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Homology-Based Signatures for Decoding Black-Box Predictions: A Topological Approach to Model Explanation

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ABSTRACT

The increasing deployment of complex machine learning models in high-stakes environments has created a pressing need for interpretable methodologies that can explain model behavior without sacrificing predictive performance. This paper introduces a topological framework for understanding how black-box classifiers partition high-dimensional feature spaces. By constructing persistent homology representations of decision boundaries and analyzing their connected components, loops, and voids, we demonstrate that topological features provide human-interpretable signatures of model decision strategies. Unlike existing explanation methods that rely on local linear approximations or feature attribution scores, our approach captures global structural properties of the model's decision regions. We provide theoretical guarantees on the stability of topological explanations and validate our framework on synthetic manifolds and real-world benchmark datasets. The results indicate that topological summaries enable practitioners to detect undesirable model behaviors, including disconnected decision regions and spurious class boundaries, that remain invisible to conventional explanation tools.

The abstract describes a new way to understand how complex machine learning models, like deep neural networks or gradient boosting machines, actually make decisions. These models are often called "black boxes" because even if they predict accurately, it's nearly impossible to see inside them. This is a serious problem in high-stakes areas such as medical diagnosis, criminal justice, or autonomous driving, where a wrong prediction can cause real harm. The paper's solution is to use topology, a branch of mathematics that studies shapes and their properties things like how many pieces a shape has, whether it has holes, or if it contains empty cavities.

Instead of trying to explain a single prediction at a time (which is what most current methods do, like LIME or SHAP), the authors look at the whole decision boundary. In a classification problem, the model carves up the feature space into regions, one for each class. The boundary between these regions is a geometric object. By applying a technique called persistent homology, the researchers can track how this boundary changes as you zoom in or out. Persistent homology reveals which topological features connected blobs, loops, tunnels, voids are robust across different scales and which are just noise.

What makes this approach different is that it captures the global structure of the model's decisions. For example, a linear model will produce decision regions that are simple and convex, with no holes. A very complex model might split the same class into several disconnected islands, or create a donut-shaped region where one class completely surrounds another. Those patterns are not visible with standard explanation tools. The paper provides mathematical proofs that these topological summaries are stable: small changes to the model or the data lead to only small changes in the topological signature. This stability is important because it means the explanations are trustworthy and not just artifacts of random noise.

The authors test their framework on two kinds of data. First, they use synthetic manifolds artificially created geometric shapes where the true decision boundary is known. This lets them verify that the topological method correctly identifies what is actually there. Second, they apply it to real benchmark datasets that are commonly used in machine learning research. The results show that topological summaries can reveal problems that would otherwise go unnoticed. Two specific examples are mentioned: disconnected decision regions (the model says that widely separated clusters of points all belong to the same class, even though there is no path between them that stays within that class) and spurious class boundaries (the model draws extra, unnecessary separations inside what should be a single, smooth region). Both are signs that the model is doing something unnatural, possibly overfitting or relying on irrelevant features.

In essence, the abstract argues that topology gives the practitioner a new lens. Instead of asking "which features are important for this prediction?" you can ask "what is the shape of the model's reasoning?" That shape can

be described in plain language "the class A region has two separate components" or "class B wraps around class C like a ring" which is human-interpretable and immediately useful for debugging or certifying a model before deployment.

INTRODUCTION

Machine learning models have achieved remarkable success across domains ranging from computer vision to clinical diagnostics. However, the most accurate models deep neural networks, gradient-boosted ensembles, and complex kernel methods operate as black boxes whose internal decision logic resists straightforward interpretation. This opacity poses significant challenges for regulatory compliance, error analysis, and scientific discovery.

Existing interpretability methods fall into two broad categories. Feature attribution techniques, such as SHAP and LIME, assign importance scores to input features based on local perturbations around individual predictions. While useful for identifying which variables influence a specific output, these methods provide no information about the global geometric structure of the decision boundary. Activation-based approaches for neural networks reveal internal representations but require access to model architecture and parameters, which is often unavailable in proprietary systems.

This paper addresses a fundamental question: Can we characterize the global topology of a black-box model's decision boundary using only input-output queries? Our answer draws upon persistent homology, a tool from computational topology that captures multiscale features of geometric objects. The key insight is that decision boundaries in high-dimensional spaces possess topological invariants numbers of connected components, tunnels, and cavities that remain stable under small perturbations of the model.

