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DEEP LEARNING ON ABSTRACT SIMPLICIAL COMPLEXES

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Introduction

Most of the deep learning techniques used today are based on models which learn a partition of the set of smooth functions defined on euclidean domains into human friendly equivalence classes...

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Chapter 1

Preliminaries on topology

Category Theory

The essential idea in algebraic topology is to convert problems about topological spaces and continuous functions into problems about algebraic objects and their homomorphisms, this way one hopes to end up with an easier problem to solve. The language of category theory shall be our main tool to formally describe this conversion.

Definition 1.1. A *category* $\mathbf{C}$ consists of three ingerdients:
a class of *objects* $Obj(\mathbf{C})$; sets of *morphisms* $Hom(A, B)$ for every ordered pair $(A, B) \in Obj(\mathbf{C})$; a composition $Hom(A, B) \times Hom(B, C) \to Hom(A, C)$, denoted by $(f, g) \mapsto f \circ g$ for every $A, B, C \in Obj(\mathbf{C})$, satisfying the following axioms:

(i) the family of $Hom(A, B)$ is pairwise disjoint,

(ii) the composition, when defined, is associative,

(iii) for each $A \in Obj(\mathbf{C})$ there exists an *identity* $1_A \in Hom(A, A)$ such that for $f \in Hom(A, B)$ and $g \in Hom(C, A)$ we have that $1_A \circ f = f$ and $g \circ 1_A = g$.

Theorem 1.2. *Topological spaces and continuous functions are a category* ***Top****, whose equivalences are called homeomorphisms.*

Instead of writing $f \in Hom(A, B)$, we usually write $f : A \to B$. For other examples of categories see [1].

Definition 1.3. Let $\mathbf{A}$ and $\mathbf{C}$ be categories, a *functor* $T : \mathbf{A} \to \mathbf{C}$ is a function, that is,

(i) $A \in Obj(\mathbf{A}) \implies TA \in Obj(\mathbf{C})$,

(ii) $f : A \to A' \implies Tf : TA \to TA' \quad A, A' \in Obj(\mathbf{A})$,

(iii) if f, g are morphisms in $\mathbf{A}$ for which $g \circ f$ is defined, then $T(g \circ f) = (Tg) \circ (Tf)$,

(iv) $T(1_A) = 1_{TA} \quad \forall A \in \mathbf{A}$.

The property *(iii)* of the previous definition actually defines what we shall call *covariant functors.* If instead we require $T(g \circ f) = (Tf) \circ (Tg)$, we are defining a so called *contravariant functor.*

Definition 1.4. An *equivalence* in a category $\mathbf{C}$ is a morphism $f : A \to B$ for which there exists a morphism $g : B \to A$ such that $f \circ g = 1_B$ and $g \circ f = 1_A$.

Theorem 1.5. *If $\boldsymbol{A}$ and $\boldsymbol{C}$ are categories and $T : \boldsymbol{A} \to \boldsymbol{C}$ is a functor of either variance, then whenever f is an equivalence on $\boldsymbol{A}$ then Tf is an equivalence on $\boldsymbol{C}$.*

Proof. We apply T to the equations $f \circ g = 1_B$ and $g \circ f = 1_A$, that for a covariant functor leads to $(Tf) \circ (Tg) = T(1_B) = 1_{TB}$ and $(Tg) \circ (Tf) = T(1_A) = 1_{TA}$. $\square$

Simplicial Complexes

We shall now introduce algebraic objects called simplicial complexes and see how they are related to compact topological spaces. In order to do that we require the definitions of convex envelope and affine independence of points in $\mathbb{R}^n$.

Definition 1.6. Let I be a finite set of indexes, we define the *convex envelope* of the points $\{x_i\}_{i\in I} \subset \mathbb{R}^n$ to be

$$[x_i]_{i\in I} := \{\sum_{i\in I} \lambda_i x_i : \lambda_i \in \mathbb{R},\ \lambda_i \geq 0,\ \sum_{i\in I} \lambda_i = 1\}.$$

It is easy to see that convex envelopes are convex and compact sets with respect to the standard topology in $\mathbb{R}^n$. From now, if not otherwise specified, we shall assume I to be a finite set of indexes.

Proposition 1.7. *Let $\{x_i\}_{i\in I} \subset \mathbb{R}^n$ then $[x_i]_{i\in I}$ is the smallest convex set containing X.*

The order by which we define the smallest convex set is the one given by the relation $\subseteq$.

