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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

Simplicial complexes

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, the discussion of which can be found in [1], shall be our main tool to formally describe this conversion, i.e. via functors. Functors are a formal way to transport equivalences from one world to another, if for instance two objects in the world A are A-equal and one can define a functor to the world B, then the images of those two objects must be B-equal in the world B and this implication is strictly directed. Usually, though, one moves to the world B because the A-equivalence classes are unknown, then from a knowledge of the B-equivalence classes in B, one can use the contrapositive implication to understand if the objects in A are not equal.

First of all we shall 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 1.1. 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 compact 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 1.2. *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 1.3. 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 1.4. 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 1.5. 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 1.6. 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 1.7. 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 1.8. 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 $\phi(x_i) \in Vert(\mathcal{H})\, \forall i \in I$.

In the beginning of the section we said that in some world A there are A-equivalence classes, in the language of category theory we might say that from the morphisms of some category A one can define an A-equivalence as invertible morphism between two objects, and let there be a functor to another category B, then the image via this functor of the A-equivalence is a B-equivalence.

Theorem 1.9. *Simplicial complexes and simplicial maps are a category* $\boldsymbol{G}$.

Definition 1.10. 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 1.11. 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 1.12. *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 1.13. 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 1.14. $|\ | : \boldsymbol{G} \to \boldsymbol{Top}$ *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 1.15. 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 1.16. 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 1.17. 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 1.18. *Abstract simplicial complexes and simplicial maps are a category* $\boldsymbol{A}$.

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 1.19. 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 1.20. *Let $\mathcal{A}$ be a d-dimentional abstract simplicial complex, it admits a geometric realization in $\mathbb{R}^{2d+1}$.*

Kuratowski theorem proves the prevuois statement to be also sharp.

The geometric realization of a simplicial complex is not unique in the simplicial complexes, but it is in their equivalence classes, which we still denote as $\mathcal{G}$ for simplicity.

Theorem 1.21. *The geometric realization is a functor $\boldsymbol{A} \to \boldsymbol{G}$.*

Since the composition of functors is a functor, the functor $\mathbf{A} \to \mathbf{G} \to \mathbf{Top}$ implies that the underlying spaces of any geometric realization of the same $\mathbf{A}$-equivalence class are homeomorphic.

Forms and integration on abstract simplicial complexes

Definition 1.22. Linear space of simplicial p-chains
Let $\mathcal{A}$ be an abstract simplicial complex, and let $\mathcal{A}_p := \{\sigma \in \mathcal{A} : dim(\sigma) = p\}$, we define the linear space $C_p = C_p(\mathcal{A})$ of simplicial p-chain on $\mathcal{A}$ to be

$$C_p = \{\sum_{\sigma\in\mathcal{A}_p} \lambda^\sigma \sigma, \quad \lambda^\sigma \in \mathbb{Z}_2\},$$

where the formal operations of the linear space are given by the defitnition itself.
(Possible extension from $\mathbb{Z}_2$ to $\mathbb{R}$, naming C_p by the dual notation Λ_p)

The set $\mathcal{A}^p$ is a canonical base of p-simplexes for C_p.

Definition 1.23. Boundary operator on C_{p+1}
Let σ be an element of the canonical base of C_{p+1} we define $\partial : C_{p+1} \to C_p$ such that

$$\partial\sigma = \sum_{i=0}^{p+1} (-1)^i \sigma_i,$$

where if $\sigma = \{x_0, ..., x_{p+1}\} \in C_{p+1}$ we define $\sigma_i := \{x_0, ..., x_{i-1}, x_{i+1}, ..., x_{p+1} \in C_p\}$.
Furthermore we extend this operator linearly on the whole space C_{p+1}

$$\partial \left(\sum_{\sigma\in\mathcal{A}_p} \lambda^\sigma \sigma \right) = \sum_{\sigma\in\mathcal{A}_p} \lambda^\sigma \partial\sigma \ .$$

Lemma 1.24. *Let $\sigma \in \mathcal{A}_{p+2}$, $p \geq 0$ then $\partial^2\sigma = 0$.*

Proof. We have

$$
\begin{aligned}
(\partial^2\sigma)_x &= \sum_{i=0}^{p+2}(-1)^i(\partial\sigma)_i \\
&= \sum_{i=0}^{p+2}(-1)^i\left[\sum_{j=0}^{i-1}(-1)^j\sigma_{ij} + \sum_{j=i+1}^{p+2}(-1)^{j-1}\sigma_{ij}\right] \\
&= \sum_{i=0}^{p+2}\sum_{j=0}^{i-1}(-1)^{i+j}\sigma_{ij} - \sum_{i=0}^{p+2}\sum_{j=i+1}^{p+2}(-1)^{i+j}\sigma_{ij} = 0.
\end{aligned}
$$

