

TDA Review

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Math Basics



Injective

A function $f: X \to Y$ is injective if $f(x_1) = f(x_2)$ implies $x_1 = x_2$.

Surjective

A function $f: X \to Y$ is surjective if $y \in Y$ implies there exists $x \in X$ such that f(x) = y.

Bijective

A function $f: X \to Y$ is bijective if it is both injective and surjective. (Equivalently f is bijective if f has both a left and right inverse.)

Pre-image

The pre-image of $y \in Y$ under $f: X \to Y$ is the set of all $x \in X$ such that f(x) = y. This can be extended to whole subsets of Y by letting the pre-image of $U \subseteq Y$ be the set of all $x \in X$ such that $f(x) \in U$.

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Let X be a set. A topology τ on X is a collection of subsets of X called open sets such that:

- 0 $\emptyset, X \in \tau$,
- 2 the union of an arbitrary collection of subsets of τ is in τ , and
- lacksquare the intersection of a finite collection of subsets of au is in au.

We call (X, τ) a topological space.

We could have just as easily defined a topology in terms of closed sets. However, the relationship between open and closed sets of a topological space is easy enough. Let $C \subseteq X$, if $X - C \in \tau$, then C is closed.

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Bases Lemmas

A basis \mathcal{B} of τ is a collection of subsets of X such that:

- **1** for every $x \in X$, there is at least one $B \in \mathcal{B}$ such that $x \in B$, and
- ② if $x \in X$ belongs to the intersection of $\{B_1, \ldots, B_n\} \subseteq \mathcal{B}$, then there exists $B \in \mathcal{B}$ such that $B = \bigcap_{i=1}^{n} B_i$, where $x \in B$.

Lemma 13.1 in Munkres

Let (X, τ) be a topological space. Let \mathcal{B} be a basis of τ on X. Then for every $U \in \tau$ there exists a collection of basis elements $\{B_{\alpha}\}_{\alpha \in J}$ such that $U = \bigcup_{\alpha \in I} B_{\alpha}$.

Lemma 13.2 in Munkres

Let (X, τ) be a topological space. Suppose there exists a collection of open sets C such that for every open set U of X and every $x \in U$, there exists $C \in \mathcal{C}$ such that $x \in C$. Then \mathcal{C} is a basis of τ .

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Let (X, τ) be a topological space. A point $x \in X$ is a limit point of a subset $A \subseteq X$ if every neighborhood of x contains a point of A. Here we say that a neighborhood of x is a set N such that $x \in N$ and $N \in \tau$.

Corollary 17.7 in Munkres

A subspace of a topological space is closed if and only if it contains all of its limit points.

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Hausdorff Spaces

A topological space (X, τ) is Hausdorff if for every $x, y \in X$, $x \neq y$ implies that x and y have disjoint neighborhoods.

This definition says something about the separability of a topological space. Interestingly, it means that elements of a Hausdorff space are distinct. Especially considering limit points of certain sequences.

The T_1 axiom is a weaker version of the Hausdorff axiom that says that every finite set is closed.

Theorem 17.10 in Munkres

If X is Hausdorff, then a sequence $\{x_n\}$ in X converges to at most one $x \in X$.

Continuos Functions



A function $f: X \to Y$ is continuous if for every open subset $V \subseteq Y$, the subset $f^{\text{pre}}(V) \subseteq X$ is open.

Theorem 18.1 in Munkres

Let (X, τ_X) and (Y, τ_Y) be topological spaces; let $f: X \to Y$. Then the following are equivalent:

- f is continuous,
- ② for every subset $A \subseteq X$, $f(\overline{A}) \subset \overline{f(A)}$,
- **3** for every closed subset $C \subseteq Y$, the set $f^{pre}(C)$ is closed, and
- for each $x \in X$ and neighborhood V of f(x), there exists a neighborhood U of x such that $f(U) \subset V$.

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Continuos Functions



Homeomorphisms

Let (X, τ_X) and (Y, τ_Y) be topological spaces. A bijection $f: X \to Y$ is a homeomorphism if f is continuous and f^{-1} is continuous. (Note that since f is a bijection, f^{-1} always exists.)

This can be restated in terms of open sets as follows: let f be a bijection such that f(U) is open if and only if U is open. Then f is a homeomorphism.

Having a one-to-one correspondence between open sets gives us a way to map the topology of one space to the topology of another. Therefore, for any property of X that is characterized entirely by the topolog of X, the same property holds for Y if f is a homeomorphism. This property is then called a topological property.

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Metric Topology



A metric space is a set X together with a function $d: X \times X \to \mathbb{R}$ satisfying the following conditions:

- 0 $d(x,y) \ge 0$ for all $x,y \in X$,
- d(x, y) = 0 if and only if x = y,
- d(x, y) = d(y, x) for all $x, y \in X$,
- $d(x,y) \le d(x,z) + d(z,y) \text{ for all } x,y,z \in X.$

The function d is called a metric on X.

