Towards Neural Homology Theory

MACHINE LEARNING
DEPARTMENT

William H. Guss [1,2] Ruslan Salakhutdinov [1]
{wguss, rsalakhu}@cs.cmu.edu

[1]Carnegie Mellon University

[2]Machine Learning at Berkeley

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The problem of architecture selection

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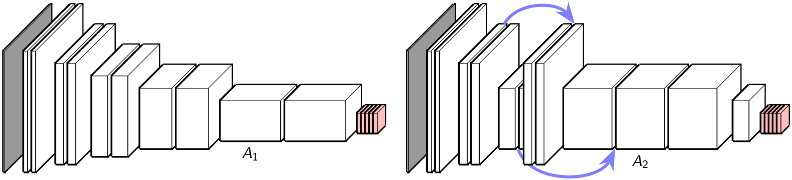

Figure: Examples of two competing convolutional architecture A_1 and A_2.

In computer vision, for example, a large body of work focuses on improving the initial architectural choices of AlexNet.

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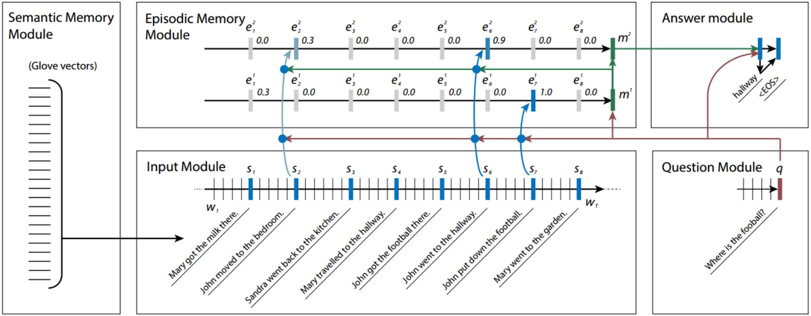

Architectures are becoming **hyperspecialized**.

Despite the success of this approach, **there are still not general principles for choosing architectures in arbitrary settings**.

To scale deep learning to new problems without *expert architecture designers*, the problem of architecture selection must be understood.

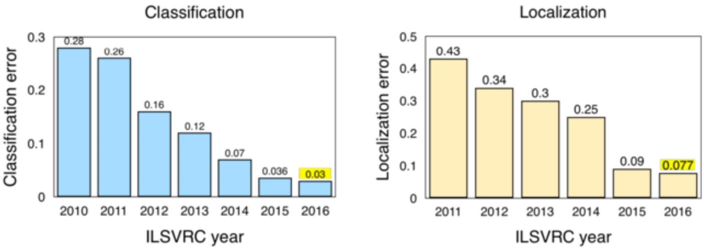

Figure: Graduate student ascent on the ImageNet dataset by year.

A partial solution: neural expressivity theory

Neural expressivity theory: properties of neural networks → expressivity and generalization capability ([RPK+16], [DFS16], [Gus16]).

E.g. shallow networks need exponentially many more units to express certain functions than deeper ones; deep networks can express curvature more efficiently, etc.

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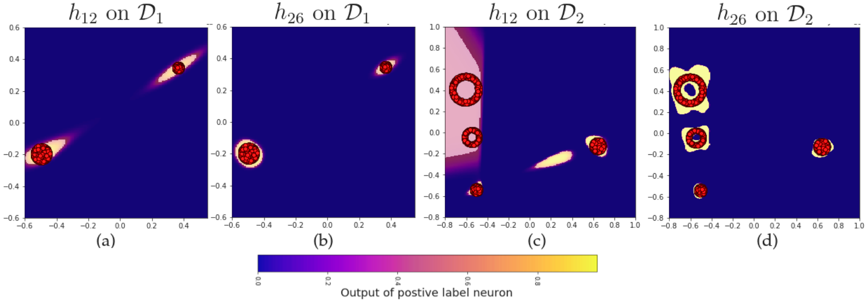
This can only be used to determine an architecture in practice if it is understood how expressive a model need be in order to solve a problem

Our approach: data-first architecture selection

Given a learning problem (some dataset), which architectures are suitably regularized and expressive enough to learn and generalize on that problem?



DAS: develop some objective measure of data complexity, and then characterize neural architectures by their ability to learn subject to that complexity.

