Scuola di Scienze Dipartimento di Fisica e Astronomia Corso di Laurea in Fisica

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. Moreover, one could also consider such a convolution to be defined on the translation group itself, represented by some \mathbb{R}^n . In the same way one can define a convolution on the group $(\mathbb{Z}, +)$ as $(a*b)_n = \sum_{i \in \mathbb{Z}} a_i b_{n-i}$. Such definitions of convolution operators are equivariant with respect to the action of the group they are defined upon. In image recognition translation invariance is necessary, but graphs and simplicial complexes do not in general need this simmetry.

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Chapter 1

Preliminaries on topology

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.

Simplicial Complexes

In this section we shall define structures called simplicial complexes and discuss some of their properties. In order to define these structures we need the definitions of convex hull and affine independence in \mathbb{R}^n . For a deeper insight into simplicial complexes we refer the reader to [1, 2].

Definition 1.1. Let $A \subset \mathbb{R}^n$, we define A to be *convex* if

$$x, y \in A \Rightarrow tx + (1+t)y \in A$$

for all $t \in [0, 1]$.

Definition 1.2. Let $\sigma := \{x_i\}_{i \in I}$ be a finite subset of \mathbb{R}^n , we define σ to be affinely independent if $\{x_0 - x_i\}_{i \in I - \{0\}}$ is linearly independent.

For the definition of affine independence of $\sigma = \{x_i\}_{i \in I} \subset \mathbb{R}^n$ to be well stated we need it to be independent of the choice of x_0 . In fact had we chosen x_j with $j \in I$, we would have that if $\{x_j - x_i\}_{i \in I - \{j\}}$ is linearly independent also $\{x_0 - x_i\}_{i \in I - \{0\}}$ is. To prove this let $f : span(\{x_j - x_i\}) \to span(\{x_0 - x_i\})$ be the identity mapping $(x_j - x_i) \mapsto (x_0 - x_i) - (x_0 - x_j)$, mapping the vector e_i in the base $\{x_j - x_i\}$ to the vector $e_i - e_j$ in the "base" $\{x_0 - x_i\}$. This mapping is represented by the square matrix

$$F := \begin{pmatrix} I & \cdots & O \\ -1 & \cdots & -1 \\ O & \cdots & I \end{pmatrix},$$

where the j-th raw is (-1,...,-1). Adding all the raws to the j-th we obtain the diagonal matrix diag(1,...,1,-1,1,...,1), therefore detF = -1. From the non-zero determinant we can conclude that f is an isomorphism, which makes our definition well stated.

Definition 1.3. Let $\sigma := \{x_i\}_{i \in I}$ be a finite subset of \mathbb{R}^n , we define the *covex set generated by* σ to be the smallest convex set containing X according to the inclusion relation.

Since the intersection of convex sets is convex, the convex set generated by σ can be equivalently defined as the intersection of all convex sets containing σ .

Theorem 1.4. Let $\sigma := \{x_i\}_{i \in I}$ be a finite subset of \mathbb{R}^n , if X is affinely independent then the convex set generated by X is

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

Furthermore for any point $x \in [\sigma]$ we have that

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

where $\lambda_i, \mu_i \geq 0$ and $\sum_{i \in I} \lambda_i = \sum_{i \in I} \mu_i = 1$.

Proof. Let $C := \{ \bigcap_{\alpha} C_{\alpha} : \sigma \in C_{\alpha}, C_{\alpha} \text{ convex} \}$, we want to show that:

(i) $C \subset [\sigma]$

This is true if $[\sigma]$ is convex and contains σ . The proof that it contains σ is trivial. In fact

for every vertex $x_j = \sum_{i \in I} \delta_{ij} x_i$, and $\sum_{i \in I} \delta_{ij} = 1$. To prove that it is convex we chose two points $a = \sum_{i \in I} a_i x_i$, $b = \sum_{i \in I} b_i x_i$ where $a_i, b_i \geq 1$ $0 \forall i \in I \text{ and } \sum_{i \in I} a_i = \sum_{i \in I} b_i = 1. \text{ For } t \in [0, 1]$

$$ta + (1-t)b = t\sum_{i \in I} a_i x_i + (1-t)\sum_{i \in I} b_i x_i = \sum_{i \in I} (ta_i + (1-t)b_i)x_i.$$

It follows that $ta_i + (1-t)b_i \ge 0$ and $\sum_{i \in I} (ta_i + (1-t)b_i) = t \sum_{i \in I} a_i + (1-t) \sum_{i \in I} b_i = 1$ for all $i \in I$, therefore (i) is proven.