Let (X, d) be a metric space. Given $\epsilon > 0$ the set

$$B_{\epsilon}(x) = \{ y \in X \mid d(x, y) < \epsilon \}$$

is called the ϵ -ball centered at x.

A basis for a topology on X is the collection of all $B_{\epsilon}(x)$ for every $\epsilon > 0$ and $x \in X$. This topology is known as the metric topology induced by d.

Metric Topology



Metrizability

A topological space (X, τ) is metrizable if there exists a metric d on Xthat induces the topology of X. A metric space is a metrizable space Xtogether with a specific metric d that gives the topology of X.

Having a metrizable topological space is useful because it allows us to use the metric in order to prove certain theorems in topology. Therefore, we'd like to be able to show that a given topological space is metrizable. This is where the Urysohn Metrization Theorem comes in (among others).

Urysohn Metrization Theorem

Every regular space X with a countable basis is metrizable.

A space is regular if for each pair consisting of a point x and a closed set C not containing x, there exists disjoint neighborhoods containing x and C respectively.

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Connectedness

Let (X, τ) be a topological space. A separation of X is a pair of disjoint non-empty open sets $U, V \subseteq X$ whose union is X. A space is connected if it has no separation. Connectedness is a topological property which is invariant.

Put differently a space X is connected if and only if the only subsets of X that are both open and closed in X are X and \emptyset .

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Connectedness Theorems

Let (X, τ) be a topological space.

Theorem 23.2 in Munkres

If sets C and D form a separation of X, and if $Y \subseteq X$ is connected, then Y is either a subset of C or a subset of D.

Theorem 23.4 in Munkres

Let $A \subseteq X$ be connected. If $A \subseteq B \subseteq \overline{A}$, then B is also connected.

Theorem 23.5 in Munkres

The image of a connected space under a continuous map is connected.

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Compactness

A collection \mathcal{C} of subsets of a topological space (X, τ) covers X if $\bigcup_{C \in \mathcal{C}} C = X$. It is said to be an open cover if each $C \in \mathcal{C}$ is open.

A space X is covering compact if every open cover of X has a finite subcover. From now on we shorten covering compact to simply compact.

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Compactness Theorems

Theorem 26.2 in Munkres

Every closed subspace of a compact space is compact.

Theorem 26.3 in Munkres

Every compact subspace of a Hausdorff space is closed.

Theorem 26.5 in Munkres

The image of a compact space under a continuous map is compact.

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Limit Point Compactness



A topological space (X,τ) is limit point compact if every infinite subset of X has a limit point. Limit point compactness is a weaker property than compactness, but the two coincide if X is metrizable. In fact compactness implies limit point compactness, but not the other way round.

The space X is said to be sequentially compact if every sequence of points in X has a convergent subsequence.

Theorem 28.2 in Munkres

Let X be metrizable. Then the following are equivalent:

- 1 X is compact.
- 2 X is limit point compact.
- 3 X is sequentially compact.

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Abstract Topology



Homotopy

Let (X, τ) be a topological space. A homotopy from $f: A \to X$ to $g:A\to X$, both continuos, is a continuous map $H:A\times [0,1]\to X$ such that H(a,0) = f(a) and H(a,1) = g(a) for all $a \in A$. The homotopy H is parametrized by $t \in [0,1]$, which may be thought of as time. Essentially H represents a continuos deformation of f into g.

Now suppose that we are considering two maps $f, f' : [0,1] \to X$ which happen to be paths in X with the same initial point x_0 and final point x_1 . If there exists a continuous map $P:[0,1]\times[0,1]\to X$ such that

$$P(s,0) = f(s), \quad P(s,1) = f'(s), \quad P(0,t) = x_0, \quad P(1,t) = x_1$$

for every $s, t \in [0, 1]$, then we say that f and f' are homotopic with P being the path homotopy. As Munkres says, "the first condition says that P represents a continuous way of deforming the path f to the path f', and the second condition says that the end points of the path remain fixed during the deformation."

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Abstract Topology



Homotopy

It turns out that both homotopy and path homotopy form equivalence relations on their respective sets of maps. For our purposes we will focus on path homotopy with its equivalence relation denoted as \simeq_p and its equivalence class denoted as [f].

If f is a path in X with initial point x_0 and final point x_1 , and if f' is another path in X with initial point x_1 and final point x_2 , we define the product f * f' to be the path h, which is defined as

$$h(s) = \begin{cases} f(2s) & \text{, if } 0 \le s \le \frac{1}{2} \\ f'(2s-1) & \text{, if } \frac{1}{2} \le s \le 1 \end{cases}.$$

Since f and f' are continuous paths in X, we know that h is also a continuous path in X.