Definition 1.8. Let $\{x_i\}_{i\in I} \subset \mathbb{R}^n$ we define the points $\{x_i\}_{i\in I}$ to be *affinely independent* if and only if

$$\sum_{i\in I} \lambda_i x_i = \sum_{i\in I} \mu_i x_i \quad \Rightarrow \quad \lambda_i = \mu_i \ \forall i \in I,$$

whenever $\sum_{i\in I} \lambda_i = \sum_{i\in I} \mu_i = 1$.

For a more intuitive understanding of this definition one can say that n points in some euclidean space are affinely independent if and only if they do not belong to the same $n-2$ dimensional affine space.

Example 1.9. Let $A, B, C, D \subset \mathbb{R}^n$ representing the four vertxes of a square and let A, D be opposite vertxes, one can easily see that

$$D = A + (B - A) + (C - A) = (-1)A + (1)B + (1)C + (0)D = (0)A + (0)B + (0)C + (1)D\,,$$

therefore A, B, C, D are not affinely independent. In fact the 4 vertexes of a square are coplanar, i.e. they belong to the same 2 dimensional affine space.

Definition 1.10. We define a *p-simplex* to be a convex envelop $[x_i]_{i\in I}$ where $\{x_i\}_{i\in I} \subset \mathbb{R}^n$ are affinely independent and $|I| = p + 1$, where $|I|$ is the cardinality of I.

One denotes the vertex set $\{x_i\}_{i\in I}$ of a simplex $\sigma = [x_i]_{i\in I}$ by $Vert(\sigma)$.

Definition 1.11. Let σ be a $p-simplex$, we say that another t-simplex τ is a *face* of σ or equivalently that σ is a *coface* of τ, by our notiation $\tau \leq \sigma$, if and only if $\tau \subset \sigma$, where $t \leq p$.

Simplexes can therefore be points, segments, triangles, tetrahedra or higher dimensional sets which I cannot name, if these particularly simple sets can describe topological spaces we can stop complicating things and try to define a category of simplexes. Unfortunately convex spaces are not able to describe topological spaces with holes.

Definition 1.12. We define a *simplicial complex* $\mathcal{G}$ to be a collection of simplexes such that

(i) $\tau \leq \sigma \in \mathcal{G} \Rightarrow \tau \in \mathcal{G}$,

(ii) $\sigma, \tau \in \mathcal{G} \Rightarrow \sigma \cap \tau \in \mathcal{G}$.

Let A, B, C be vertexes of a triangle, with the simplicial complex $\{[A], [B], [C], [A, B], [B, C], [C, A]\}$ one can describe the boundary of a triangle, which has a hole that could not be described by any simplex.

Simplicial complexes are the objects of our category, we now look for appropriate morphisms.

Definition 1.13. Let $\mathcal{G}, \mathcal{H}$ be simplicial complexes, then a *simplicial map* $\phi : \mathcal{G} \to \mathcal{H}$ is a function such that whenever $[x_i]_{i\in I} \in \mathcal{G}$, then $\phi([x_i]_{i\in I}) = [\phi(v_i)]_{i\in I} \in \mathcal{H}$, where $\phi(x_i) \in Vert(\mathcal{H})\,\forall i \in I$.

Theorem 1.14. *Simplicial complexes and simplicial maps are a category* $\boldsymbol{G}$*, whose equivalences are called isomorphisms..*

Definition 1.15. Let $\mathcal{G}$ be a simplicial complex, we define its *underlying space* $|\mathcal{G}| = \bigcup_{\sigma\in\mathcal{G}} \sigma$, provided with the standard topology inherited from $\mathbb{R}^n$.

Since the union of compact sets is compact the underlying space of a simplicial complex in $\mathbb{R}^n$ is a compact topological subspace of $\mathbb{R}^n$.

Definition 1.16. A topological space X is called *polyhedron* if there exists a simplicial complex $\mathcal{G}$ and a homeomorphism $h : |\mathcal{G}| \to X$. The ordered pair $(\mathcal{G}, h)$ is called a *triangulation* of X.

One understands that in order to have a homeomorphism between the compact underlying space of a simplcial complex and another topological space, this other space has to be compact.

Lemma 1.17. *Let a topological space X be a finite union of closed subsets $X = \bigcup_{i\in I} X_i$. If, for some space Y, there are continuous maps $f_i : X_i \to Y$ that agree on overlaps $f_i|_{X_i\cap X_j} = f_j|_{X_i\cap X_j}$, there there exist a unique continuous function $f : X \to Y$ such that $f|_{X_i} = f_i\,\forall i \in I$.*

Definition 1.18. Let $\phi : \mathcal{G} \to \mathcal{H}$ be a simplicial map, let then $\sigma \in \mathcal{G}$ we define $f_\sigma : \sigma \to |\mathcal{H}|$ to be $\sum_{v\in Vert(\sigma)} \lambda_v v \mapsto \sum_{v\in Vert(\sigma)} \lambda_v \phi(v)$. The continuity of this functions in σ and the intersection property of the definition of simplicial complex allow us to use the previous lemma to uniquely define a function $|\phi| : |\mathcal{G}| \to |\mathcal{H}|$ which we shall name *piecewise linear map.*

The unique association of simplicial complexes and their underlying spaces and of simlicial maps and piecewise linear maps leads to the definition of a functor from the category of simplicial complexes and maps to the category of topological spaces and continuous functions.

