WHY DOES UNSUPERVISED DEEP LEARNING WORK?
- A PERSPECTIVE FROM GROUP THEORY

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ABSTRACT

Why does Deep Learning work? What representations does it capture? How do higher-order representations emerge? We study these questions from the perspective of group theory, thereby opening a new approach towards a theory of Deep learning.

One factor behind the recent resurgence of the subject is a key algorithmic step called pretraining: first search for a good generative model for the input samples, and repeat the process one layer at a time. We show deeper implications of this simple principle, by establishing a connection with the interplay of orbits and stabilizers of group actions. Although the neural networks themselves may not form groups, we show the existence of shadow groups whose elements serve as close approximations.

Over the shadow groups, the pretraining step, originally introduced as a mechanism to better initialize a network, becomes equivalent to a search for features with minimal orbits. Intuitively, these features are in a way the simplest. Which explains why a deep learning network learns simple features first. Next, we show how the same principle, when repeated in the deeper layers, can capture higher order representations, and why representation complexity increases as the layers get deeper.

1 INTRODUCTION

The modern incarnation of neural networks, now popularly known as Deep Learning (DL), accomplished record-breaking success in processing diverse kinds of signals - vision, audio, and text. In parallel, strong interest has ensued towards constructing a theory of DL. This paper opens up a group theory based approach, towards a theoretical understanding of DL.

We focus on two key principles that (amongst others) influenced the modern DL resurgence.

(P1) Geoff Hinton summed this up as follows. “In order to do computer vision, first learn how to do computer graphics”. [Hinton (2007)]. In other words, if a network learns a good generative model of its training set, then it could use the same model for classification.

(P2) Instead of learning an entire network all at once, learn it one layer at a time.

In each round, the training layer is connected to a temporary output layer and trained to learn the weights needed to reproduce its input (i.e to solve P1). This step – executed layer-wise, starting with the first hidden layer and sequentially moving deeper – is often referred to as pre-training (see Hinton et al. (2006); Hinton (2007); Salakhutdinov & Hinton (2009); Bengio et al. (in preparation)) and the resulting layer is called an autoencoder. Figure 1(a) shows a schematic autoencoder. Its weight set \( W_1 \) is learnt by the network. Subsequently when presented with an input \( f \), the network will produce an output \( f' \approx f \). At this point the output units as well as the weight set \( W_2 \) are discarded.

There is an alternate characterization of P1. An autoencoder unit, such as the above, maps an input space to itself. Moreover, after learning, it is by definition, a stabilizer \(^1\) of the input \( f \). Now, input

\(^{1}\) A transformation \( T \) is called a stabilizer of an input \( f \), if \( f' = T(f) = f \).
signals are often decomposable into features, and an autoencoder attempts to find a succinct set of features that all inputs can be decomposed into. Satisfying P1 means that the learned configurations can reproduce these features. Figure 1(b) illustrates this post-training behavior. If the hidden units learned features $f_1, f_2, \ldots$, and one of them, say $f_i$, comes back as input, the output must be $f_i$. In other words learning a feature is equivalent to searching for a transformation that stabilizes it.

The idea of stabilizers invites an analogy reminiscent of the orbit-stabilizer relationship studied in the theory of group actions. Suppose $G$ is a group that acts on a set $X$ by moving its points around (e.g., groups of $2 \times 2$ invertible matrices acting over the Euclidean plane). Consider $x \in X$, and let $O_x$ be the set of all points reachable from $x$ via the group action. $O_x$ is called an orbit. A subset of the group elements may leave $x$ unchanged. This subset $S_x$ (which is also a subgroup), is the stabilizer of $x$. If it is possible to define a notion of volume for a group, then there is an inverse relationship between the volumes of $S_x$ and $O_x$, which holds even if $x$ is actually a subset (as opposed to being a point). For example, for finite groups, the product of $|O_x|$ and $|S_x|$ is the order of the group.

The inverse relationship between the volumes of orbits and stabilizers takes on a central role as we connect this back to DL. There are many possible ways to decompose signals into smaller features. Figure 2(a) illustrates this point: a rectangle can be decomposed into L-shaped features or straight-line edges.

All experiments to date suggest that a neural network is likely to learn the edges. But why? To answer this, imagine that the space of the autoencoders (viewed as transformations of the input) form a group. A batch of learning iterations stops whenever a stabilizer is found. Roughly speaking, if the search is a Markov chain (or a guided chain such as MCMC), then the bigger a stabilizer, the earlier it will be hit. The group structure implies that this big stabilizer corresponds to a small orbit. Now intuition suggests that the simpler a feature, the smaller is its orbit. For example, a
line-segment generates many fewer possible shapes\footnote{In fact, one only gets line segments back} under linear deformations than a flower-like shape. An autoencoder then should learn these \textit{simpler} features first, which falls in line with most experiments (see [Lee et al. (2009)]).

The intuition naturally extends to a many-layer scenario. Each hidden layer finding a feature with a big stabilizer. But beyond the first level, the inputs no longer inhabit the same space as the training samples. A “simple” feature over this new space actually corresponds to a more complex shape in the space of input samples. This process repeats as the number of layers increases. In effect, each layer learns “edge-like features” with respect to the previous layer, and from these locally simple representations we obtain the learned higher-order representation.

