Alma Mater Studiorum · Università di Bologna

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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. Although this approach has been successful in modern machine learning, it only deals with a really small set of domains. The goal of geometric deep learning is to extend this method to data defined on manifolds and simplicial complexes.
Convolution on euclidean domains is itself based on the translation invariance of such domains. In fact the convolution of a function $f : \mathbb{R}^n \to \mathbb{R}$, with some filter $g : \mathbb{R}^n \to \mathbb{R}$ is $(f * g)(x) = \langle f, g \circ T^{-1} \rangle_{L^2}$, where $T : \mathbb{R}^n \to \mathbb{R}^n$ is a translation represented by the vector x. Luckily convolutions can be define for functions define on groups with a measure, therefore we could also see the $\mathbb{R}^n$ with the measure dx as a representation of the group of translations $\mathbf{T}$ with measure dT, i.e. $(f * g)(x) = \int_{\mathbf{T}} dT f(T) g(x - T)$.

Contents

Chapter 1

Preliminaries on topology

Simplicial Complexes

We want to introduce algebraic objects called simplicial complexes and see how they are related to compact topological spaces. In order to do this we need 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 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 1.2. *Let $X = \{x_i\}_{i\in I} \subset \mathbb{R}^n$ 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 envelope $[x_i]_{i\in I}$ 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 $Vert(\sigma)$. We call the x_i the vertexes of $\sigma = [x_i]_{i\in I}$ and we denote the vertex set of a simplex by $Vert(\sigma)$.

Definition 1.6. Let σ be a p-simplex and $p, t \in \mathbb{N}$, we say that another t-simplex τ is a *face* of σ or equivalently that σ is a *coface* of τ, and we write $\tau \leq \sigma$, if $\tau \subset \sigma$, where $t \leq p$.

Now we are ready for our main definitions.

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

(i) if any simplex $\tau \leq, \sigma \in \mathcal{G}$ then $\tau \in \mathcal{G}$,

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

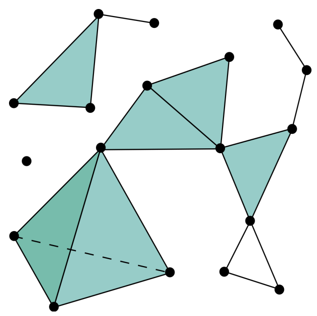

Figure 1.1: Example of simplicial complex.

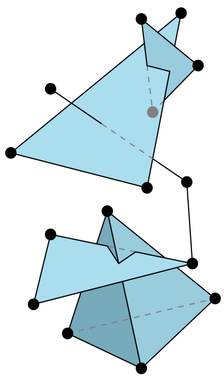

Figure 1.2: Set of simplexes which is not a simplicial complex.

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 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]. Firstly we want to equip our simplicial complexes with an orientation.

Definition 1.8. 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.

Secondly we define on the simplicial complex a vector space structure.

Definition 1.9. 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 $\{0, \dots, p\}$. We shall call C_p the space of *simplicial p-chains*.

In the study of chains' spaces a special role is played by a particular linear operator called boundary operator.

Definition 1.10. We define the *boundary* 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.

The set of all chains' spaces with their respective boundary operators is a special category that we call a *chain complex*, the property that defines a chain complex is the following.

Theorem 1.11. $\partial^2 = 0$.

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

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

□

We are interested in boundary operators because they allow us to define the p-holes, which mathematically can be thought as the p-cycles, p-chains that have no boundary, that are not boundary of any higher dimensional simplex. It is possible to show that the p-holes form a vector space and if two simplicial complex are isomorphic also their p-holes' spaces are. This, given what we said in the previous section, allows us to decide if two topological spaces are not homeomorphic by looking at the p-holes' spaces of their triangulations.

Definition 1.12. 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

In order to define data on simplicial complexes we are interested in studying the dual of the simplicial chain complex which we shall call a simplicial cochain complex.

Definition 1.13. 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 1.14. The dual of the boundary operator which we shall call *coboundary operator*, is defined to be

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

One could also show that the property $d^2 = 0$ is verified in the so defined cochain complex. The homology group could in general be define for any chain complex, in particulare for the simplicial cochain complex it takes the name of cohomology group.