Theorem 1.19. $|\ | : \boldsymbol{G} \to \boldsymbol{Top}$ *is a functor.*

Notice that there is no obvious functor from **Top** to **G**, therefore the implications reguarding equivalences are strictly directed.

Although this approach provides simplicial complexes with the topology inherited from the metric space it hides the power of simplicial complexes to describe those networks and interactions which would happily exist without that topology, to make this distinction clear enough we will treat simplicial complexes as a realization of more abstract objects called abstract simplicial complexes.

Definition 1.20. Let $\mathcal{V}$ be a finite set we define an *abstract simplicial complex* $\mathcal{A}$ to be

$$\mathcal{A} := \{\sigma \subset \mathcal{V} : \tau \subset \sigma \Rightarrow \tau \in \mathcal{A}\}$$

where σ are called *abstract simplexes* of $\mathcal{A}$.

One calls $\mathcal{V}$ the *vertex set* of $\mathcal{A}$ and denotes it by $Vert(\mathcal{A})$; since the vertex set is finite we expect every abstract simplex to be also finite, therefore we might use the notation $\sigma = \{v_i\}_{i\in I_\sigma}$, which so far we consider invariant under arbitrary permutations of the finite index set I_σ.

Definition 1.21. Let $\mathcal{A}$ be an abstract simplicial complex we define its *dimension* to be

$$dim\mathcal{A} := max_{\sigma\in\mathcal{A}}(|\sigma| - 1),$$

where by $|\sigma|$ we denote the cardinality of σ.

One calls an abstract simplex of dimension p an *abstract p-simplex*, according to our definition the empy set is a (-1)-simplex. A *graph* is a one dimensional abstract simplicial complex.

Definition 1.22. Let $\mathcal{A}, \mathcal{B}$ be abstract simplicial complexes, then a *simplicial map* $\phi : \mathcal{A} \to \mathcal{B}$ is a function such that whenever $\sigma = \{v_i\}_{i\in I_\sigma} \in \mathcal{A}$, then $\phi(\{v_i\}_{i\in I_\sigma}) = \{\phi(v_i)\}_{i\in I_\sigma} \in \mathcal{B}$, where $\phi(v_i) \in Vert(\mathcal{B})\, \forall i \in I_\sigma$.

Although the vertex to vertex mapping is a quite selective condition on the function we did not prevent it from cramming abstract simplexes into lower dimensional ones.

Theorem 1.23. *Abstract simplicial complexes and simplicial maps are a category* $\boldsymbol{A}$*, whose equivalences are called isomorphisms.*

One can show that under some dimensional conditions one can define a functor from the category of abstract simplicial complexes to the category of simplicial complexes.

Definition 1.24. Let $\mathcal{G}$ be a simplicial complex, we call the abstract simplicial complex

$$\mathcal{A} := \{\{x_i\}_{i\in I} \subset Vert(\mathcal{G}) : [x_i]_{i\in I} \in \mathcal{G}\}$$

a vertex scheme for $\mathcal{G}$ or equivalently we might say that $\mathcal{G}$ is a *geometric realization* of $\mathcal{A}$.

Theorem 1.25. *Let* $\mathcal{A}$ *be a d-dimensional abstract simplicial complex, it admits a geometric realization in* $\mathbb{R}^{2d+1}$.

Kuratowski theorem proves the prevuois statement to be also sharp.

One could also show that that geometric realizations of isomorphic abstract simplicial complexes are themselves isomorphic.

Simplicial Homology

An important field in algebraic topology is homology theory. We shall discuss homology theory to the extent that allows us to define the laplacian operator on simplicial complexes, for further readings see [2].

Definition 1.26. An *oriented* simplicial complex $\mathcal{A}$ is a simplicial complex and a partial order on $Vert(\mathcal{A})$ whose restriction to the vertices of any simplex in $\mathcal{A}$ is a linear order.

