Topology of Singular Fibers for Visualization

Osamu Saeki
(Institute of Mathematics for Industry, Kyushu Univ.)

Joint work with
Shigeo Takahashi, Daisuke Sakurai, Hsiang-Yun Wu, Keisuke Kikuchi, Hamish Carr, David Duke, Takahiro Yamamoto

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Who am I?

Got PhD in Mathematics (at the Univ. of Tokyo) in 1992.
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Main interest: Singularity Theory, 3- and 4-Dimensional Topology

Proposed the Theory of Singular Fibers of Differentiable Maps.

Osamu Saeki

Topology of Singular Fibers of Differential Maps

K = 1

K = 2

K = 3
My recent interests include collaboration with industrial partners or computer scientists on enhancing **visualization of multi-variate data** from the viewpoint of **topology**.
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Unique institute where quite a few "**pure mathematicians**" (like me) also collaborate.
Main idea of today’s talk

§1. Visualizing Scalar Field Data  §2. Visualizing Multi-field Data  §3. Visualizing 2-Variate Volume Data  §4. Examples of Visualization

“Topological Approach to Visualization of Scientific Data”

- Use techniques from **Differential Topology**, especially those of **Singularity Theory**: Topology is essential for extracting global features of given data.
- Visualize **Multi-fields**, instead of Scalar fields.
- Apply visualization techniques to **Mathematics** itself.
§1. Visualizing Scalar Field Data
\[ N^n : \text{differentiable manifold of dimension } n \text{ (or a region in } \mathbb{R}^n) \]
\[ f : N^n \rightarrow \mathbb{R} \quad \text{differentiable function (scalar field)} \]
$N^n$ : differentiable manifold of dimension $n$ (or a region in $\mathbb{R}^n$)
$f : N^n \to \mathbb{R}$ differentiable function (scalar field)

**Definition 1.1** For $c \in \mathbb{R}$, set

$$f^{-1}(c) = \{p \in N^n | f(p) = c\},$$

which is called a **level set**.
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**Definition 1.1** For $c \in \mathbb{R}$, set

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which is called a **level set**.

In general, a level set is of dimension $n - 1$ (but may not be a manifold). For $n = 2$, it is a curve; for $n = 3$, it is a surface, etc.

**Example 1.2** Altitude from the sea level (height function):
level set = contour line
Example of level sets

1. Visualizing Scalar Field Data
2. Visualizing Multi-field Data
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\[ N \rightarrow \mathbb{R}^f \]
Example of level sets

One can grasp the global feature of the data by chasing the level sets.
Example of level sets

§1. Visualizing Scalar Field Data  §2. Visualizing Multi-field Data  §3. Visualizing 2-Variate Volume Data  §4. Examples of Visualization

One can grasp the global feature of the data by chasing the level sets. We have some **critical level sets** where **topological transitions of level sets** occur.
Morse lemma

§1. Visualizing Scalar Field Data §2. Visualizing Multi-field Data §3. Visualizing 2-Variate Volume Data §4. Examples of Visualization

\[ f : N^n \rightarrow \mathbb{R} \] differentiable function (scalar field)
Morse lemma

\[ f : \mathbb{R}^n \rightarrow \mathbb{R} \] differentiable function (scalar field)

\( p \in \mathbb{R}^n \) is a **critical point** of \( f \) if

\[
\frac{\partial f}{\partial x_1}(p) = \frac{\partial f}{\partial x_2}(p) = \cdots = \frac{\partial f}{\partial x_n}(p) = 0.
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**Theorem 1.3 (Morse lemma)** *If $f$ is **generic** enough, then around each critical point, $f$ is expressed as*

$$f = \pm x_1^2 \pm x_2^2 \pm \cdots \pm x_n^2 + c$$

*w.r.t. certain local coordinates for some constant $c$.***
Morse lemma

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For the study of level-set changes, the Morse lemma is essential!
$f : N^3 \to \mathbb{R}$ \hspace{1em} (dim $N^3 = 3$)

Level sets are surfaces “with singularities”.

