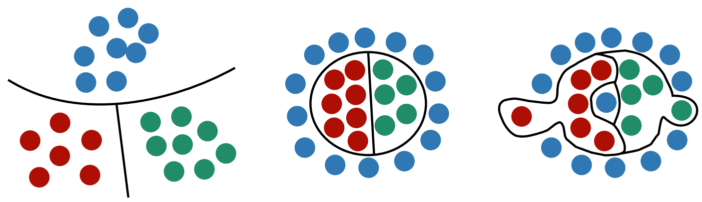

Figure 3: Decision regions and boundaries for three different classification problems with three labels. The black lines represent decision boundaries given by FCFNNs. The different decision regions are separated by decision boundaries. Decision regions and boundaries give valuable information on the neural network used in each case. Classification problems are ordered from left to right by increasing *complexity*. For the left and central classification problems, the decision regions and boundaries are *simple*, in the sense that they seem to properly classify the inputs of the domain without visible outliers or *strange* regions. However, the neural network for the central classification problem seems to have a more complex output, since the blue decision region has one hole that does not exist in the first case. This could be, for example, an indicator of the inherent difficulty of the problem. The right decision regions and boundary are more complicated. The blue decision region has two connected components and one hole, and the red and green regions have two *odd* protuberances which appeared due to outliers in the training data. Although protuberances cannot be detected by the use of usual topological techniques, the extra connected component is detected by the homology of the blue decision region. See Section 2.3 for more details.

2.3 Topological data analysis

Many tools from topological data analysis have been used within machine learning. Among them, persistent homology and Mapper graphs have so far been the most relevant in the study of deep learning methods. In this section, we provide a concise overview of both. The book by Munkres (2000) is a standard reference for general topology. For an introduction to computational topology and to most of the concepts used in this survey, we refer the reader to the book by Edelsbrunner and Harer (2022).

2.3.1 Persistent homology

The most widely used tool from topological data analysis to analyze neural networks in this survey is persistent homology, which studies the evolution of homology groups along an ordered family of simplicial complexes.

An *abstract simplicial complex* is a collection K of non-empty finite subsets of a set P such that $\{p\}$ is in K for all $p \in P$ and such that $\sigma \in K$ whenever $\sigma \subseteq \sigma'$ with $\sigma' \in K$. Elements of P are called *vertices* and elements of K are called *simplices*. A simplex σ has *dimension* d if its cardinality is $d+1$, and the dimension of a finite simplicial complex K is the maximum dimension of its simplices. Graphs $G=(V,E)$ are 1-dimensional simplicial complexes with $P=V$, where each edge in E is a simplex $\{v,w\}$ with $v \neq w$.

Each finite simplicial complex K with a prescribed order in its set of vertices has an associated family of *homology groups* $H_n(K)$ for $n \in \mathbb{N}$, defined as follows. An *n-chain* is a finite sum of n-dimensional simplices of K with coefficients in $\mathbb{Z}$, and the *boundary* of an ordered n-simplex $\sigma = (v_0, \ldots, v_n)$ is the alternating sum $\sum_i (-1)^i (v_0, \ldots, \hat{v}_i, \ldots, v_n)$, where v_i is omitted. An n-chain is an *n-cycle* if its boundary is zero. Then $H_n(K)$ is defined as a quotient of the abelian group of n-cycles modulo the subgroup of n-boundaries. Hence, generators of $H_n(K)$ can be interpreted as n-dimensional "cavities" in K. If coefficients in a field $\mathbb{F}$ are used to define n-chains, then $H_n(K)$ becomes an $\mathbb{F}$-vector space. For convenience, we will work with such vector spaces in most of what follows. If no coefficient field is explicitly selected, we will assume that the one used is the field $\mathbb{F}_2$ of two elements. The dimension of $H_n(K)$ as an $\mathbb{F}$-vector space is called the n-th *Betti number* of K and denoted by $b_n(K)$. The zeroth Betti number counts the number of connected components of K. For a detailed introduction to homology, we refer to Edelsbrunner and Harer (2022).

