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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

Category Theory

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 shall be our main tool to formally describe this conversion.

Definition 1.1. A category C consists of three ingerdients:

a class of objects $Obj(\mathbf{C})$; sets of morphisms Hom(A, B) for every ordered pair $(A, B) \in Obj(\mathbf{C}) \times Obj(\mathbf{C})$; a composition $Hom(A, B) \times Hom(B, C) \to Hom(A, C)$, denoted by $(f, g) \mapsto f \circ g$ for every $A, B, C \in Obj(\mathbf{C})$, satisfying the following axioms:

- (i) the family of Hom(A, B) is pairwise disjoint,
- (ii) the composition, when defined, is associative,
- (iii) for each $A \in Obj(\mathbb{C})$ there exists an *identity* $1_A \in Hom(A, A)$ such that for $f \in Hom(A, B)$ and $g \in Hom(C, A)$ we have that $1_A \circ f = f$ and $g \circ 1_A = g$.

Instead of writing $f \in Hom(A, B)$, we usually write $f : A \to B$.

Definition 1.2. Let **A** and **C** be categories, a functor $T: \mathbf{A} \to \mathbf{C}$ is a function, that is,

- (i) $A \in Obj(\mathbf{A}) \implies TA \in Obj(\mathbf{C}),$
- (ii) $f: A \to A' \implies Tf: TA \to TA' \quad A, A' \in Obj(\mathbf{A}),$
- (iii) if f, g are morphisms in **A** for which $g \circ f$ is defined, then $T(g \circ f) = (Tg) \circ (Tf)$,
- (iv) $T(1_A) = 1_{TA} \quad \forall A \in \mathbf{A}$.

The property (iii) of the previous definition actually defines what we shall call *covariant functors*. If instead we require $T(g \circ f) = (Tf) \circ (Tg)$, we are defining a so called *contravariant functor*.

Definition 1.3. An equivalence in a category C is a morphism $f: A \to B$ for which there exists a morphism $q: B \to A$ such that $f \circ q = 1_B$ and $q \circ f = 1_A$.

Theorem 1.4. If A and C are categories and $T: A \to C$ is a functor of either variance, then whenever f is an equivalence on A then Tf is an equivalence on C.

Proof. We apply T to the equations $f \circ g = 1_B$ and $g \circ f = 1_A$, that for a covariant functor leads to $(Tf) \circ (Tg) = T(1_B) = 1_{TB}$ and $(Tg) \circ (Tf) = T(1_A) = 1_{TA}$.

A category that will be used in the following section is the category of topological spaces and continuous functions.

Theorem 1.5. Topological spaces and continuous functions are a category **Top**, whose equivalences are called homeomorphisms.

Other examples of categories can be found in [1].

Simplicial Complexes

We shall now 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 1.6. 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

$$[x_i]_{i \in I} := \{ \sum_{i \in I} \lambda_i x_i : \lambda_i \in \mathbb{R}, \ \lambda_i \ge 0, \ \sum_{i \in I} \lambda_i = 1 \}.$$

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 1.7. 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 1.8. 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 1.9. 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 1.10. 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 1.11. 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 1.12. We define a simplicial complex \mathcal{G} to be a collection of simplexes such that

- (i) $\tau < \sigma \in \mathcal{G} \Rightarrow \tau \in \mathcal{G}$,
- (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 1.13. 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 1.14. Simplicial complexes and simplicial maps are a category G, whose equivalences are called isomorphisms..

Definition 1.15. 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 1.16. 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 simple complex and another topological space, this other space has to be compact.

Lemma 1.17. 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 1.18. 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 1.19. $| \cdot | : G \rightarrow Top \text{ is a functor.}$

Notice that there is no obvious functor from \mathbf{Top} to \mathbf{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 1.20. 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 1.21. 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 empty set is a (-1)-simplex. A graph is a one dimensional abstract simplicial complex.

Definition 1.22. 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 1.23. Abstract simplicial complexes and simplicial maps are a category A, whose equivalences are called isomorphisms.