We make three primary contributions. First, we formalize the relationship between persistent homology and decision boundary geometry, proving that topological summaries satisfy Lipschitz continuity with respect to model parameter changes. Second, we develop an algorithm for constructing persistence diagrams from random point samples of the input space, requiring no gradient information or internal model access. Third, we demonstrate through controlled experiments that topological features correlate with specific model pathologies, enabling practitioners to identify overfitting, underfitting, and unstable decision regions.

Machine learning models keep surprising us with what they can do. They beat humans at image recognition, they detect tumors in CT scans that radiologists miss, they predict equipment failures from vibration patterns. But the models that work best deep neural networks with millions of parameters, gradient-boosted trees with hundreds of decision splits, kernel methods that map data into impossible-to-visualize feature spaces are also the most opaque. You feed in an input, you get an output, but what happens inside is anyone’s guess. This isn’t just an academic annoyance. When a model denies a loan or misdiagnoses a patient, you need to explain why. Regulators demand it. Developers need it to debug their systems. Scientists trying to discover new phenomena from data need to trust that the model’s logic matches physical reality. A black box won’t cut it.

So people have built tools to peek inside. The popular ones fall into two camps. First there are feature attribution methods SHAP and LIME are the best known. The idea is simple: tweak the input slightly, see how the prediction changes, and assign importance scores to each feature based on those local perturbations. This works well if you only care about one prediction at a time. For a single patient, you can say “the model flagged this X-ray because it saw a spiculated mass in the upper left lobe.” But these methods don’t tell you anything about the overall shape of the decision boundary. You might know which pixels matter for each image, but you won’t know whether the boundary that separates “cancer” from “healthy” is a single smooth sheet or a tangled mess of disconnected islands. The second camp is activation-based methods for neural networks things like feature visualization or layer-wise relevance propagation. They show you what internal neurons respond to. The catch: you need full access to the model’s architecture and weights. That works fine for open-source models, but many real-world systems are proprietary. Banks don’t hand out their fraud detection networks. Tech companies don’t let you run backpropagation through their recommendation engines. So you’re left with a black box that only answers queries: give it an input, get an output, nothing more.

This paper asks whether that’s actually enough. Can we characterize the global shape of a black-box decision boundary using nothing but input-output queries? I think the answer is yes, and the key comes from a branch of math called computational topology. Specifically, persistent homology. The idea is to take point samples from the input space, label each point by which side of the decision boundary it falls on, and then build a filtration a nested sequence of simplicial complexes that tracks how the shape of the boundary changes as you zoom in or out. Every decision boundary has certain topological invariants: how many separate pieces it has (connected components), how many tunnels or holes go through it (one-dimensional loops), and how many enclosed cavities it contains (two-dimensional voids). These

numbers are stable. Make a small change to the model's parameters, and the boundary might wiggle but its topology won't flip unless something drastic happens. That's the Lipschitz property we prove in Section 3.

What we contribute is three things. First, a formal proof that persistence diagrams those multiset summaries of topological features vary continuously with the model parameters. No gradient needed, just the fact that small parameter changes produce small shifts in the decision boundary under mild regularity assumptions. Second, an algorithm that constructs these diagrams from random point samples. You pick points uniformly from a bounded region of input space, query the model for each one, and build a Vietoris–Rips or alpha complex. The algorithm doesn't need gradients, doesn't need internal activations, doesn't even need the model's confidence scores just yes/no or class labels. Third, a set of experiments showing that these topological summaries aren't just mathematical curiosities. We find that overfitted models produce decision boundaries with many tiny disconnected components little bubbles of one class floating inside the other. Underfitted models produce boundaries with fewer features than expected, often missing the necessary tunnels or cavities that separate natural data clusters. And unstable regions, where the model flips predictions wildly under small input changes, show up as persistent topological noise across many scales. Practitioners can use this to diagnose their models without ever opening the black box.

The rest of the paper is organized as follows. Section 2 reviews persistent homology and the sampling theory that makes our approach work. Section 3 states our continuity theorem and sketches the proof. Section 4 describes the random sampling algorithm and gives practical recommendations for choosing sample sizes and scales. Section 5 presents the experimental results on synthetic datasets and two real-world benchmarks. Section 6 discusses limitations computational cost for very high dimensions, sensitivity to sampling density near the boundary and suggests directions for future work.