Abstract Topology



The Fundamental Group

The product operation * may also be used to induce an operation on the set of equivalence classes of paths. Let [f] and [f'] be two equivalence classes of paths in X, then we have [f] * [f'] = [f * f'].

The fundamental group of a topological space (X,τ) is the set of equivalence classes of paths in X with the * operation. The fundamental group is denoted as $\pi_1(X,x_0)$ where x_0 is a chosen fixed point in X. This fixed point is called the base point and we consider only those paths which start and end at the base point. This way we guarantee that the fundamental group is indeed a group.

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Topological data analysis, or TDA, is a relatively new field of mathematics which began as a branch of algebraic topology. The goal of TDA is to extract information about a data set by using topological methods. The data set is usually a finite set of points in \mathbb{R}^n with some notion of distance between points, however, we may also use more abstract sets as well.

The first step in TDA is to construct a simplicial complex from the data set. For our purposes we will be using abstract simplicial complexes which along with their geometric realizations form a topological space. We will then use the topological space to compute the homology groups of the simplicial complex at various scales.



Simplicial Complexes

Abstract Simplicial Complex

An abstract simplicial complex K is a collection of finite sets that is closed under subsets. The sets $\sigma \in K$ are called simplices and the subsets of σ are called faces. The dimension of a simplex σ is one less than its cardinality. The dimension of K is the maximum dimension of any simplex in K.

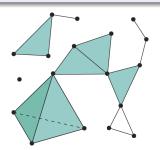


Figure: A geometric realization of an abstract simplicial complex.

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Chain Groups

Chain Group

Let K be an abstract simplicial complex. The chain group $C_p(K)$ is the free abelian group generated by the p-simplices of K. The elements of $C_p(K)$ are called p-chains.

Elements of $C_p(K)$ are formal sums of p-simplices with coefficients over a field or ring. Most often the coefficients are taken from \mathbb{Z}_2 in order to denote the presence or absence of a simplex in a chain. Further, elements of $C_p(K)$ are added component-wise. E.g., if c and c' are p-chains such that $c = \sum_{i=1}^n a_i \sigma_i$ and $c' = \sum_{i=1}^n b_i \sigma_i$, then $c + c' = \sum_{i=1}^n (a_i + b_i) \sigma_i$. (Note that this is equivalent to the symmetric difference when using \mathbb{Z}_2 coefficients.)

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The Boundary Operator

Boundary Operator

Let K be an abstract simplicial complex. The boundary operator $\partial_p: C_p(K) \to C_{p-1}(K)$ is the unique homomorphism such that $\partial_p(\sigma) = \sum_{i=0}^p (-1)^i \sigma_{[i]}$ for every p-simplex σ in K.

The boundary operator is a linear map which gives us a way to move between the chain groups of different dimensions. The image of a chain group under the boundary operator is called the boundary group. Similarly, the kernel of the boundary operator is called the cycle group.

Formally, we have $B_p(K) = \operatorname{im}(\partial_{p+1})$ and $Z_p(K) = \ker(\partial_p)$.

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Homology

Homology Group

Let K be an abstract simplicial complex. The p-th homology group of K is the quotient group $H_p(K) = Z_p(K)/B_p(K)$ where $Z_p(K)$ is the p-th cycle group and $B_p(K)$ is the p-th boundary group.

The homology groups of a simplicial complex are a topological invariant which give information about the connected components, holes, tunnels, voids, etc. of the complex. The order/rank of the homology groups is given by

$$\operatorname{rank}(H_p(K)) = \dim(Z_p(K)) - \dim(B_p(K)).$$

Further, the rank of the p-th homology group is the same as the number of p-dimensional holes in the complex, i.e., its p-dimensional Betti number β_p .

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Euler Characteristic

As a last note on the theoretical underpinnings of TDA, we have the following theorem.

Euler-Poincaré Theorem

Let K be an abstract simplicial complex. Then the alternating sum of the ranks of the homology groups of K, i.e. β_p , is equal to the Euler characteristic of K.

$$\chi(K) = \sum_{p \ge 0} (-1)^p \beta_p.$$

It is important to note that the Euler characteristic is a topological invariant. This means that we can use the Euler characteristic to compare the topological properties of different data sets. Further, we might be able to use the Euler characteristic as a measure of the complexity and performance of a machine learning model.

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Applications of TDA to DL



Watanabe and Yamana (2021)

Methodologies as proposed by Watanabe and Yamana (2021) can be summarized as having relevant applications in the following areas:

- OPH can be used to detect the shortage of training data,
- and for selecting the best model architecture.

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Applications of TDA to DL



Corneanu et al. (2019)

Methodologies as proposed by Corneanu et al. (2019) can be summarized as having relevant applications in the following areas:

- OPH can be used to detect when the model is over-fitting,
- and find the examples where the model fails to generalize to unseen data.

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