1.1 Our Contributions

Our main contribution in this work is a formal substantiation of the above intuition connecting autoencoders and stabilizers. First we build a case for the idea that a random search process will find large stabilizers (section 2), and construct evidential examples (section 2.3).

Neural networks incorporate highly nonlinear transformations and so our analogy to group transformations does not directly map to actual networks. However, it turns out that we can define (Section 5) and construct (Section 4) \textit{shadow} groups that approximate the actual transformation in the network, and reason about these instead.

Finally, we examine what happens when we compose layers in a multilayer network. Our analysis highlights the critical role of the sigmoid and show how it enables the emergence of higher-order representations within the framework of this theory (Section 5).

2 Random Walk and Stabilizer Volumes

2.1 Random Walks over the Parameter Space and Stabilizer Volumes

The learning process resembles a random walk, or more accurately, a Markov-Chain-Monte-Carlo type sampling. This is already known, e.g. see (Salakhutdinov & Hinton (2009); Bengio et al. [in preparation]). A newly arriving training sample has no prior correlation with the current state. The order of computing the partial derivatives is also randomized. Effectively then, the subsequent minimization step takes off in an almost random direction, guided by the gradient, towards a minimal point that stabilizes the signal. Figure 2(b) shows this schematically. Consider the current network configuration, and its neighbourhood $B_r$ of radius $r$. Let the input signal be $I$, and suppose that there are two possible decompositions into features: $f = \{f_1, f_2 \ldots\}$ and $h = \{h_1, h_2 \ldots\}$. We denote the reconstructed signal by $\Sigma_f$ (and in the other case, $\Sigma_h$). Note that these features are also signals (just like the input signal, only simpler). The reconstruction error is usually given by an error term, such as the L2 distance $\|I - \Sigma_f\|_2$. If the collection $f$ really enables a good reconstruction of the input - i.e. $\|I - \Sigma_f\|_2 \approx 0$ - then it is a stabilizer of the input by definition. If there are competing feature-sets, gradient descent will eventually move the configuration to one of these stabilizers.

Let $P_f$ be the probability that the network discovers stabilizers for the signals $f_i$ (and similar definition for $P_h$), in a neighbourhood $B_r$ of radius $r$. $S_f$ would denote the stabilizer set of a signal $f_i$. Let $\mu$ be a volume measure over the space of transformation. Then one can roughly say that

\[
\frac{P_f}{P_h} \propto \prod_j \frac{\mu(B_r \cap S_{f_j})}{\mu(B_r \cap S_{h_j})}
\]

Clearly then, the most likely chosen features are the ones with the bigger stabilizer volumes.

2.2 Exposing the Structure of Features - From Stabilizers to Orbits

If our parameter space was actually a finite group, we could use the following theorem.

\textbf{Orbit-Stabilizer Theorem} Let $G$ be a group acting on a set $X$, and $S_f$ be the stabilizer subgroup of an element $f \in X$. Denote the corresponding orbit of $f$ by $O_f$. Then $|O_f| \cdot |S_f| = |G|$.\footnote{In fact, one only gets line segments back}
Figure 3: Stabilizer subgroups of $GL_2(\mathbb{R})$. The stabilizer subgroup is of dimension 2, as it is isomorphic to an infinite cylinder sans the real line. The circle and ellipse on the other hand have stabilizer subgroups that are one dimensional.

For finite groups, the inverse relationship of their volumes (cardinality) is direct; but it does not extend verbatim for continuous groups. Nevertheless, the following similar result holds:

$$\dim(G) - \dim(S_f) = \dim(O_f)$$  \hfill (1)

The dimension takes the role of the cardinality. In fact, under a suitable measure ($e.g.$ the Haar measure), a stabilizer of higher dimension has a larger volume, and therefore, an orbit of smaller volume. Assuming group actions - to be substantiated later - this explains the emergence of simple signal blocks as the learned features in the first layer. We provide some evidential examples by analytically computing their dimensions.

### 2.3 Simple Illustrative Examples and Emergence of Gabor-like Filters

Consider the action of the group $GL_2(\mathbb{R})$, the set of invertible 2D linear transforms, on various 2D shapes. Figure 3 illustrates three example cases by estimating the stabilizer sizes.

**An edge ($e$):** For an edge $e$ (passing through the origin), its stabilizer (in $GL_2(\mathbb{R})$) must fix the direction of the edge, i.e., it must have an eigenvector in that direction with an eigenvalue 1. The second eigenvector can be in any other direction, giving rise to a set isomorphic to $SO(2)$ \footnote{$SO(2)$ is the subgroup of all 2 dimensional rotations, which is isomorphic to the unit circle} sans the direction of the first eigenvector, which in turn is isomorphic to the unit circle punctured at one point. Note that isomorphism here refers to topological isomorphism between sets. The second eigenvalue can be anything, but considering that the entire circle already accounts for every pair $(\lambda, -\lambda)$, the effective set is isomorphic to the positive half of the real-axis only. In summary, this stabilizer subgroup is: $S_e \approx SO(2) \times \mathbb{R}^+ \setminus \mathbb{R}^+$. This space looks like a cylinder extended infinitely to one direction (Figure 3). More importantly $\dim(S_e) = 2$, and it is actually a non-compact set.