2. Mathematical Preliminaries

2.1 Topological Spaces and Homology

Let X⊂RdX⊂Rd denote the input space equipped with the standard Euclidean metric. For a given classification model f:Rd→{0,1,…,K−1}f:Rd→{0,1,…,K−1}, the decision region for class kk is the preimage Rk=f−1(k)Rk=f−1(k). The decision boundary B=⋃k≠ℓ(∂Rk∩∂Rℓ)B=⋃k□ =ℓ(∂Rk∩∂Rℓ) is the set of points where the predicted class changes.
Homology groups Hp(Rk)Hp(Rk) capture pp-dimensional holes in the region RkRk. The rank of H0H0 equals the number of connected components. The rank of H1H1 counts independent loops or tunnels. The rank of H2H2 counts enclosed cavities or voids. For most machine learning applications, p∈{0,1,2}p∈{0,1,2} suffices, as higher-dimensional holes rarely occur in decision boundaries of practical models.

We're looking at a classification problem where the input space is a subset XX of RdRd with the usual Euclidean distance. The model ff assigns to each point a label from 00 to K−1K−1. For a given class kk, the decision region RkRk is simply all points that map to kk under ff. The decision boundary BB is where the class changes specifically, the union over all pairs of distinct classes of the intersection of their region boundaries. In plain terms, these are the points where a tiny movement can flip the prediction.

Now, homology comes in to describe the shape of each decision region. Homology groups Hp(Rk)Hp(Rk) capture different kinds of "holes" in RkRk. The rank of H0H0 is just the number of connected components how many separate pieces the region breaks into. The rank of H1H1 counts independent loops, like tunnels or handles that go through the region (think of a donut hole). The rank of H2H2 counts enclosed cavities or voids, like the interior of a hollow ball.
For most machine learning scenarios, we only care about p=0,1,2p=0,1,2. Why? Because in practice, the decision boundaries of typical models think neural networks with smooth activations, or SVMs, or decision trees tend to be reasonably nice geometric objects in low to moderate dimensions. Higher-dimensional holes (like a 3-dimensional void in a 4-dimensional space) almost never appear in the decision regions of models we actually use. The data and the classifiers are usually such that the regions have at most surfaces, curves, and isolated components nothing that requires tracking 3-cycles or beyond. So homology up to dimension 2 is enough to capture the relevant topological features: how many pieces, how many independent loops, and how many cavities.

2.2 Persistent Homology for Sublevel Sets

Rather than computing homology at a single scale, persistent homology tracks how topological features appear and disappear as we vary a threshold parameter. For a continuous function g:Rd→Rg:Rd→R, the sublevel set Lt={x:g(x)≤t}Lt={x:g(x)≤t} grows with increasing tt. The persistence diagram Dgmp(g)Dgmp(g) records each pp-dimensional feature as a point (b,d)(b,d) where bb is the threshold at which the feature appears (birth) and dd is the threshold at which it disappears (death).

To apply persistence to classification, we construct a function whose sublevel sets approximate the decision regions. Define the signed distance to the decision boundary:
hk(x)={−ρ(x,B)if f(x)=k+ρ(x,B)otherwisehk(x)={−ρ(x,B)+ρ(x,B)if f(x)=kotherwise

where ρ(x,B)=inf⁡y∈B‖ x−y‖ 2ρ(x,B)=infy∈B‖ x−y‖ 2. Then the sublevel set {x:hk(x)≤t}{x:hk(x)≤t} corresponds exactly to points within distance ∣ t∣ ∣ t∣ of RkRk when t<0t<0. As tt increases from −∞−∞ to 00, the sublevel sets trace the expansion of RkRk outward from its interior.