Definition 1.27. Let $\mathcal{A}$ be an oriented simplicial complex, on $\mathcal{A}$ we define a formal sum in order to obtain a vector space on the real numbers, that is

$$C_p(\mathcal{A}) := \{\sum_i \lambda_i \sigma_i^p \quad \lambda_i \in \mathbb{R}\},$$

where σ_i^p are oriented p-simplexes of $\mathcal{A}$.
All $\sigma_i^p = [v_0, \dots, v_p]$ can have two possible orientations that satisfy $[v_0, \dots, v_p] = sgn(\pi)[v_{\pi 0}, \dots, v_{\pi p}]$, where π is a permutation of $\{0, \dots, p\}$.

Definition 1.28. We define the linear operator $\partial_{p+1} : C_{p+1} \to C_p$ by setting

$$\partial_{p+1}([v_0, \dots, v_p]) = \sum_{i=0}^{p} (-1)^i [v_0, \dots, \hat{v}_i, \dots, v_p]$$

(where $\hat{v}_i$ means delete the vertex v_i) and extending by linearity.

Theorem 1.29. $\partial^2 = 0$.

Proof. Let $\partial_{p+1}([v_0, \dots, v_{p+1}]) = \sum_{i=0}^{p+1} (-1)^i [v_0, \dots, \hat{v}_i, \dots, v_{p+1}]$ then

$$\partial_p(\partial_{p+1}([v_0, \dots, v_{p+1}])) = \sum_{j=0, j\neq i}^{p+1} \sum_{i=0}^{p+1} (-1)^{i+j} [v_0, \dots, \hat{v}_i, \dots, \hat{v}_j, \dots, v_{p+1}] = 0.$$

□

Definition 1.30. We define the *p-homology group* to be

$$H_p := \frac{ker\partial_p}{im\partial_{p+1}},$$

where $im\partial_{p+1}$ is the group of simplicial p-cycles and $ker\partial_p$ is the group of simplicial p-boundaries.

The homology group is therefore the space of cycles that are not boundaries.

Simplicial Cohomology

Definition 1.31. Let $\mathbf{V}$ be the category of vector spaces and linear transformations between them, we define the *dual contravariant functor* by

$$V \in Obj(\mathbf{V}) \mapsto V^* \in Obj(\mathbf{V})$$

$$\partial \in Hom(U, V) \mapsto \partial^* \in Hom(V^*, U^*) : \partial^*(\phi) = \phi \circ \partial.$$

Definition 1.32. Let C_p be the space of simplicial p-chains, we define the space of *simplicial cochains* to be $C^p := Hom(C_p, \mathbb{R})$, i.e. the dual space of C_p.

Definition 1.33. By means of the dual functor we are able to define the dual of the boundary operator which we shall call *coboundary operator*, which is defined to be

$$d_{p+1} : C^p \to C^{p+1} \quad d_p(\sigma^*) = \sigma^* \circ \partial_{p+1}.$$

Definition 1.34. We define the *p-cohomology group* to be

$$H^p := \frac{kerd_{p+1}}{imd_p},$$

where imd_{p-1} is the group of simplicial p-cocycles and $kerd_p$ is the group of simplicial p-coboundaries.

Definition 1.35. We define the scalar product called *integration* $\langle , \rangle : C_p \times C_p \to \mathbb{R}$ on the canonical basis of C_p to be

$$\langle i, j \rangle = \delta_{ij},$$

where i, j are any two p-simplexes in the canonical basis of C_p and δ_{ij} is the Kronecker Delta.

It is convenient, from now on, to write cochains σ^* as bra vectors $\langle\sigma|$, chains σ as ket vectors $|\sigma\rangle$, and the scalar product $\langle i, j\rangle$ as the bra-ket product $\langle i|j\rangle$.

Definition 1.36. Let $d_{p+1} : C^p \to C^{p+1}$ be the coboundary operator, then for any $\sigma^* \in C^p, \tau \in C_{p+1}$ we can define its dual representation $\partial^\dagger_{p+1}$ by

$$(d_{p+1}\sigma^*)(\tau) = (d_{p+1}\langle\sigma|)|\tau\rangle = \langle\partial^\dagger_{p+1}\sigma|\tau\rangle.$$

It is easy to notice that our definitions lead to the restatement of the equivalent of the generalized Stokes' theorem on simplicial complexes according to the integration previously defined, i.e. $(d\langle\sigma|)|\tau\rangle = \langle\sigma|\partial\tau\rangle$.

Theorem 1.37. $H_p \simeq H^p$

Laplacian Operators

Definition 1.38. We define the *p-Laplacian* operator to be

$$\Delta_p = \partial_{p+1}\partial^\dagger_{p+1} + \partial^\dagger_p\partial_p =: \Delta^+_p + \Delta^-_p.$$

Proposition 1.39. $\Delta^\dagger_p = \Delta_p$.