An $\mathbb{R}$-indexed *persistence module* is a family $\mathbb{V} = (V_t)_{t\in\mathbb{R}}$ of vector spaces over a field $\mathbb{F}$ equipped with $\mathbb{F}$-linear maps $f_{s,t} \colon V_s \to V_t$ for $s \le t$, such that $f_{s,t} \circ f_{r,s} = f_{r,t}$ if $r \le s \le t$ and $f_{t,t} = \mathrm{id}$ for all t. Given a filtration of simplicial complexes $(K_t)_{t\in\mathbb{R}}$ ordered by inclusion, the family $(H_*(K_t))_{t\in\mathbb{R}}$ is a persistence module, where $H_*(K_t)$ denotes the direct sum of $H_n(K_t)$ for all $n \in \mathbb{N}$. The $\mathbb{F}$-linear maps $f_{s,t} \colon H_*(K_s) \to H_*(K_t)$ are induced by the inclusions $K_s \subseteq K_t$. Persistence modules are discussed in detail in the book by Chazal et al. (2016). We denote the persistence module given by the n-th homology H_n of a filtration of simplicial complexes $(K_t)_{t\in\mathbb{R}}$ and fixed field $\mathbb{F}$ by $\mathbb{V}_n^{\mathbb{F}}(K)$. We drop the superscript denoting the field when it is clear from the context.

A persistence module $\mathbb{V}$ is of *finite type* if V_t is finite-dimensional for all t and equal to zero for $t < t_0$ for some t_0, and the maps $f_{s,t}$ are isomorphisms in a neighbourhood of every index value t except for a finite set $\{t_1, \ldots, t_k\}$ at which $f_{t_i,t}$ is an isomorphism if $t_i \le t < t_i + \varepsilon$ for some $\varepsilon > 0$, yet f_{s,t_i} fails to be an isomorphism if $t_i - \varepsilon < s < t_i$.

A vector $v \in V_b$ is said to be *born* at a parameter value b if it is not in the image of $f_{s,b}$ for any $s < b$, and a vector $v \in V_s$ *dies* at a parameter value d if $f_{s,d}(v) = 0$ and $f_{s,t}(v) \neq 0$ for $s \le t < d$. As explained in (Chazal et al., 2016, Theorem 1.4), the lifetime intervals $[b, d) \subset \mathbb{R}$ of a full collection of (arbitrarily chosen) basis elements of a persistence module $\mathbb{V}$ of finite type represent $\mathbb{V}$ up to isomorphism. The intervals $[b, d)$ form a *multiset*, since they can be repeated, so every interval is given with a multiplicity. This multiset is called a *barcode* of $\mathbb{V}$. We assume that $d \in \bar{\mathbb{R}}$ since death parameter values are infinite in the case of vectors $v \in V_s$ for which $f_{s,t}(v) \neq 0$ for all t.

Barcodes are more efficiently represented by means of *persistence diagrams*, which are multisets of points in a coordinate plane with a point (b, d) with $b < d$ and $d \in \bar{\mathbb{R}}$ for each interval $[b, d)$ in the barcode of a persistence module $\mathbb{V}$. We denote by $D(\mathbb{V}) = \{(b_i, d_i)\}_{i\in L}$ the persistence diagram of a persistence module $\mathbb{V}$, where L is the multiset of intervals $[b_i, d_i)$ in its associated barcode; see Figure 4.

In the case of a filtration $(K_t)_{t\in\mathbb{R}}$ of simplicial complexes, the persistence diagram of $(H_*(K_t))_{t\in\mathbb{R}}$ describes the evolution of homology generators along thefiltration. Thus, a representative n-cycle ζ can be associated with each point (b, d) in homological degree n, so that b is the birth parameter of ζ and d is the value at which ζ becomes a boundary.

