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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...

Contents

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 process, i.e. via functors. Functors are a formal way to transpose 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 he has no idea whether the two objects in A are equal or not, therefore 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 envelopes 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 give 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 $\sum_{i\in I} \lambda_i = \sum_{i\in I} \mu_i = 1$.

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.

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 $|I| = p + 1$.

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 $t \leq p$.

Definition 1.7. We define a *simplicial complex* $\mathcal{G}$ to be a collection of simplexes such that

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

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

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 $\phi(x_i) \in Vert(\mathcal{H})\, \forall i \in I$.

Theorem 1.9 (**G** is a category)**.**

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 too.

Lemma 1.12 (gluing lemma, Rotman)**.**

Definition 1.13 (Piecewise linear map)**.**

Theorem 1.14 ($|\;| :$ **G** $\to$ **Top** is a functor)**.**

(The directionality of this functor gives a direction to implications reguarding identities)
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 [1].

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. *All abstract simplicial complexes and simplicial maps are a category* $\boldsymbol{A}$ *whose identities are called isomorphisms.*

Although abstract simplicial complex can be used to model any kind of vertex interaction they lack of a topology, we wish therefore to define some structures in a euclidean space that can be related unequivocally(i.e. via a functor) to abstract simplicial complexes. We shall call those geometric simplicial complexes to avoid misunderstandings.

Definition 1.19. *Geometric realization of an abstract simplicial complex*
Let $\mathcal{K}$ be a geometric simplicial complex, and let $Vert(\mathcal{K}) := \{\sigma \in \mathcal{K} : dim(\sigma) = 0\}$, we call the abstract simplicial complex $\mathcal{A} := \{\{x_i\}_{i \in I} \subset Vert(\mathcal{K}) : \langle x_i \rangle_{i \in I} \in \mathcal{K}\}$ a vertex scheme for $\mathcal{K}$ or equivalently we might say that $\mathcal{K}$ 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.

Forms and integration on abstract simplicial complexes

Definition 1.21. 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 1.22. 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 1.23. *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 1.24. 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

$$+ : \Lambda^p \times \Lambda^p \to \Lambda^p \qquad (\omega + \eta)(\sigma) = \omega(\sigma) + \eta(\sigma) \quad \sigma \in C_p,\ \omega, \eta \in \Lambda^p,$$

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

Proposition 1.25. *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 1.26. 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 1.27. *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 1.28. 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 1.29. *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.