Theorem 1 (Stability). For two classifiers ff and f′f′ with decision boundaries BB and B′B′, let dB=sup⁡x∈Rd∣ ρ(x,B)−ρ(x,B′)∣ dB=supx∈Rd∣ ρ(x,B)−ρ(x,B′)∣ denote the Hausdorff distance between boundaries. Then the bottleneck distance between persistence diagrams satisfies:
dB(Dgmp(hk),Dgmp(hk′))≤2dB(B,B′)dB(Dgmp(hk),Dgmp(hk′))≤2dB(B,B′)

Proof sketch. The functions hkhk and hk′hk′ differ by at most 2dB(B,B′)2dB(B,B′) pointwise. Standard stability theorems for persistent homology (Cohen-Steiner et al., 2007) then imply the bottleneck bound. ■

This theorem guarantees that small changes in the decision boundary produce small changes in the persistence diagram, making topological summaries robust to sampling noise and model perturbations.

We start with a continuous function g:Rd→Rg:Rd→R. For each real number tt, the sublevel set Lt={x:g(x)≤t}Lt ={x:g(x)≤t} is just the set of points where the function value is at most tt. As tt increases, these sets grow: Ls⊆LtLs⊆Lt whenever s≤ts≤t. Persistent homology looks at how the topology (holes, connected components, etc.) of these sublevel sets changes with tt. A topological feature say a connected component that appears at t=bt=b and later merges into another component at t=dt=d is recorded as a point (b,d)(b,d) in a persistence diagram. The birth bb is the first tt where the feature exists; the death dd is the tt where it disappears. Features that live forever (e.g., the whole space) are usually recorded as having death +∞+∞, but often we ignore those.

Now how does this help classification? Suppose we have a binary classifier (the idea extends to multiple classes) with a decision boundary B⊂RdB⊂Rd. The classifier assigns a label kk to points on one side of BB and a different label to the other side. We want a function whose sublevel sets approximate the region for class kk. The signed distance to BB does this. Define

hk(x)={−ρ(x,B)if f(x)=k,+ρ(x,B)otherwise,hk(x)={−ρ(x,B)+ρ(x,B)if f(x)=k,otherwise,
where ρ(x,B)=inf⁡y∈B‖ x−y‖ 2ρ(x,B)=infy∈B‖ x−y‖ 2 is the Euclidean distance from xx to the boundary. So inside the region labeled kk, hkhk is negative and its absolute value equals the distance to the boundary. Outside that region, hkhk is positive and again its value is the distance to BB.

Now look at the sublevel set {x:hk(x)≤t}{x:hk(x)≤t}. For t<0t<0, this set is exactly the set of points in the kk-region that are at most ∣ t∣ ∣ t∣ away from the boundary. In other words, it is the kk-region "eroded" inward by distance ∣ t∣ ∣ t∣ . As tt increases from −∞−∞ to 00, the sublevel sets grow from the empty set (if the kk-region is bounded) to the whole kk-region (at t=0t=0). For t>0t>0, the sublevel set includes also points from the other side that are within distance tt of BB. So the expansion traces not only the kk-region but also a "buffer" around it.

The topological features of these sublevel sets holes, connected components, etc. are intimately related to the shape of the decision region. For instance, if the kk-region has a narrow passage that closes as we go inward, that will appear as a feature in the persistence diagram.

Stability. If we have two classifiers ff and f′f′ with decision boundaries BB and B′B′, we can measure how far apart the boundaries are by the Hausdorff distance

dB(B,B′)=sup⁡x∈Rd∣ ρ(x,B)−ρ(x,B′)∣ .dB(B,B′)=x∈Rdsupρ(x,B)−ρ(x,B′).
Intuitively, if the two boundaries are close in this sense, then the functions hkhk and hk′hk′ (built from BB and B′B′) are close pointwise: ∣ hk(x)−hk′(x)∣ ≤2dB(B,B′)∣ hk(x)−hk′(x)∣ ≤2dB(B,B′) for every xx. This is because the signed distance changes at most by the Hausdorff distance of the zero sets.

A classic result in topological data analysis (Cohen-Steiner et al., 2007) says that if two real-valued functions are uniformly close, then their persistence diagrams are close in the bottleneck distance. The bottleneck distance measures how far you have to move points in the diagram to match one diagram to the other. More precisely, if ‖ g−g′‖ ∞≤ε‖ g−g′‖ ∞≤ε, then the bottleneck distance between their persistence diagrams is at most εε (for sublevel sets). Applying this to hkhk and hk′hk′ with ε=2dB(B,B′)ε=2dB(B,B′) gives

dB(Dgm⁡p(hk),Dgm⁡p(hk′))≤2dB(B,B′).dB(Dgmp(hk),Dgmp(hk′))≤2dB(B,B′).
The theorem is powerful because it tells us that if the decision boundary changes only a little (due to different training sets, slight model variations, or noise), the topological summary also changes only a little. Hence the persistence diagram is a robust signature of the classifier's decision region. In classification tasks, this stability means that small perturbations do not create spurious topological features or destroy real ones. We can therefore use persistence diagrams as features for learning or for comparing classifiers without worrying about oversensitivity.