There are several ways to construct filtrations of simplicial complexes given a set of points or a weighted graph. For sets of points P equipped with a symmetric function

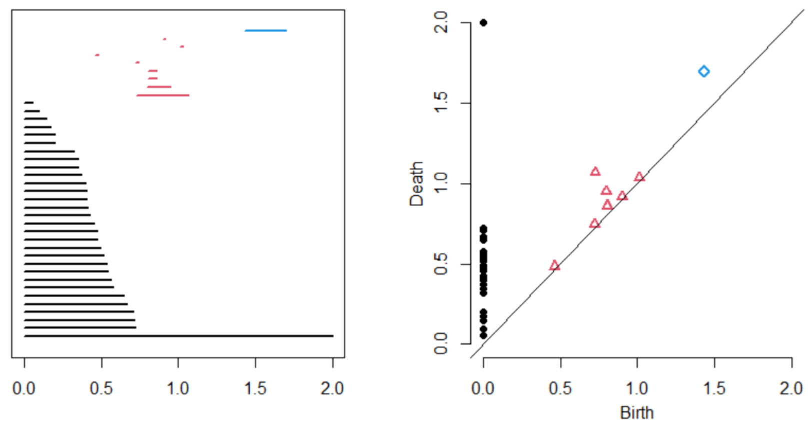

Figure 4: Barcode and persistence diagram of a Vietoris–Rips persistence module of a point cloud with 30 points sampled from the surface of a 3D sphere of radius 1.

$d\colon P \times P \to \bar{\mathbb{R}}$ such that $d(x,x) \leq d(x,y)$ for all $x, y \in P$, called a *dissimilarity*, the most frequent choice is the *Vietoris–Rips filtration*, defined as

$$\mathrm{VR}_t(P,d) = \{\sigma \in \mathcal{P}(P) \setminus \emptyset \,:\, \mathrm{diam}(\sigma) \leq t\}\,.$$

We refer to such pairs (P,d) as *point clouds*. Figure 5 shows simplicial complexes for different values of t of a Vietoris–Rips filtration for a point cloud with eight points and the Euclidean distance. For practical purposes, there are situations in which we may want to limit the dimension of the Vietoris–Rips simplicial complexes to a maximum value $k_{\max}$. In this case, we only take simplices up to dimension $k_{\max}$. We denote dimension-limited Vietoris–Rips filtrations and simplicial complexes by

$$\mathrm{VR}_t^{k_{\max}}(P,d) = \{\sigma \in \mathrm{VR}_t(P,d) \,:\, \dim(\sigma) \leq k_{\max}\}\,.$$

If the point cloud P is a subset of a metric space (X,d), then another popular indexed family of simplicial complexes is the *Čech filtration*

$$\check{C}_t(P,X,d) = \left\{\sigma \in \mathcal{P}(P) \setminus \emptyset \,:\, \textstyle\bigcap_{x\in\sigma} \bar{B}(x,t/2) \neq \emptyset\right\},$$

where $\bar{B}(x,\varepsilon) = \{y \in X : d(x,y) \leq \varepsilon\}$ denotes the closed ball centered at x of radius ε.

Similar ideas can be applied to weighted graphs. Let (G, w_V, w_E) be a weighted graph, where $w_V\colon V(G) \to \mathbb{R}$ and $w_E\colon E(G) \to \mathbb{R}$ are weight functions for the vertices and the edges of G, respectively. By requiring that $w_V(v) \leq w_E(e)$ for all $v \in V(G)$ and all $e \in E(G)$ incident to v, the weighted graph G can be treated as a point cloud. Points correspond to the vertices of G and distances between points are given by the weight functions w_V and w_E, where the lack of an edge between two vertices is encoded as an infinite distance. Thus the distance from a point to itself need not be zero. Formally,

$$d(v,w) = \begin{cases} w_V(v) & \text{if } v = w, \\ w_E(\{v,w\}) & \text{if } \{v,w\} \in E(G), \\ +\infty & \text{otherwise.} \end{cases} \tag{6}$$