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DEEP LEARNING ON ABSTRACT SIMPLICIAL COMPLEXES

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Chapter 1

Preliminaries on topology

Before discussing deep learning on graphs and manifolds we will give a definition of graph and higher dimensional structures called abstract simplicial complexes, in order to define convolutions on those structures we will define the Laplace operator by translating De Rham cohomology on oriented simplicial complexes. Furthermore we shall discuss other possible definitions of convolution based on the invariance of oriented simplicial complexes under some group of transformations i.e. even permutations of indexes.

Simplicial complexes

In this section we shall define simplicial complexes, which, as abstract as they might look, can be used to model interactions among individuals, traffic and road networks, as well as shapes, and to approximate functions on some compact manifold.

Definition 1.1. 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 finite, therefore we might use the notation $\sigma = \{v_i\}_{i\in I_\sigma}$, which so far we consider invariant under arbitrary permutations on the index set I_σ.

Definition 1.2. 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 $|\sigma|$ is 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 1.3. 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 1.4. *All abstract simplicial complexes and simplicial maps are a category $\mathfrak{A}$ 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 1.5. 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

$$\langle x_i \rangle_{i\in I} := \{a = \sum_{i\in I} \lambda_i x_i : \lambda_i \in \mathbb{R},\ \lambda_i > 0,\ \sum_{i\in I} \lambda_i = 1\},$$

which is the smallest convex set containing $\{x_i\}_{i\in I}$.

Definition 1.6. 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

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

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

Definition 1.7. We define a *geometric p-simplex* to be a convex envelop $\langle x_i \rangle_{i\in I}$ where $\{x_i\}_{i\in I} \subset \mathbb{R}^n$ are affinely independent and $|I| = p + 1$.

Definition 1.8. Let σ be a geometric 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 1.9. We define a *geometric simplicial complex* $\mathcal{G}$ to be a collection of geometric simplexes such that

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

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

Definition 1.10. *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 1.11. *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 1.12. 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 1.13. 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 1.14. *Let $\sigma \in \mathcal{A}_{p+2}$, $p \geq 0$ then $\partial^2\sigma = 0$.*

Proof. We have

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

$\square$

Definition 1.15. 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 1.16. *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 1.17. 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 1.18. *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 1.19. 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 1.20. *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

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

while

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

□

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