Example of topological transitions of level-surfaces for a 3-dimensional scalar field around \textbf{critical level sets}.
\[ f : N^n \rightarrow \mathbb{R} \quad \text{a scalar field} \]
$f : \mathbb{N}^n \rightarrow \mathbb{R}$ a scalar field

The space (or graph) obtained by contracting each connected component of the level set to a point is called a **Reeb graph** (or contour tree, volume skeleton tree, Stein factorization, ...).
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Reeb graph

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Vertices of a Reeb graph $\iff$ Critical points of a function

Reeb graph is indispensable for visualizing scalar fields.
Direct volume rendering

§1. Visualizing Scalar Field Data  §2. Visualizing Multi-field Data  §3. Visualizing 2-Variate Volume Data  §4. Examples of Visualization

An example of an application of Reeb graph:

- Big Size
- Complicated Structure
- Noise

Volume Data → Analysis → Transfer Function Design → Rendering

- Reeb graph
- Scalar function $\mathbb{R}^3 \rightarrow \mathbb{R}$
- Topology of level sets
- Topologically accentuated!

Visual Feedback
§2. Visualizing Multi-field Data
We study several functions at the same time, rather than a single scalar valued function.

For technical reasons, topological analysis of such multi-variate data has just recently begun.

We can attack this problem, using the recently developed “Joint Contour Net”, a novel technique in Computer Science, on the basis of Singularity Theory, a sophisticated discipline in Mathematics.
$N^n$: differentiable manifold of dimension $n$ (or a region in $\mathbb{R}^n$)

$f : N^n \to \mathbb{R}^m \ (m \geq 1)$ differentiable map (or multi-field)

\[ f(x) = (f_1(x), f_2(x), \ldots, f_m(x)) \]
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For $c \in \mathbb{R}^m$, $f^{-1}(c)$ is called a fiber (rather than a level set).
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**Definition 2.1**

For $c \in \mathbb{R}^m$, $f^{-1}(c)$ is called a fiber (rather than a level set).

Generically, we have $\dim f^{-1}(c) = n - m$.

Usually, we assume $n \geq m$. 
Remark 2.2
Mathematically, a fiber is, in fact, NOT just a subset in $\mathbb{N}^n$, but a MAP around a pre-image.
More precisely...

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Mathematically, a fiber is, in fact, NOT just a subset in $N^n$, but a MAP around a pre-image.

$$f : N^n \rightarrow \mathbb{R}^m, \ g : L^n \rightarrow \mathbb{R}^m$$ multi-fields
For points $c \in \mathbb{R}^m$ and $d \in \mathbb{R}^m$, fibers over $c$ and $d$ are equivalent (or the points have the same singular fiber type) if
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$$
\begin{array}{ccc}
(f^{-1}(U), f^{-1}(c)) & \xrightarrow{\cong} & (g^{-1}(V), g^{-1}(d)) \\
\downarrow f & & \downarrow g \\
(U, c) & \xrightarrow{\cong} & (V, d)
\end{array}
$$

for some neighborhoods $c \in U \subset \mathbb{R}^m$ and $d \in V \subset \mathbb{R}^m$. 

Singular fibers for scalar fields

Equivalence classes of singular fibers for Morse functions on surfaces
Example of fibers

\[ n = 3, \quad N^3: \text{sea water, } f : N^3 \rightarrow \mathbb{R}^2 \]
\[ f = (\text{temperature, salt density}) \]
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Salinity Constant Curves on Temperature Constant Constant Surfaces

Temperature Constant Surfaces

Singular Fiber

Singular Point
Example of fibers

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Salinity Constant Curves on Temperature Constant Surfaces

A fiber containing a singular point is called a **singular fiber**. This is important in grasping the topological feature of the given data!
Singual points and Jacobi set

§1. Visualizing Scalar Field Data §2. Visualizing Multi-field Data §3. Visualizing 2-Variate Volume Data §4. Examples of Visualization

\[ f : N^n \rightarrow \mathbb{R}^m \quad (n \geq m) \quad \text{differentiable map (multi-field)} \]
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**Definition 2.3** For a point \( p \in N^n \), the **differential**

\[
df_p : T_p N^n \rightarrow T_{f(p)} \mathbb{R}^m
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is the linear map associated with the **Jacobian matrix** of \( f \) (the \( m \times n \) matrix whose entries are the first order partial derivatives of \( f \)).
Singular points and Jacobi set