□

Definition 1.25. p-forms on abstract simplicial complexes
Let $\mathcal{A}$ be an abstract simplical complex we define the linear space of p-forms $\Lambda^p = \Lambda^p(\mathcal{A})$ to be

$$\Lambda^p := \{\omega : C_p \to \mathbb{R}\}, \textit{such that}$$

$$\omega\left(\sum_{\sigma\in\mathcal{A}_p}\lambda^\sigma\sigma\right) = \sum_{\sigma\in\mathcal{A}_p}\lambda^\sigma\omega(\sigma) \quad \forall\omega\in\Lambda^p,\ \lambda_\sigma\in\mathbb{Z}_2\ ,$$

with linear space operations defined as

$$
\begin{aligned}
+ : \Lambda^p\times\Lambda^p\to\Lambda^p \qquad & (\omega+\eta)(\sigma) = \omega(\sigma)+\eta(\sigma) \quad \sigma\in C_p,\ \omega,\eta\in\Lambda^p, \\
\cdot : \mathbb{R}\times\Lambda^p\to\Lambda^p \qquad & (\lambda\omega)(\sigma) = \lambda\omega(\sigma) \quad \sigma\in C_p,\ \omega\in\Lambda^p,\ \lambda\in\mathbb{R}.
\end{aligned}
$$

Proposition 1.26. *A canonical base of elementary forms for Λ^p is*

$$\{\sigma^*\in\Lambda^p : \sigma\in\mathcal{A}_p,\ \sigma^*(\tau) = \delta_{\sigma\tau} \quad \tau\in\mathcal{A}_p\},$$

therefore giving us an expression for every other p-form

$$\omega = \sum_{\sigma\in\mathcal{A}_p}\omega_\sigma\sigma^*, \quad \omega_\sigma\in\mathbb{R}.$$

Definition 1.27. Exterior derivative of a p-form
Let $\omega\in\Lambda^p$ we define $d : \Lambda^p\to\Lambda^{p+1}$ on its coordinates to be

$$(d\omega)_\sigma = \sum_{i=0}^{p+2}(-1)^i\omega_{\sigma_i}\ .$$

Lemma 1.28. *Let $\omega\in\Lambda^p$, $p\geq 0$ then $d^2\omega = 0$.*

Proof. We have for $\sigma\in\mathcal{A}_{p+2}$

$$
\begin{aligned}
(d^2\omega)_\sigma &= \sum_{i=0}^{p+2}(-1)^i(d\omega)_{\sigma_i} \\
&= \sum_{i=0}^{p+2}(-1)^i\left[\sum_{j=0}^{i-1}(-1)^j\omega_{\sigma_{ij}} + \sum_{j=i+1}^{p+2}(-1)^{j-1}\omega_{\sigma_{ij}}\right] \\
&= \sum_{i=0}^{p+2}\sum_{j=0}^{i-1}(-1)^{i+j}\omega_{\sigma_{ij}} - \sum_{i=0}^{p+2}\sum_{j=i+1}^{p+2}(-1)^{i+j}\omega_{\sigma_{ij}} = 0.
\end{aligned}
$$

□

Definition 1.29. Integration of p-forms on p-chains
Let $\omega \in \Lambda^p$ and $\tau \in C_p$ we define the integral of ω on τ to be a bilinear form $\Lambda^p \times C_p \to \mathbb{R}$

$$(\omega, \tau)_p := \sum_{\sigma \in \mathcal{A}_p} \omega_\sigma \tau^\sigma,$$

where $\omega = \sum_{\sigma \in \mathcal{A}_p} \omega_\sigma \sigma^*$ and $\tau = \sum_{\sigma \in \mathcal{A}_p} \tau^\sigma \sigma$.
(This might be extended by adding a non trivial permutation invariant measure on $\mathcal{A}_p$)

Theorem 1.30. *Let* $\omega = \sum_{\sigma \in \mathcal{A}_p} \omega_\sigma \sigma^*$ *and* $\tau = \sum_{\sigma \in \mathcal{A}_{p+1}} \tau^\sigma \sigma$ *the following identity holds*

$$(d\omega, \tau)_{p+1} = (\omega, \partial\tau)_p \,,$$

i.e. the operators $d : \Lambda^p \to \Lambda^{p+1}$ *and* $\partial : C_{p+1} \to C_p$ *are dual.*

Proof. We have

$$(d\omega, \tau)_{p+1} = \sum_{\sigma \in \mathcal{A}_{p+1}} \tau^\sigma \, (d\omega, \sigma)_{p+1} \;\; , \qquad (d\omega, \sigma)_{p+1} = (d\omega)_\sigma = \sum_{i=0}^{p+1} (-1)^i \omega_{\sigma_i},$$

while

$$(\omega, \partial\tau)_p = \sum_{\sigma \in \mathcal{A}_{p+1}} \tau^\sigma \, (\omega, \partial\sigma)_p \;\; , \qquad (\omega, \partial\sigma)_p = \left(\omega, \sum_{i=0}^{p+1} (-1)^i \sigma_i \right)_p = \sum_{i=0}^{p+1} (-1)^i \omega_{\sigma_i} \; .$$

□

This theorem can be seen as the generalized Stokes' theorem on abstract simplicial complexes.

The Laplace Operator

Bibliography

[1] Joseph J. Rotman. *An Introduction to Algebraic Topology*. Graduate Texts in Mathematics. Springer-Verlag New York, 1988.