As an example, consider the forces that are studied in the context of protein interaction, such as electrostatics and van der Waals. The van der Waals potential decays rapidly, possibly proportional to the sixth power of the distance to the source, while the electrostatic potential decays much slower, proportional to the distance. It is thus believed that the electrostatic potential influences the interaction at an early stage, while the proteins are relatively far apart, by steering them towards each other. Once in close contact, the van der Waals force takes over, which may be the reason why stable interactions require a good amount of local shape complementarity [10]. It would be interesting to put this hypothesis to a computational test in which we can visualize the relationship between different energy potentials through their Jacobi sets. Maybe the hypothesis is more true for some and less for other proteins. On top of visualizing the relationship, it would be useful to quantify the agreement and disagreement between the potentials. It is not entirely clear how to go about constructing such a test. The natural domain for the mentioned potentials is $\mathbb{R}^3$, but it might be more convenient to use two-dimensional domains, such as molecular surfaces [6] and interfaces between proteins [2].

Solar system. Similar to the electrostatic potential, the gravitational potential exerted by a heavenly body decays at a rate that is proportional to the distance. At any moment in time, the gravitational force acting on a point in our solar system depends on its mass and the distance from the

sun, the planets and the moons. Let $\mathbb{M} = \mathbb{R}^3 \times \mathbb{R}$ represent space-time in our solar system and let $g : \mathbb{M} \to \mathbb{R}$ be the gravitational potential obtained by adding the contributions of the sun, the planets and the moons. The function is smooth except at the centers of the bodies, where g goes to infinity. At a fixed time t, we have a map from $\mathbb{R}^3$ to $\mathbb{R}$, which generically has four types of critical points. These points trace out curves, which we model as the Jacobi set of g and a second function f that maps every space-time point $(x, t) \in \mathbb{R}^3 \times \mathbb{R}$ to its time: $f(x, t) = t$. Every level set of f is the gravitational potential at some fixed moment in time, so it should be obvious that $\mathbb{J}(f, g)$ is indeed the 1-manifold traced out by the critical points.

The Lagrange points used by NASA in planning the flight paths of their space-crafts are related to these curves but more complicated because they are defined in terms of the interaction between the gravitational force and the momentum of the moving space-craft. It would be interesting to see whether the Lagrange points can also be modeled using the framework of Jacobi sets.

7   Discussion

The main contribution of this paper is an algorithm that constructs the Jacobi set of a collection of piecewise linear continuous functions on a common triangulated manifold. The crucial concept in the definition of the Jacobi set is the notion of a critical point of a piecewise linear function. Our decision to use reduced Betti numbers was in part guided by computational convenience and feasibility. The weaker definition based on the Euler characteristic of the lower link used by Banchoff [3] is also possible but misses important portions of the set. The stronger definition that requires the thickened lower link of a regular point be homeomorphic to a ball leads to an undecidable recognition problem for links of dimension 5 or higher [14].

We conclude this section with a list of open questions raised by the work presented in this paper. This list does not include the questions stated in earlier sections.

- The algorithm in Section 4 may be applied more generally than just to manifolds, such as for example to homology manifolds. By definition, these cannot be distinguished from manifolds if we classify links using homology. What is the most general class of simplicial complexes for which our algorithm is meaningful?

- Initial computational experiments indicate that coarse triangulations lead to poor approximations of the Jacobi set. This suggests we need an adaptive meshing method that locally refines the triangulation depending on the available information on the Jacobi set.

- Definition (5) of Jacobi sets extends to the case of $k + 1 > d$ Morse functions. According to [11], $\mathbb{J}$ has co-dimension $k - d + 2$ and thus dimension $2d - k - 2$.

What is the significance of the Jacobi set of $k + 1 > d$ Morse functions for scientific applications?

- Finally, it would be interesting to explore whether the methods of this paper can be extended to more general vector fields, in particular to smooth vector fields that are not gradient fields.

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