Proof. Let $|\sigma\rangle, |\tau\rangle \in C_p$

$$\begin{aligned}\langle\sigma|\Delta_p\tau\rangle &= \langle\sigma|(\partial_{p+1}\partial^\dagger_{p+1} + \partial^\dagger_p\partial_p)\tau\rangle = \\ &= \langle(\partial_{p+1}\partial^\dagger_{p+1} + \partial^\dagger_p\partial_p)^\dagger\sigma|\tau\rangle = \\ &= \langle(\partial_{p+1}\partial^\dagger_{p+1} + \partial^\dagger_p\partial_p)\sigma|\tau\rangle = \langle\Delta_p\sigma|\tau\rangle.\end{aligned}$$

□

According to the spectral theorem there exists a basis of eigenchains of the Laplacian, and since all $\Delta_p, \Delta^+_p, \Delta^-_p$ are self-adjoint we can say that they all admit a basis of eigenchains.

Proposition 1.40. *Let* $\Delta_p|\sigma\rangle = \lambda_\sigma|\sigma\rangle$ *then* $\lambda_\sigma \geq 0$.

Proof. Let $\Delta^+_p|\sigma\rangle = \lambda^+_\sigma|\sigma\rangle$, we see that

$$\langle\sigma|\Delta^+_p\sigma\rangle = \langle\partial^\dagger_{p+1}\sigma|\partial^\dagger_{p+1}\sigma\rangle \geq 0$$

$$\langle\sigma|\Delta^+_p\sigma\rangle = \lambda^+_\sigma\langle\sigma|\sigma\rangle \geq 0 \implies \lambda+_\sigma \geq 0.$$

Let then $\Delta^-_p|\sigma\rangle = \lambda^-_\sigma|\sigma\rangle$, we see that

$$\langle\sigma|\Delta^-_p\sigma\rangle = \langle\partial_p\sigma|\partial_p\sigma\rangle \geq 0$$

$$\langle\sigma|\Delta^-_p\sigma\rangle = \lambda^-_\sigma\langle\sigma|\sigma\rangle \geq 0 \implies \lambda-_\sigma \geq 0.$$

Furthermore, since $\Delta^+_p\Delta^-_p = \Delta^-_p\Delta^+_p = 0$ we have that $[\Delta^+_p, \Delta^-_p] = 0$, thence $[\Delta_p, \Delta^\pm_p] = 0$, therefore $\Delta_p, \Delta^+_p, \Delta^-_p$ share a basis of eigenchains. Let $|\sigma\rangle$ be in that common basis then $\Delta_p|\sigma\rangle = \lambda_\sigma|\sigma\rangle$, where $\lambda_\sigma = \lambda^+_\sigma + \lambda^-_\sigma \geq 0$. □

Theorem 1.41 (Eckmann's Theorem). *ker*$\Delta_p \simeq H_p$.

Proof.

$$\Delta_p = \partial_{p+1}\partial_{p+1}^{\dagger} + \partial_p^{\dagger}\partial_p =: \Delta_p^+ + \Delta_p^-$$

$$\Delta_p^+\Delta -_p = \Delta_p^-\Delta_p^+ = 0(hom.lem.) \implies ker\Delta_p^{\pm} \subset im\Delta_p^{\mp}$$

$$ker\Delta_p = ker\Delta_p^+ \cap ker\Delta_p^-$$

$$ker\partial_{p+1}^{\dagger} \cap ker\partial_p \subset ker\Delta_p(trivial)$$

$$\partial_{p+1}^{\dagger}\sigma \in im\partial_{p+1}^{\dagger}, \sigma \in ker\Delta_p \implies \partial_{p+1}^{\dagger}\sigma \in ker\partial_{p+1} = (im\partial_{p+1}^{\dagger})^{\perp}$$

$$\partial_p\sigma \in im\partial_p, \sigma \in ker\Delta_p \implies \partial_p\sigma \in ker\partial_p^{\dagger} = (im\partial_p)^{\perp}$$

$$\partial_p\sigma = \partial_{p+1}^{\dagger}\sigma \subset im\partial_{p+1}^{\dagger} \cap (im\partial_{p+1}^{\dagger})^{\perp} = im\partial_p \cap (im\partial_p)^{\perp} = 0$$

$$ker\Delta_p = ker\partial_{p+1}^{\dagger} \cap ker\partial_p = (im\partial_{p+1})^{\perp} \cap ker\partial_p \simeq H_p$$

□

[4]

Chapter 2

Simplicial Neural Networks

Convolutional Neural Networks

Graph Neural Networks

Simplicial Neural Networks

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