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 1.24. 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 1.25. Let A be a d-dimensional abstract simplicial complex, it admits a geometric realization in \mathbb{R}^{2d+1} .

Kuratowski theorem proves the prevuois statement to be also sharp.

One could also show that that geometric realizations of isomorphic abstract simplicial complexes are themselves isomorphic.

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 1.26. 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 1.27. 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 $\sigma_i^p = [v_0, \ldots, v_p]$ can have two possible orientations that satisfy $[v_0, \ldots, v_p] = sgn(\pi)[v_{\pi 0}, \ldots, v_{\pi p}]$, where π is a permutation of $\{0, \ldots, p\}$. 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 1.28. We define the boundary operator $\partial_{p+1}: C_{p+1} \to C_p$ by setting

$$\partial_{p+1}([v_0,\ldots,v_p]) = \sum_{i=0}^p (-1)^i [v_0,\ldots,\hat{v_i},\ldots,v_p]$$

(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 1.29. $\partial^2 = 0$.

Proof. Let
$$\partial_{p+1}([v_0,\ldots,v_{p+1}]) = \sum_{i=0}^{p+1} (-1)^i [v_0,\ldots,\hat{v_i},\ldots,v_{p+1}]$$
 then

$$\partial_p(\partial_{p+1}([v_0,\ldots,v_{p+1}])) = \sum_{j=0,j\neq i}^{p+1} \sum_{i=0}^{p+1} (-1)^{i+j} [v_0,\ldots,\hat{v_i},\ldots,\hat{v_j},\ldots,v_{p+1}] = 0.$$

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 1.30. 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. The cochain complex is the image of the chain complex via a special functor, i.e. the dual contravariant functor.

Definition 1.31. Let V be the category of vector spaces and linear transformations between them, we define the *dual contravariant functor* by

$$V \in Obj(\mathbf{V}) \mapsto V^* := Hom(V, \mathbb{R}) \in Obj(\mathbf{V})$$

$$\partial \in Hom(U,V) \mapsto \partial^* \in Hom(V^*,U^*) : \partial^*(\phi) = \phi \circ \partial.$$

By applying this functor to the spaces of simplicial chains we are able to define the space of simplicial cochains, and their respective coboundary operator.

Definition 1.32. 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 1.33. By means of the dual functor we are able to define the dual of the boundary operator which we shall call *coboundary operator*, which is defined to be

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

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 1.34. We define the *p-cohomology group* to be

$$H^p := \frac{kerd_{p+1}}{imd_n},$$

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 1.35. 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 ∂^{\dagger} .

Definition 1.36. 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 ∂_{p+1}^{\dagger} by

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

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 1.37. 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 1.38. $\Delta_p^{\dagger} = \Delta_p$.

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 1.39. 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

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

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

Let then $\Delta_p^-|\sigma\rangle=\lambda_\sigma^-|\sigma\rangle,$ we see that

$$\langle \sigma | \Delta_p^- \sigma \rangle = \langle \partial_p \sigma | \partial_p \sigma \rangle \ge 0$$

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

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 $\lambda_\sigma = \lambda_\sigma^+ + \lambda_\sigma^- \ge 0$.

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 1.40. $ker\Delta_p \simeq H_p$.

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:

$$\begin{split} \partial_{p+1}^{\dagger}\sigma &\in im\partial_{p+1}^{\dagger}, \sigma \in ker\Delta_{p} \implies \partial_{p+1}^{\dagger}\sigma \in ker\partial_{p+1} = (im\partial_{p+1}^{\dagger})^{\perp}, \\ \partial_{p}\sigma &\in im\partial_{p}, \sigma \in ker\Delta_{p} \implies \partial_{p}\sigma \in ker\partial_{p}^{\dagger} = (im\partial_{p})^{\perp}, \\ \partial_{p}\sigma &= \partial_{p+1}^{\dagger}\sigma \in im\partial_{p+1}^{\dagger} \cap (im\partial_{p+1}^{\dagger})^{\perp} = im\partial_{p} \cap (im\partial_{p})^{\perp} = 0, \end{split}$$

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

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Definition 2.1 (relu).
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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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