Towards a measure of data complexity

A brief introduction to topology

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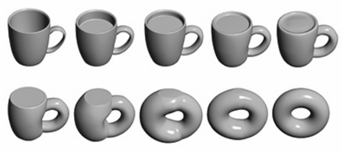

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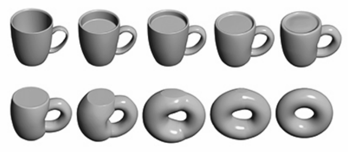
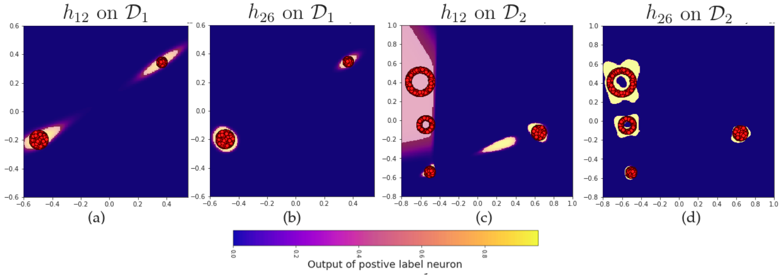


Topology can differentiate sets in a meaningful way that discards certain irrelevant properties such as rotation, translation, curvature, etc.

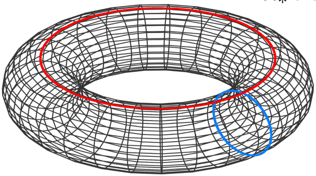
In this view $\mathcal{D}_1 \not\cong \mathcal{D}_2$. Furthermore h_{12} cannot express decision boundaries with the topology of $\mathcal{D}_2$.



We can characterize architectures by topological expressivity.

Algebraic topology lets us explicitly compute which spaces are equivalent to eachother.

$$H_* : \mathsf{Top}^2 \longrightarrow \mathsf{AbGrp}$$



$$\xrightarrow{H_1(\mathbb{T}) = \mathbb{Z} \oplus \mathbb{Z}}$$

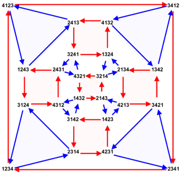


Figure: An illustration of the core philosophy of algebraic topology: 'functoraly' reduce hard problems in topology to easy ones in group theory.

Homology: a tool for computing topology

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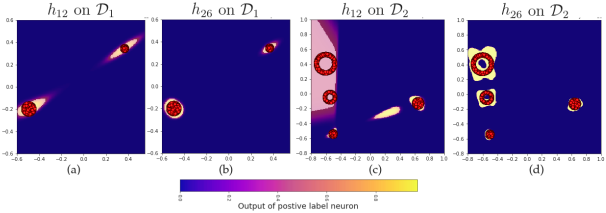

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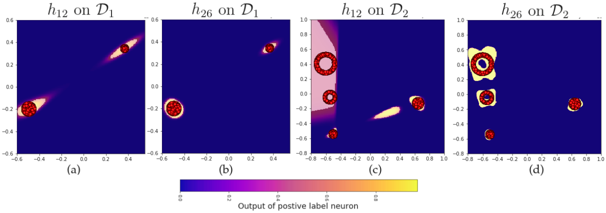

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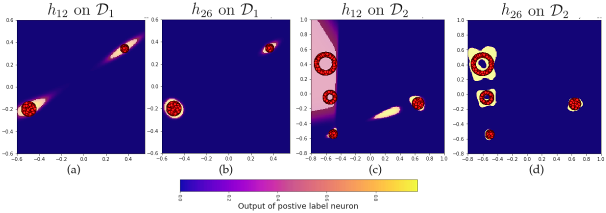

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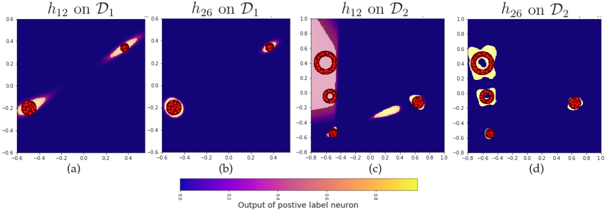

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$H(\mathcal{D}_1) \leqslant H(\mathcal{D}_2)$ **and $\mathcal{D}_2$ requires more complex architectures**

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Def (Homology). If X is a topological space, then

- $H_n(X) = \mathbb{Z}^{\beta_n}$ is called **the** n**th homology group of** X if β_n is the number of 'holes' of dimension n in X.
- the homology of X is defined as $H(X) = \{H_n(X)\}_{n=0}^{\infty}$.

Theorem (Bredon). If $X \cong Y$ then $H(X) = H(Y)$.