METHODOLOGY

3.1 Sampling Strategy for Decision Boundary Proximity

Computing hk(x)hk(x) requires knowledge of the distance to the decision boundary BB. For black-box models, BB is not explicitly available. We therefore estimate ρ(x,B)ρ(x,B) through binary search along random directions.

Given a query point xx, sample mm unit vectors u1,…,umu1,…,um uniformly from the sphere Sd−1Sd−1. For each direction, perform binary search to find the smallest λ≥0λ≥0 such that f(x+λuj)≠f(x)f(x+λuj)□ =f(x). Let λj∗ λj∗ be this distance. Then:

ρ^(x,B)=min⁡1≤j≤mλj∗ ρ^(x,B)=1≤j≤mminλj∗
For points whose nearest boundary point lies within a region of approximately linear decision boundary, this estimate converges to ρ(x,B)ρ(x,B) as m→∞m→∞. In practice, we find m=50m=50 directions suffices for dimensions up to 20.

3.2 Constructing Persistence Diagrams from Samples

To build persistence diagrams for a class RkRk, we generate NN points uniformly from a bounded domain Ω⊂RdΩ⊂Rd that contains the training data. For each point xixi, compute h^k(xi)=(2· 1[f(xi)=k]−1)· ρ^(xi,B)h^k(xi)=(2· 1[f(xi)=k]−1)· ρ^(xi,B), which yields negative values inside RkRk and positive values outside.
We then construct the Vietoris-Rips complex on the set of points at varying distance thresholds. For each threshold εε, we connect points with Euclidean distance less than εε. The resulting simplicial complex approximates the sublevel set geometry. Using the Dionysus library, we compute persistence diagrams for p=0,1,2p=0,1,2.

The goal is to build persistence diagrams for a specific class, call it RkRk. Here's how it works step by step.
First, you take a bounded domain Ω⊂RdΩ⊂Rd that contains all your training data. Inside this domain, you generate NN points uniformly at random. These points act as a sample set where you will evaluate a certain function.
For each sampled point xixi, you compute a value h^k(xi)h^k(xi). The formula is:
h^k(xi)=(2· 1[f(xi)=k]−1)· ρ^(xi,B)h^k(xi)=(2· 1[f(xi)=k]−1)· ρ^(xi,B)

Here:

- 1[f(xi)=k]1[f(xi)=k] is an indicator: 1 if the true label of xixi is class kk, else 0.
- The term (2· indicator−1)(2· indicator−1) becomes +1+1 when xixi belongs to class kk, and −1−1 otherwise.
- ρ^(xi,B)ρ^(xi,B) is some estimated distance (or density-related value) from xixi to the boundary between classes. The exact definition of ρ^ρ^ is not given here, but presumably it is positive.

Multiplying gives: inside class kk the value is negative (since +1+1 times a positive ρ^ρ^ would be positive? Wait: inside RkRk, indicator = 1, so 2∗ 1−1=+12∗ 1−1=+1, then times positive ρ^ρ^ yields positive. That contradicts the statement. Let me read carefully: the original says "yields negative values inside RkRk and positive values outside". That means they likely define the sign differently, or they take the negative of the whole thing. Probably they mean (1−2· 1[…])(1−2· 1[…]) instead. But the text as written says 2· 1−12· 1−1. So either it's a typo, or they later flip interpretation. Anyway, the important point: the function h^kh^k is negative on points of class kk, positive elsewhere.

So it acts like a signed distance to the class region.
Once you have these function values on the NN random points, you build a Vietoris–Rips complex. You vary a distance threshold εε. For each εε, you connect any two points whose Euclidean distance is less than εε. That gives a graph. Then you add higher-dimensional simplices whenever all their edges are present (the usual Rips construction). This simplicial complex approximates the sublevel set geometry of the function h^kh^k. Why? Because the points are sampled uniformly, and the function values are attached to them. The sublevel set {x:h^k(x)≤t}{x:h^k(x)≤t} for a negative threshold tt captures the region inside RkRk. By varying εε in the Rips complex, you are effectively varying a scale parameter that captures connectivity and holes in that region.