Definition 1.15. 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.

To have a mirrored intuition of what the coboundary operator actually does we equipe our simplicial chain spaces with an inner product. This finite dimensional Hilbert space structure shall allow us to represent the action of a cochain σ^* on the chain τ as the scalar product $\langle \sigma, \tau \rangle$.

Definition 1.16. 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 $\langle i | j \rangle$.
The same Hilbert space structure allows us to represent the coboundary operator d in the space of chains with its integral kernel $\partial^\dagger$.

Definition 1.17. 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. $(d\langle \sigma |) | \tau \rangle = \langle \sigma | \partial \tau \rangle$. One can therefore think of the coboundary operator as a discrete exterior derivative acting on cochains.

Laplacian Operators

An important role in the definition of a convolution on simplicial complexes is played by the Laplaciano operator, especially by its eigenfunctions and spectrum.

Definition 1.18. We define the *p-Laplacian* operator to be

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

The Laplacian operator is defined to be self-adjoint and positive definite.

Proposition 1.19. $\Delta_p^{\dagger} = \Delta_p$.

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

$$\langle\sigma|\Delta_p\tau\rangle = \langle\sigma|(\partial_{p+1}\partial_{p+1}^{\dagger} + \partial_p^{\dagger}\partial_p)\tau\rangle =$$
$$= \langle(\partial_{p+1}\partial_{p+1}^{\dagger} + \partial_p^{\dagger}\partial_p)^{\dagger}\sigma|\tau\rangle =$$
$$= \langle(\partial_{p+1}\partial_{p+1}^{\dagger} + \partial_p^{\dagger}\partial_p)\sigma|\tau\rangle = \langle\Delta_p\sigma|\tau\rangle.$$

□

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 1.20. *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

$$\langle\sigma|\Delta_p^{+}\sigma\rangle = \langle\partial_{p+1}^{\dagger}\sigma|\partial_{p+1}^{\dagger}\sigma\rangle \geq 0$$

$$\langle\sigma|\Delta_p^{+}\sigma\rangle = \lambda_\sigma^{+}\langle\sigma|\sigma\rangle \geq 0 \implies \lambda+_\sigma \geq 0.$$

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 $[\Delta_p, \Delta_p^{\pm}] = 0$, 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 $\lambda_\sigma = \lambda_\sigma^{+} + \lambda_\sigma^{-} \geq 0$. □

Another really interesting property that was first proven by Beno Eckmann in 1944, is that the kernel of the p-Laplacian is isomorphic to the p-homology group.

Theorem 1.21. $ker\Delta_p \simeq H_p$.

Proof. We have

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

According to Theorem 1.29 it is true that

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

It is trivial to see that since $ker\Delta_p = ker\Delta_p^{+} \cap ker\Delta_p^{-}$

$$ker\partial_{p+1}^{\dagger} \cap ker\partial_p \subset ker\Delta_p,$$

less trivial is the opposite inclusion:

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

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

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

therefore $ker\partial_{p+1}^{\dagger} \cap ker\partial_p \subset ker\Delta_p$. Finally we notice that

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

□

Chapter 2

Simplicial Neural Networks

Convolutional Neural Networks

The goal of machine learning is teaching machines to approximate expert observers. Thinking of the space of possible machines as possibly convex and compact, one is able by varying a finite number of parameters to find a unique best approximation of any expert observer. The rappresentation of a random initialized machine is

Definition 2.1 (relu).

Definition 2.2 (convolutional layer).

Definition 2.3 (pooling layer).

Definition 2.4 (drop out).

Definition 2.5 (CNN).

Definition 2.6 (gradient descent).

Simplicial Neural Networks

Applications of simplicial complexes

Definition 2.7 (convolution on a simplicial complex).

Definition 2.8 (heat equation on a simplicial complex).

Definition 2.9 (pooling on a simplicial complex).

Definition 2.10 (pooling on a graph).

Definition 2.11 (simplicialNN).

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