Homological Characterization of Neural Architectures

The power of homological characterization

Homology is a stringent measure for characterizing neural architectures:

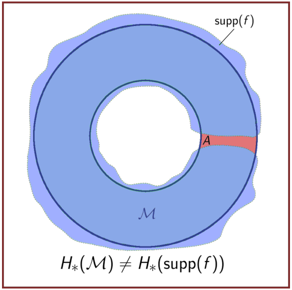

Figure: When homology cannot be expressed, there exists a misclassified set.

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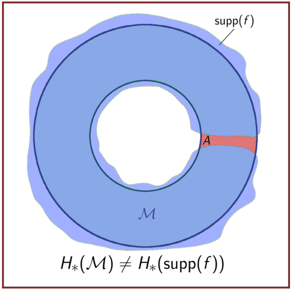

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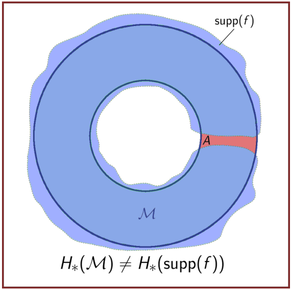
Let $H_S(f)$ be the homology of the support of f, i.e. $H_S(f) = H(\{x \ : \ f(x) > 0\})$.



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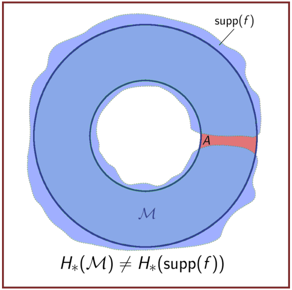
Theorem (The Homological Principle of Generalization). If for all $f \in \mathcal{F}$, $H_S(f) \neq H(\mathcal{M})$, then there exists $A \subset X$ such that f missclassifies A.



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Architecture selection in the lense of topology

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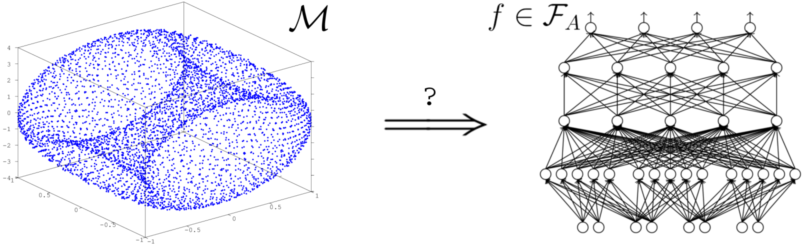

An empirical approach

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An empirical approach: Synthetic data

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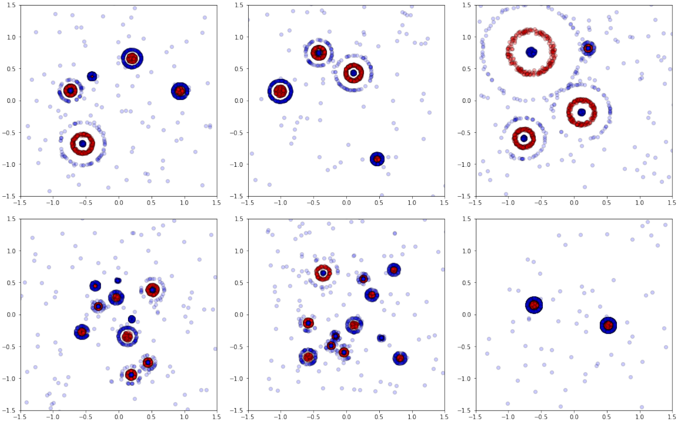

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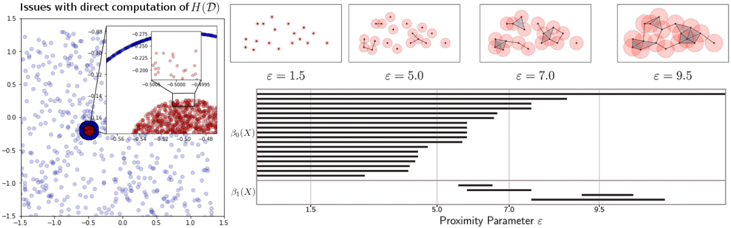

Figure: Left: The local disconnectedness of datasets prevents direct computation of their homology. Right: An illustration of computing persistent homology on a collection of points ([TZH15])

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2. (Sanity check) Real data is homologically rich!