Finally, you use the Dionysus library (a common software for persistent homology) to compute persistence diagrams. You do this for homology dimensions p=0,1,2p=0,1,2. Dimension 0 tracks connected components, dimension 1 tracks loops (cycles), dimension 2 tracks voids (cavities). The persistence diagram records when these topological features appear and disappear as the threshold εε changes.
In short, the method converts a classification problem into a function on a point cloud, then uses persistent homology to describe the shape of the class region RkRk from a finite sample.

3.3 Topological Signatures for Model Comparison

A persistence diagram is an infinite multiset of points in the plane, which is not directly usable as a feature vector. We extract three numerical summaries:

Persistence entropy: For a diagram with points {(bi,di)}{(bi,di)}, define persistence ℓi=| di−bi| ℓi=| di−bi| . The entropy is E=−∑ipilog⁡piE=−∑ipilogpi where pi=ℓi/∑jℓjpi=ℓi/∑jℓj. Higher entropy indicates more complex topological structure.

Maximum persistence: M=max⁡iℓiM=maxiℓi. Large values indicate dominant topological features that persist across many scales.

Birth-death correlation: The Pearson correlation between birth and death values. High correlation suggests that features appearing early also die late, characteristic of well-separated decision regions.

These three quantities for each homology dimension and each class produce a compact signature vector of length 3×3×K3×3×K, where KK is the number of classes.

When you have a persistence diagram from something like a Vietoris–Rips filtration, you get a bunch of points (b, d) in the plane. Each point corresponds to a topological feature (a connected component, a loop, a void, etc.) that appears at scale b and disappears at scale d. The diagram is just a multiset you can't directly feed it into a classifier or regression model. So you need numbers, or a vector of numbers, that capture the shape of that diagram.

The text gives three common numerical summaries. I'll go through each one in plain terms.

Persistence entropy First you compute the persistence ℓ_i = |d_i b_i| for each point. That's the "lifetime" of the feature. Then you normalise these lifetimes to probabilities: p_i = ℓ_i / (sum of all ℓ_j). The entropy is –Σ p_i log p_i.What does this measure? If all lifetimes are about the same, the probabilities are roughly equal and entropy is high. If one feature dominates (say one huge bar and many tiny ones), then most probability mass is on that one bar, so entropy is low. In practice, higher entropy means the diagram has a richer mix of persistence scales many features lasting for different amounts. Low entropy might mean a single prominent scale or many very short-lived features that don't contribute much.

Maximum persistence That's just M = max_i ℓ_i. This is straightforward: the longest bar in the diagram. A large M means there's at least one topological feature that survives over a wide range of scales. That often indicates something meaningful about the underlying shape e.g., a big hole in a point cloud or a clear separation between clusters. In model comparison, if one model's diagrams consistently have higher M than another's, it might be capturing more persistent structure.

Birth-death correlation You take all the (b_i, d_i) pairs and compute the Pearson correlation coefficient between the births and the deaths.If the correlation is positive and high, then features that are born early also tend to die late. That suggests a kind of hierarchical or well-separated structure: think of clusters that appear early and stay separate, so their loops or components persist. If the correlation is low or negative, births and deaths are less tied maybe many short features that appear and die quickly, or long features that appear late. This can tell you something about how "regular" the topology is across scales.

Putting it together These three numbers are computed for each homology dimension separately usually dimension 0 (connected components), dimension 1 (cycles/loops), and sometimes dimension 2 (voids/cavities). The text says "for each homology dimension and each class". So if you have K classes (say in a classification problem, where each class has its own set of persistence diagrams, perhaps from different trained models or different subsets of data), then you get a vector of length 3 × 3 × K.

For example:

- 3 summaries (entropy, max persistence, birth-death correlation)
- for each of 3 dimensions (H0, H1, H2)
- for each of K classes.

That gives you 9K numbers. You can then use that vector as input to another classifier, or as a distance metric between models. The idea is that two models that behave similarly in terms of these topological signatures will have similar geometric properties decision boundaries, cluster shapes, etc. even if their internal parameters look different.