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**Singular point** is a point $p \in N^n$ such that $\text{rank } df_p < m$. The set of singular points

$$J(f) = \{ p \in N^n \mid \text{rank } df_p < m \}$$

is called the **Jacobi set** (or the **singular point set**) of $f$. 
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Generically, the Jacobi set \( J(f) \) is of dimension \( m - 1 \).
For multi-fields, any theorem like the Morse lemma for scalar fields?
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**Definition 2.4** $f : N^n \to \mathbb{R}^m$, $g : L^n \to \mathbb{R}^m$ multi-fields
For singular points $p \in N^n$ and $q \in L^n$ of $f$ and $g$, respectively, they have the same **singularity type** if
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for some neighborhoods \( p \in U \subset N^n, q \in V \subset L^n, f(p) \in U' \subset \mathbb{R}^m, \) and \( f(q) \in V' \subset \mathbb{R}^m \).
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**Morse lemma** says that a non-degenerate critical point of a Morse function has the same singularity type as the critical point of a quadratic function $\pm x_1^2 \pm x_2^2 \pm \cdots \pm x_n^2$. 

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**Example 2.5** When \( n = 2 \) and \( m = 2 \).
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Types of singularities: **fold** and **cusp** (Whitney, 1955)
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**Example 2.5** When $n = 2$ and $m = 2$.
Types of singularities: *fold* and *cusp* (Whitney, 1955)
Suppose $n \geq m = 2$ and $f$ is generic.
\[ f : N^n \rightarrow \mathbb{R}^m \]

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**fold**: A generalization of the Morse critical points for scalar fields
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- **cusp**: A degeneration of fold singularities
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For $m \geq 4$, the situation is much more complicated.
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For $m = 3$, a **swallowtail** may appear, which is a degeneration of cusp singularities.

For $m \geq 4$, the situation is much more complicated.

\[ \implies \text{still studied in Singularity Theory as one of its central problems.} \]
Assume that data (of the $f$-values) are given at a discrete set of points in the domain $\mathbb{N}^n$. 
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**Known Techniques**

[Bachthaler & Weiskopf, 2008] **Continuous Scatterplots:**
Refinement of scatterplots for discrete data values
\[\mapsto\] Curves of the Jacobi set image can be vaguely grasped.
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[Lehmann & Theisel, 2010] **Discontinuities in Continuous Scatterplots**: More sophisticated algorithm for detecting the Jacobi set image. Posed the problem of counting the number of fiber components.
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**Discontinuities in Continuous Scatterplots:**
More sophisticated algorithm for detecting the Jacobi set image.
Posed the problem of counting the number of fiber components.

Unfortunately, these studies are apparently not fully based on mathematical theories.
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1. Identify the Jacobi set $J(f)$ in the domain, and identify their **singularity types**;
2. Identify the Jacobi set image $f(J(f))$, and identify their **singular fiber types**.
For visualization of multi-variate data, we need to

1. Identify the Jacobi set \( J(f) \) in the domain, and identify their singularity types;
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[Edelsbrunner & Harer, 2002]

**Jacobi Sets of Multiple Morse Functions:**
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**Jacobi Sets of Multiple Morse Functions:**
Suggested an algorithm for obtaining the Jacobi set. However, it does not identify the singularity types.

Singularity theory of differentiable mappings

\[\downarrow\]

One can identify the singularity types and the singular fiber types (to a certain extent...)

For a generic $f : \mathbb{N}^n \to \mathbb{R}^m$, we have $\dim J(f) = \dim f(J(f)) = m - 1$. Jacobi set image $f(J(f))$ divides the range $\mathbb{R}^m$ into some regions.
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Example of Jacobi set image of a map of a surface into $\mathbb{R}^2$
For visualizing a multi-field $f$, the following is expected.
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1. Visualize $J(f)$ in $N^n$, and $f(J(f))$ in $\mathbb{R}^m$,
2. Visualize the *singularity types* for $J(f)$, and the *singular fiber types* for $f(J(f))$,
3. Visualize the *regular fibers* corresponding to the connected components of $\mathbb{R}^m \setminus f(J(f))$. 
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In fact, when a singularity theorist (like me) analyzes a given multi-field, he/she tries to visualize it by the above method (but, with hand calculation and almost always without success !)
For visualizing a multi-field \( f \), the following is expected.

1. Visualize \( J(f) \) in \( N^n \), and \( f(J(f)) \) in \( \mathbb{R}^m \),
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3. Visualize the **regular fibers** corresponding to the connected components of \( \mathbb{R}^m \setminus f(J(f)) \).

In fact, when a singularity theorist (like me) analyzes a given multi-field, he/she tries to visualize it by the above method (but, with hand calculation and almost always without success !)