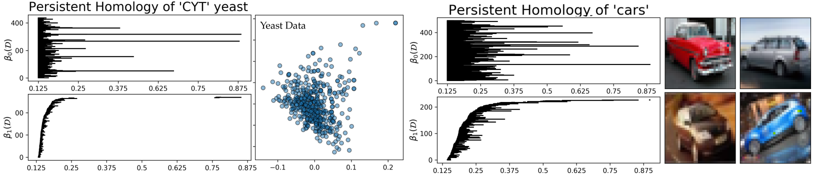

Figure: The persistent homology barcodes of classes in the CIFAR-10 and UCI Protein Localization Datasets.

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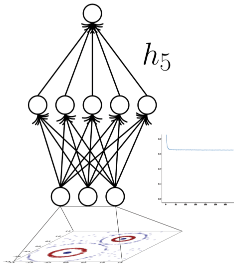

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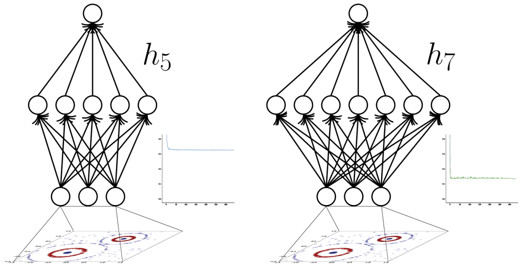

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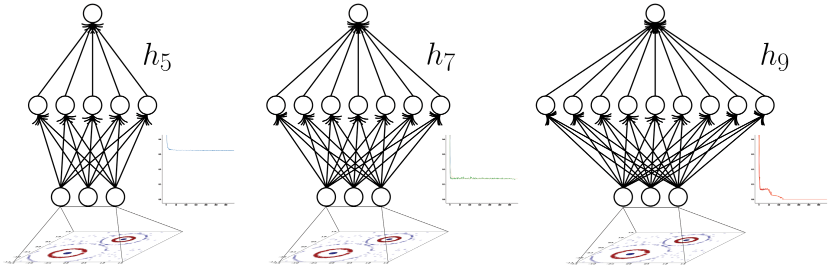

Empirical results: Topological phase transitions

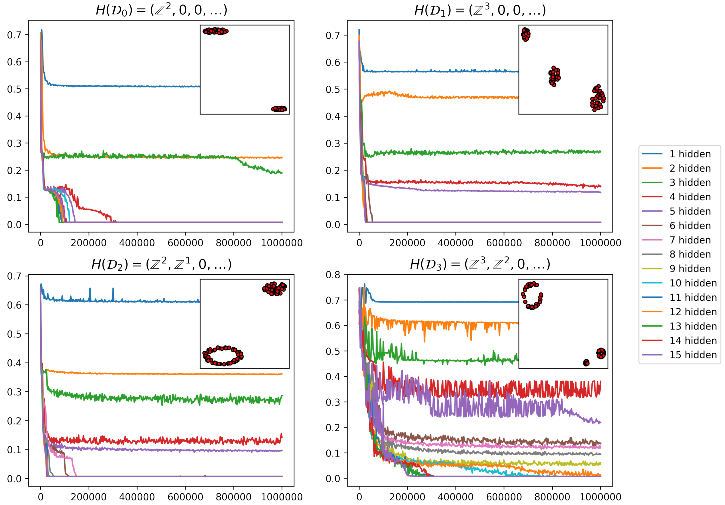

Figure: Average testing error of different architectures on datasets of increasing homological complexity.

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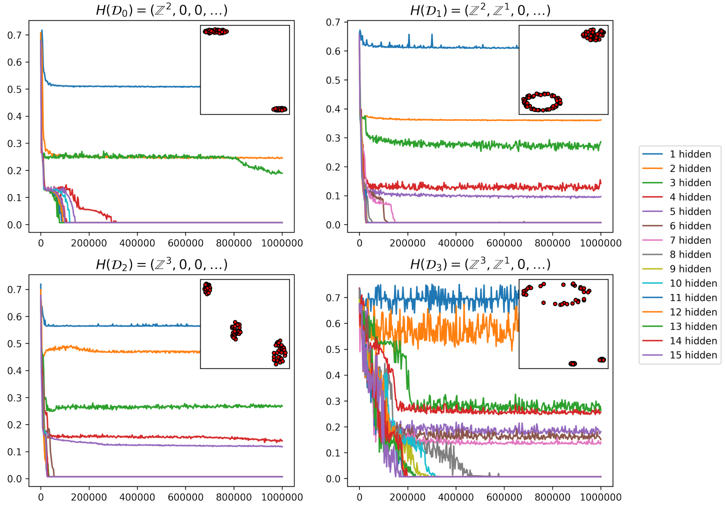