(ii) $[\sigma] \subset C$

(iii)
$$\sum_{i \in I} \lambda_i x_i = \sum_{i \in I} \mu_i x_i \Rightarrow \lambda_i = \mu_i \forall i \in I$$

A proof of theorem 1.4 can be found in [1]. The set $[\sigma]$ is often called *covex hull* of σ .

Example 1.5. 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 1.6. We define a p-simplex $[\sigma]$ to be the convex hull of an affinely independent set $\sigma := \{x_i\}_{i \in I} \subset \mathbb{R}^n$, where p = |I| - 1 is called dimension of the p-simplex.

Theorem 1.4 gives us the possibility to represent a point in a simplex $[\sigma]$ via a finite set of real parameters defined in the range [0, 1] and satisfying the normalisation condition $\sum_{i \in I} \lambda_i = 1$. Such parameters are called *baricentric coordinates* of $[\sigma]$.

The points in σ are called *vertexes* of the simplex $[\sigma]$, accordingly we define the vertex set of a simplex $[\sigma]$ to be $Vert([\sigma]) = \sigma$.

Definition 1.7. Let $[\sigma]$ be a p-simplex and $p, t \in \mathbb{N}$, we say that another t-simplex $[\tau]$ is a face of $[\sigma]$ or equivalently that $[\sigma]$ is a *coface* of $[\tau]$, and we write $[\tau] \leq [\sigma]$, if $\tau \subset \sigma$, where $t \leq p$.

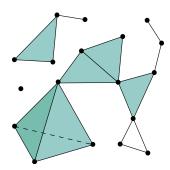


Fig. 1.1: Example of simplicial complex.

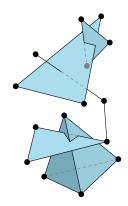


Fig. 1.2: Set of simplexes which is not a simplicial complex.

Now we are ready for our main definitions.

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

- (i) if any simplex $[\tau] \leq [\sigma], [\sigma] \in \mathcal{G}$ then $[\tau] \in \mathcal{G}$,
- (ii) if $[\sigma], [\tau] \in \mathcal{G}$ then $[\sigma] \cap [\tau] \in \mathcal{G}$.

We can see in Fig. 1.2 that the intersection property of simplicial complexes is not satisfied.

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. The discussion of abstract simplicial complexes can be found in [2].

Definition 1.9. 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 1.10. 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.

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 [3]. First we want to equip our simplicial complexes with an orientation.

Definition 1.11. 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.

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

Definition 1.12. 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 1.13. 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 1.14. $\partial^2 = 0$.

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 1.15. 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 1.16. 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 1.17. The dual of the boundary operator which we shall call *coboundary operator*, is defined to be

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

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 particular for the simplicial cochain complex it takes the name of cohomology group.

Definition 1.18. 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 1.19. 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 1.20. 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 Laplacian operator, especially by its eigenfunctions and spectrum. A more thorough discussion of this operator can be found in [4].

Definition 1.21. 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 1.22. $\Delta_p^{\dagger} = \Delta_p$.

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 1.23. 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

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

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

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 1.24. $ker\Delta_p \simeq H_p$.

Proof. We have

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

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

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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).

Appendix A

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 A.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 A.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 A.3. An equivalence in a category C is a morphism $f: A \to B$ for which there exists a morphism $g: B \to A$ such that $f \circ g = 1_B$ and $g \circ f = 1_A$.

Theorem A.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 A.5. Topological spaces and continuous functions are a category **Top**, whose equivalences are called homeomorphisms.

Other examples of categories can be found in [2].

Appendix B

Construction of Simplicial Complexes from Point Clouds

Cech, Alpha and Delauney complexes. Nerve Theorem.

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