Any way, it is important to identify the **singular fibers** and the **topological transitions of the fibers** near singular fibers.
§3. Visualizing 2-Variate Volume Data
Let us consider the case of $n = 3$ and $m = 2$: 2-variate volume data. In the following, $f : N^3 \to \mathbb{R}^2$ will be a multi-field, where $N^3$ is a bounded region (with boundary) in $\mathbb{R}^3$.

$N^3$: **spatial domain** (or **domain**)

$\mathbb{R}^2$: **data domain** (or **range**)

We assume that $f$ is differentiable and is sufficiently **generic** (or **non-degenerate**).
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We assume that \( f \) is differentiable and is sufficiently \textbf{generic} (or non-degenerate).

Jacobi set \( J(f) \) forms a smooth curve in \( N^3 \).
Let $\partial N^3$ be the boundary of the spatial domain, which is a compact surface (without boundary).

Set $f_\partial = f|_{\partial N^3} : \partial N^3 \rightarrow \mathbb{R}^2$, which is a generic differentiable map.
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We define its Jacobi set $J(f_{\partial})$ in a similar way: it forms a smooth curve in $\partial N^3$.

A fiber that passes through $J(f) \cup J(f_{\partial})$ is called a **Singular Fiber**.
For visualization, we use the technology of **Joint Contour Net** (\(\text{\textcopyright} \ JCN\)) [Carr & Duke, 2013], which decomposes the domain into regions of equivalent behavior.
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The main idea of JCN is that we **quantize** the $f$-values.

Instead of taking a point $c \in \mathbb{R}^2$, we consider a small pixel $P \subset \mathbb{R}^2$. Instead of a fiber $f^{-1}(c)$, we consider a **fat fiber** $f^{-1}(P)$.

In this way, we can identify singular fibers in a robust way, because fat fibers contain essential information on its central fiber.
Domain (3D): Tetrahedral mesh / Range (2D): Rectangular mesh
Tetrahedra in the domain are decomposed into smaller pieces according to their (quantized) values.
Unite neighboring pieces that have the same value. They correspond to the connected components of the inverse image of a pixel — a fat fiber.

At each pixel (square), put a node for each set of neighboring tetrahedra.
Encode the adjacency information of the fat fibers by edges.

For nodes in neighboring pixels, connect them by an edge if they have a common tetrahedron.
In this way, we get a graph called **Joint Contour Net**, describing the adjacency relations among the connected components of fat fibers. This, in turn, can be used to detect birth-death or merge-splitting of fibers.

We study the adjacency of the nodes of the JCN corresponding to neighboring pixels.

Birth-Death of fibers

Merge-Splitting of fibers
In fact, JCN is a graph representation of the so-called **Reeb space**.
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For a multi-field $f : \mathbb{R}^n \to \mathbb{R}^m$, the space $W_f$ obtained by contracting each connected component of the fiber to a point is called the Reeb space of $f$ [Edelsbrunner–Harer–Patel, 2008].
In fact, JCN is a graph representation of the so-called **Reeb space**.

For a multi-field $f : N^n \rightarrow \mathbb{R}^m$, the space $W_f$ obtained by contracting each connected component of the fiber to a point is called the **Reeb space** of $f$ [Edelsbrunner–Harer–Patel, 2008]. In other words, we have the decomposition

$$N^n \xrightarrow{f} \mathbb{R}^m \xrightarrow{q_f} W_f,$$

for some map $\overline{f}$, where $q_f$ is the natural quotient map. This is called the **Stein factorization** of $f$ (in singularity theory).
If $f$ is non-degenerate, then the Reeb space $W_f$ is a polyhedron (or a simplicial complex) of dimension $m$. It is a straightforward generalization of Reeb graph for scalar fields.
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The **Jacobi set image** $q_f(J(f))$ corresponds to the **boundary** (birth-death) or **bifurcation locus** (merge-splitting) of the Reeb space.

Reeb space encodes the topological transition (at least, transition of the number of connected components) of fibers.
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Using results from Singularity Theory concerning maps of manifolds with boundary [Shibata, 2000; Martins & Nabbaro 2013], we get the following classification theorem.
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**Theorem 3.1** *Connected components of singular fibers of a generic differentiable map* $f : N^3 \rightarrow \mathbb{R}^2$ *are classified as in the following lists: there are 7 fibers of codimension* $\kappa = 1$, *and 21 fibers of* $\kappa = 2$. 
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Combining JCN together with the classification theorem, we can identify the singular fiber types!
The following 7 singular fibers appear along curves in the range.