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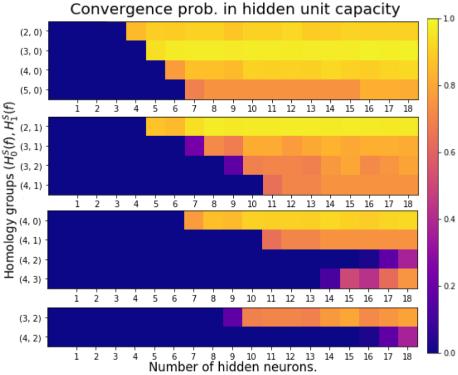

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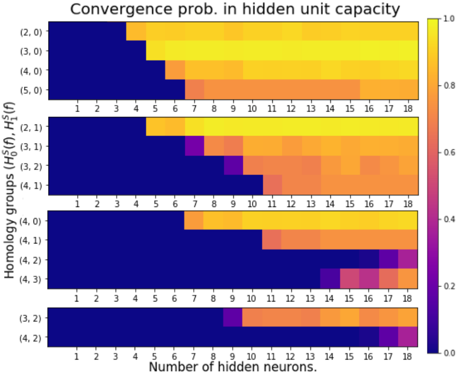

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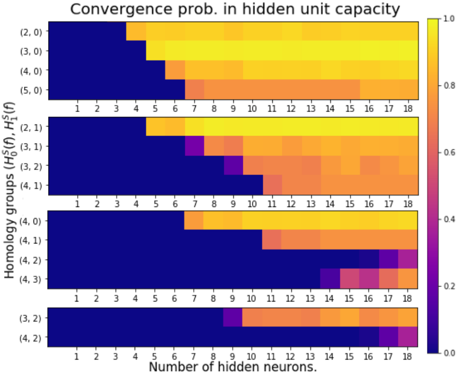

Neural Homology Theory

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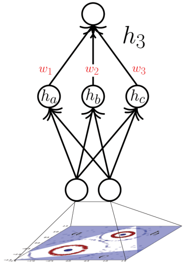

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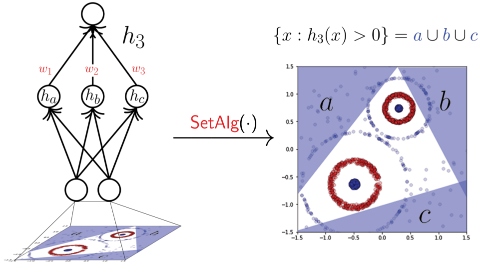

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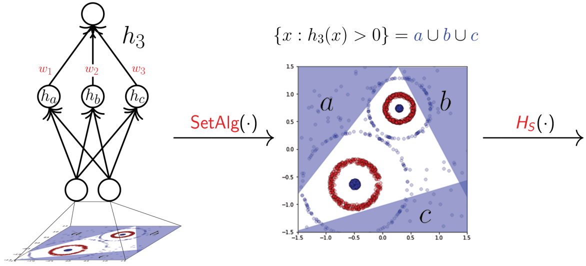

$$H_S^0(h_3) \cong \frac{a + b \oplus c}{\left(\frac{ac \oplus bc}{abc}\right)}$$

$$\boxed{\#\text{Regions} = \frac{1 \oplus 1}{\left(\frac{0 \oplus 1}{0}\right)} \approx 2 - 1 = 1}$$

Neural networks as set expressions.

Neural networks with ReLu-like functions can be converted into set expression.

1. The decision region of a single hidden unit is a halfspace.

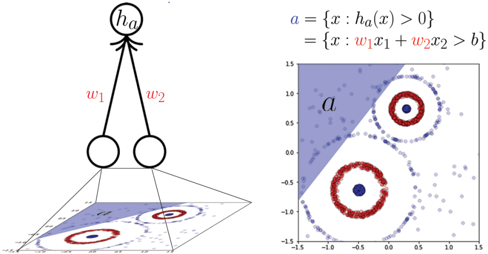

Figure: An illustration of halfspaces induced by ReLu-like networks.