One thing the text doesn't spell out: how exactly do you get a persistence diagram per class? Typically you'd take the model's prediction function (e.g., the probability outputs) and build a filtration on the data space using something like sublevel sets of that function, or use the model's internal representations. But that's a separate discussion. Here the focus is just on turning the resulting diagrams into a fixed-length vector.

EXPERIMENTAL VALIDATION

4.1 Synthetic Datasets with Known Topology

We first validate our method on synthetic data where the true decision topology is known. Consider a two-class problem in R2R2:

- **Two disks:** Class 0 forms two separated disks. Class 1 occupies the complement. Expected: H0(R0)H0(R0) has rank 2.
- **Annulus with disk:** Class 0 is an annulus (outer radius 2, inner radius 1). Class 1 is the interior disk. Expected: H1(R0)H1(R0) has rank 1.
- **Three spheres:** Class 0 consists of three disconnected spherical regions in R3R3. Class 1 is the background. Expected: H0(R0)H0(R0) rank 3, H2(R1)H2(R1) rank 1 (the background has a cavity).

We train a random forest (500 trees, max depth 10) on 10,000 labeled points from each configuration. Table 1 reports the topological signatures extracted from the trained models.

Configuration	Max Persistence H0	Max Persistence H1	Max Persistence H2	Detected Topology
Two disks	0.87	0.12	0.00	2 components □
Annulus	0.34	0.76	0.00	1 loop □
Three spheres	0.91	0.08	0.68	3 components, 1 cavity □

The persistent homology correctly identifies the ground-truth topological features. The small nonzero persistence values for features not present in the true data arise from sampling noise and the finite resolution of the decision boundary estimate.

4.2 Identifying Overfitting in High Dimensions

We construct a high-dimensional classification task where overfitting manifests as spurious holes in decision regions. Generate 2,000 points in R10R10 from two isotropic Gaussian distributions with means μ0=(0,…,0)μ0=(0,…,0) and μ1=(1,0,…,0)μ1=(1,0,…,0), both with variance 0.5. Train three classifiers:

- **Underfit:** Logistic regression with no regularization
- **Proper fit:** Random forest with 100 trees, max depth 5
- **Overfit:** Random forest with 500 trees, max depth 20, no minimum samples per leaf

We evaluate topological signatures on a holdout set of 1,000 points. Figure 1 (described narratively) shows the persistence diagrams for class 0. The underfit model produces a single connected component with no loops, as the linear decision boundary yields a convex region. The properly fit model shows minor topological complexity small loops appear but die quickly (persistence < 0.1). The overfit model exhibits a persistent loop with death-birth ratio exceeding 0.8, indicating a closed decision region that isolates a small pocket of class 0 surrounded by class 1.

Quantitatively, the overfit model has persistence entropy 1.34 for H1H1, compared to 0.28 for proper fit and 0.00 for underfit. Maximum persistence for H1H1 is 0.67, 0.12, and 0.00 respectively. These metrics provide early warning of overfitting without requiring validation accuracy curves.

4.3 Case Study: MNIST Digit Classification

We analyze a convolutional neural network trained on MNIST (test accuracy 98.7%). The network has two convolutional layers (32 and 64 filters) followed by a 128-unit dense layer and a 10-way softmax output. We focus on the decision region for the digit '8', which often exhibits topological complexity due to the digit's two-loops shape.

Generate 5,000 random points uniformly from the hypercube [0,1]784[0,1]784 after normalizing pixel values. For each point, estimate distance to decision boundary using 100 random directions. Compute persistence diagrams for the '8' region in the ambient 784-dimensional space too high-dimensional for direct geometric interpretation, but the persistence entropy provides a summary.

The persistence diagram for H0H0 shows eight features with persistence exceeding 0.3, indicating that the model's '8' region has approximately eight connected components in the high-dimensional input space. This is unexpected: we might anticipate a single connected region corresponding to all images that look like 8. Further investigation reveals that the network treats heavily rotated or scaled '8' images as separate components because the training data contained only upright, normally scaled digits. The topological signature thus exposes a limitation of the training distribution that would remain hidden when examining only classification accuracy.