In the list, squares correspond to boundary tangency points in $\partial N^3$ as in the figures on the right.
The following 21 singular fibers appear discretely. Red points correspond to $J(f) \cap \partial N^3 = J(f) \cap J(f_{\partial})$. 

\[ J(f) \cap \partial N^3 = J(f) \cap J(f_{\partial}). \]
The curve of the Jacobi set image $f(J(f)) \cup f_\delta(J(f_\delta)) \subset \mathbb{R}^2$ has 3 types of singularities.

With the help of JCN, we can also identify the curve of the Jacobi set image in the range.
Example of transition of fibers

1. Visualizing Scalar Field Data
2. Visualizing Multi-field Data
3. Visualizing 2-Variate Volume Data
4. Examples of Visualization

Fiber over each part of $f(J(f))$ and $\mathbb{R}^2 \setminus f(J(f))$
When $n = 4$, $m = 3$

§1. Visualizing Scalar Field Data  §2. Visualizing Multi-field Data  §3. Visualizing 2-Variate Volume Data  §4. Examples of Visualization

Local configurations of the Jacobi set image for maps $f : N^4 \rightarrow R^3$
An example of topological transition of fibers for a map $f : \mathbb{N}^4 \rightarrow \mathbb{R}^3$
For $n = 4$, $m = 3$, we have the following classification list.
§4. Examples of Visualization
Analytic map \( f(x, y, z) = (x, y^3 - xy + z^2) \).
A birth-death of fibers can be observed.

\[
\begin{align*}
  f^{-1}(3\varepsilon^2, -2\varepsilon^3) & \quad x = 3\varepsilon^2 \\
  y^3 - xy + z^2 & = -2\varepsilon^3
\end{align*}
\]
Same analytic map $f(x, y, z) = (x, y^3 - xy + z^2)$.

A merge-splitting of fibers can be observed.
Volume data for the Hurricane Isabel 
$f = (\text{Pressure}, \text{Temperature})$

The singular fiber in the left corresponds to the crossing in the right.
The “Hurricane Isabel” data set was produced by the Weather Research and Forecast (WRF) model, courtesy of NCAR and the U.S. National Science Foundation (NSF).
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On the other hand, our technique should be improved for visualizing general scientific data. It works relatively well for simulation data, but sometimes we have serious problems with noise or sparsity of real data.
This supports a theoretical result: the map on the left is degenerated; however, after a perturbation, two or more cusps appear. This was predicted by a theorem [Ikegami & Saeki, 2009] in singularity theory: now it has been visually verified.
For $a, b \in \mathbb{R}_+$, set

$$f_{a,b}(z, w) = z^3 + w^2 + a\bar{z} + b\bar{w}, \quad (z, w) \in \mathbb{C}^2$$

How does the family $\{f_{a,b}\}$ bifurcate if $(a, b) \in \mathbb{R}_+^2$ varies?
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$\mathbb{R}_+^2$ is divided into two regions $A$ and $B$.

The left 2 figures below show the Jacobi set images of $f_{a,b} : \mathbb{C}^2 = \mathbb{R}^4 \rightarrow \mathbb{R}^2 = \mathbb{C}$ for $(a, b) \in A$ and $(a, b) \in B$, respectively.
For $a, b \in \mathbb{R}_+$, set

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How does the family $\{f_{a,b}\}$ bifurcate if $(a, b) \in \mathbb{R}^2_+$ varies?

$\mathbb{R}^2_+$ is divided into two regions $A$ and $B$.

The left 2 figures below show the Jacobi set images of $f_{a,b} : \mathbb{C}^2 = \mathbb{R}^4 \to \mathbb{R}^2 = \mathbb{C}$ for $(a, b) \in A$ and $(a, b) \in B$, respectively.

We would be very happy if we can visualize the singular fibers for $f_{a,b}$. 
By using the **singularity theory** of differentiable mappings,

- We can **list up** singularity types and **singular fiber types** that appear generically;
- Accordingly, we can **identify** the **singularities** and **singular fibers** together with their types.
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Conversely, **these visualization techniques help singularity theory research in Mathematics!**
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I am sure!
Thank you for your attention!