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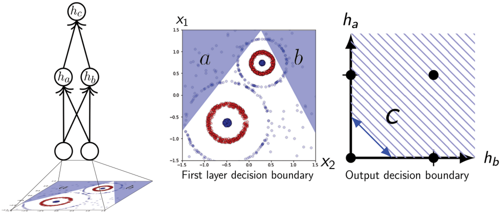

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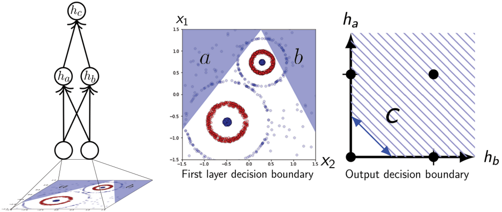

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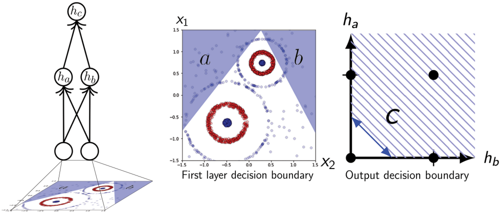

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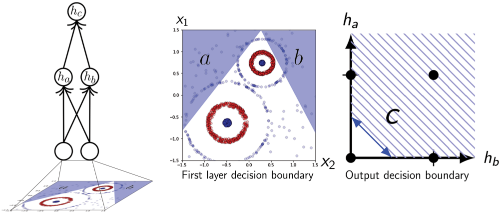

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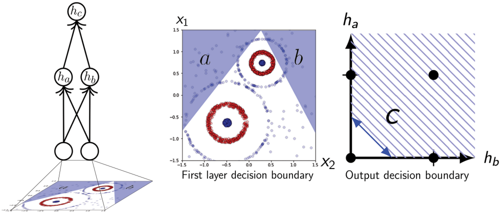

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$$= a \cup b$$

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Formally:

$$\{x : N(x) > 0\} = \bigcup_{\gamma \in S(W)} \bigcap_{h_i \in \text{hidden}} \{x : \text{sign}(\gamma_i) h_i(x) > 0\}$$

with $N(x) = ReLu(W^T h(x))$ and

$$S(W) = \{h : W^T h > 0\} \cap \{-1, 1\}^{|\text{hidden}|}.$$

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Homology of set algebra on halfspaces

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   - The "sum" of homologies $H(a) \oplus H(b)$
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For example,

$$\#\text{ holes } = \frac{a \oplus b}{ab + c \oplus d} := \frac{H(a) \oplus H(b)}{H(a \cap b \cup c) \oplus H(d)}$$

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$$\begin{aligned} H_0(a \cap b \cup c) &= ab + c \\ &= \frac{ab \oplus c}{abc} = \frac{a \oplus b \oplus c}{abc \oplus a + b} \\ &\approx 3 - H_0(a \cap b \cap c) + H_0(a \cup b). \end{aligned}$$

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Neural homology theory says **no.**

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2. Therefore

$$\# \text{ Regions} = H_0(h_3 > 0) \leqslant 3.$$

□

Remarks & Questions

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Appendix

Homology

Definition (Homology Theory, [Bre13])

A homology theory on the on Top^2 is a function $H : Top^2 \to Ab$ assigning to each pair (X, A) of spaces a graded (abelian) group $\{H_p(X, A)\}$, and to each map $f : (X, A) \to (Y, B)$, homomorphisms $f_* : H_p(X, A) \to H_p(Y, B)$, together with a natural transformation of functors $\partial_* : H_p(X, A) \to H_{p-1}(X, A)$, called the connecting homomorphism (where we use $H_*(A)$ to denote $H_*(A, \varnothing)$) such that the following five axioms are satisfied.

Definition (Homology Theory, [Bre13])

1. If $f \simeq g : (X, A) \to (Y, B)$ then $f_* = g_* : H_*(X, A) \to H_*(Y, B)$.
2. For the inclusions $i : A \to X$ and $j : X \to (X, A)$ the sequence sequence of inclusions and connecting homomorphisms are exact.
3. Given the pair (X, A) and an open set $U \subset X$ such that $cl(U) \subset int(A)$ then the inclusion $k : (X - U, A - U) \to (X, A)$ induces an isomorphism $k_* : H_*(X - U, A - U) \to H_*(X, A)$
4. For a one point space P, $H_i(P) = 0$ for all $i \neq 0$.
5. For a topological sum $X = +_\alpha X_\alpha$ the homomorphism

$$\bigoplus (i_\alpha)_* : \bigoplus H_n(X_\alpha) \to H_n(X)$$

is an isomorphism, where $i_\alpha : X_\alpha \to X$ is the inclusion.