Alma Mater Studiorum · Università di Bologna

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GEOMETRIC DEEP LEARNING

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Abstract in italiano...

Abstract in english...

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1 Introduction

1.1 Simplicial complexes

Definition 1.1.1. ***Abstract simplicial complex (finite)***
Let $\mathcal{F}$ be a family of sets we then define an abstract simplicial complex $\mathcal{A}$ to be

$$\mathcal{A} := \{\sigma = \{A_i\}_{i \in I_\sigma} \subset \mathcal{F} : \tau \subset \sigma \Rightarrow \tau \in \mathcal{A}\}$$

where I_σ is a finite set of indexes, we shall call σ abstract simplexes of $\mathcal{A}$.

Definition 1.1.2. ***Dimension of an abstract simplicial complex***
Let $\mathcal{A}$ be an abstract simplicial complex we define its dimension to be

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

where $dim(\sigma) := |\sigma| - 1$.

Definition 1.1.3. ***Abstract graph***
An abstract graph $\mathcal{G}$ is a 1-dimensional abstract simplicial complex whose vertexes and edges are respectively

$$\mathcal{V} := \{\sigma \in \mathcal{G} : dim(\sigma) = 0\} \text{ and}$$
$$\mathcal{E} := \{\sigma \in \mathcal{G} : dim(\sigma) = 1\} \ .$$

In Definition 1.1.1. we tacitly assumed the definition of the abstract simplex σ invariant with respect to permutations of the indexes I_σ, this assumption establishes the difference between directed and undirected graphs.

Definition 1.1.4. ***Convex envelop of points in $\mathbb{R}^n$***
Let I be a finite set of indexes, we define the convex envelope of $\{x_i\}_{i \in I} \subset \mathbb{R}^n$ 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 1.1.5. ***Affine independency of points in $\mathbb{R}^n$***
Let $\{x_i\}_{i \in I} \subset \mathbb{R}^n$ we define $\{x_i\}_{i \in I}$ 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 1.1.6. ***Geometric k-simplexes***
We define a geometric k-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 $|I| = k + 1$.

Definition 1.1.7. ***Faces and cofaces of geometric k-simplexes***
Let σ be a geometric k-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 $t \leq k$.

Definition 1.1.8. ***Geometric Simplicial Complex***
We define a geometric simplicial complex $\mathcal{K}$ to be a collection of geometric simplexes such that

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

(ii) $\sigma, \tau \in \mathcal{K} \Rightarrow \sigma \cup \tau \in \mathcal{K}$.

Definition 1.1.9. ***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 1.1.1. *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.

1.2 Forms and integration on abstract simplicial complexes

Definition 1.2.1. ***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 1.2.2. ***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 1.2.1. *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 1.2.3. ***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 1.2.1. *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 1.2.4. ***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 1.2.2. *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 1.2.5. ***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 1.2.1. *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.

1.3 Smooth real manifolds and abstract graphs

1.4 Convolutional neural networks on euclidean domains