For comparison, we compute topological signatures for the digit '0' region. The '0' region shows only three persistent components, reflecting the greater rotational symmetry of zeros in the training data. The H1H1 features for '0' are negligible, whereas '8' shows moderate H1H1 persistence (maximum 0.24) corresponding to the two holes in the digit's shape though these holes are not preserved in the high-dimensional decision region due to the network's invariance to small deformations.

5. Comparison with Existing Methods

We compare our topological approach with three standard interpretability methods on the overfitting detection task from Section 4.2.

LIME: For a fixed test point in class 0, LIME fits a local linear model using 500 perturbations. The resulting feature weights change by 40% when the number of perturbations varies between 100 and 1,000. More critically, LIME

provides no information about the global loop structure an analyst would need to examine many local explanations to infer the existence of a spurious hole.

SHAP: Similar to LIME, SHAP produces feature attributions based on Shapley values. For class 0 points inside the spurious loop, SHAP correctly identifies features that distinguish the pocket from the main region. However, SHAP cannot distinguish between an isolated pocket and a narrow connecting corridor between two larger regions. The topological approach explicitly detects the closed loop that defines the pocket as a separate component.

Partial Dependence Plots (PDP): For the two-dimensional projection of the data (the first two principal components), PDP shows the average predicted probability as a function of these coordinates. The overfit model produces a PDP with a small blue island (class 0) surrounded by red (class 1). While this reveals the spurious pocket, PDP requires projecting to low dimensions, which may collapse or distort topological structure in higher dimensions. Our method works directly in the original 10-dimensional space.

A quantitative comparison on 50 synthetic datasets with known topological features shows that our method achieves 94% accuracy in detecting the presence of at least one non-trivial topological feature ($\beta_1 \geq 1 \beta_1 \geq 1$ or $\beta_2 \geq 1 \beta_2 \geq 1$), compared to 31% for the best projection-based PDP approach (optimal projection chosen by an oracle) and 0% for LIME and SHAP (which are not designed for global structure detection).

6. Limitations and Practical Considerations

Several limitations warrant discussion. First, the computational cost of estimating distances to the decision boundary scales as $O(m \cdot N \cdot \log(1/\tau))O(m \cdot N \cdot \log(1/\tau))$ where mm is the number of random directions, NN the number of sample points, and $\tau\tau$ the desired precision in boundary location. For a 20-dimensional dataset with $N=5000N=5000$, $m=50m=50$, and binary search depth 20, the total number of model evaluations is 5 million. For neural networks with millisecond inference times, this is feasible (roughly 90 minutes). For slower models or higher dimensions, the method becomes impractical.

Second, the uniform sampling of the input domain fails when the domain is unbounded or when decision boundaries extend to infinity. In practice, we restrict sampling to a bounding box determined by the training data quantiles, accepting that boundary features outside this box will be missed.

Third, our method assumes the decision boundary has positive reach that is, the closest point on the boundary is unique for all points within some distance. While violated for boundaries with sharp corners, the stability theorem ensures that approximate distances still yield meaningful persistence diagrams.

Fourth, the interpretation of higher-dimensional persistence ($p \geq 3$) remains difficult for human analysts. Our experiments suggest that focusing on $p = 0, 1, 2$ captures the most practically relevant features, but pathological models may exhibit higher-dimensional holes that we would fail to detect.

CONCLUSION

This paper has presented a topological framework for interpreting black-box machine learning models based on the persistent homology of decision regions. The theoretical contribution establishes stability guarantees linking model perturbations to changes in topological summaries. The methodological contribution provides a practical algorithm that requires only query access to the model, making it applicable to proprietary systems. The empirical contribution demonstrates that topological signatures detect overfitting, reveal disconnected decision components, and distinguish classes with different intrinsic geometries. For practitioners, topological analysis offers a complementary tool to existing interpretability methods. Where LIME and SHAP answer "which features matter for this prediction?", topological methods answer "what is the global shape of the decision region?" These questions are equally important for building trustworthy models, particularly in safety-critical applications where unexpected decision boundaries could lead to catastrophic failures. Future work includes extending the framework to probabilistic classifiers, where decision boundaries are replaced by level sets of probability functions. Another direction involves developing topological regularization terms that penalize spurious holes during training, directly embedding interpretability into the learning objective. Finally, we plan to investigate the relationship between topological complexity and generalization bounds, potentially linking the geometric properties we measure to theoretical guarantees on model performance.

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