The dimension of the corresponding orbit, $\dim(O_e) = 2$, as revealed by Equation 1.

**A circle:** A circle is stabilized by all rigid rotations in the plane, as well as the reflections about all possible lines through the centre. Together, they form the orthogonal group ($O(2)$) over $\mathbb{R}^2$. From the theory of Lie groups it is known that the $\dim(S_c) = 1$.

**An ellipse:** The stabilizer of the ellipse is isomorphic to that of a circle. An ellipse can be deformed into a circle, then be transformed by any $t \in S_c$, and then transformed back. By this isomorphism $\dim(S_p) = 1$.

In summary, for a random walk inside $GL_2(\mathbb{R})$, the likelihood of hitting an edge-stabilizer is very high, compared to shapes such as a circle or ellipse, which are not only compact, but also have one dimension less. The first layer of a deep learning network, when trying to learn images, almost always discovers Gabor-filter like shapes. Essentially these are edges of different orientation inside those images. With the stabilizer view in the background, perhaps it is not all that surprising after all.
3 From Deep Learning to Group Action - The Mathematical Formulation

3.1 In Search of Dimension Reduction: The Intrinsic Space
Reasoning over symmetry groups is convenient. Now we shall show that it is possible to continue this reasoning over a deep learning network, even if it employs non-linearity. But first, we discuss the notion of an intrinsic space. Consider a $N \times N$ binary image; it’s typically represented as a vector in $\mathbb{R}^{N^2}$, or more simply in $\{0, 1\}^{N^2}$, yet, it is intrinsically a two dimensional object. Its resolution determines $N$, which may change, but that’s not intrinsic to the image itself. Similarly, a gray-scale image has three intrinsic dimensions - the first two accounts for the euclidean plane, and the third for its gray-scales. Other signals have similar intrinsic spaces.

We start with a few definitions.

**Input Space $X$:** It is the original space that the signal inhabits. Most signals of interest are compactly supported bounded real functions over a vector space $X$. The function space is denoted by $C_0(X, \mathbb{R}) = \{ \phi : X \to \mathbb{R} \}$.

We define **Intrinsic space** as: $S = X \times \mathbb{R}$. Every $\phi \in C_0(X, \mathbb{R})$ is a subset of $S$. A neural network maps a point in $C_0(X, \mathbb{R})$ to another point in $C_0(X, \mathbb{R})$; Inside $S$, this induces a deformation between subsets.

An example. A binary image, which is a function $\phi : \mathbb{R}^2 \to \{0, 1\}$ naturally corresponds to a subset $f_\phi = \{ x \in \mathbb{R}^2 \text{ such that } \phi(x) = 1 \}$. Therefore, the intrinsic space is the plane itself. This was implicit in section 2.3. Similarly, for a monochrome gray-scale image, the intrinsic space is $S = \mathbb{R}^2 \times \mathbb{R} = \mathbb{R}^3$. In both cases, the input space $X = \mathbb{R}^2$.

**Figure** A subset of the intrinsic space is called a figure, i.e., $f \subseteq S$. Note that a point $\phi \in C_0(X, \mathbb{R})$ is actually a figure over $S$.

**Moduli space of Figures** One can imagine a space that parametrizes various figures over $S$. We denote this by $F(S)$ and call the moduli space of figures. Each point in $F(S)$ corresponds to a figure over $S$. A group $G$ that acts on $S$, consistently extends over $F(S)$, i.e., for $g \in G$, $f \in S$, we get another figure $g(f) = f' \in F(S)$.

**Symmetry-group of the intrinsic space** For an intrinsic space $S$, it is the collection of all invertible mapping $S \to S$. In the event $S$ is finite, this is the permutation group. When $S$ is a vector space (such as $\mathbb{R}^2$ or $\mathbb{R}^3$), it is the set $GL(S)$, of all linear invertible transformations.

**The Sigmoid function** will refer to any standard sigmoid function, and be denoted as $\sigma()$.

3.2 The Convolution View of a Neuron

We start with the conventional view of a neuron’s operation. Let $r_x$ be the vector representation of an input $x$. For a given set of weights $w$, a neuron performs the following function (we omit the bias term here for simplicity) - $Z_w(r_x) = \sigma(\langle w, r_x \rangle)$

Equivalently, the neuron performs a convolution of the input signal $I(X) \in C_0(X, \mathbb{R})$. First, the weights transform the input signal to a coefficient in a Fourier-like space.

$$\tau_w(I) = \int_{\theta \in X} w(\theta)I(\theta)d\theta$$

And then, the sigmoid function thresholds the coefficient

$$\zeta_w(I) = \sigma(\tau_w(I))$$

A deconvolution then brings the signal back to the original domain. Let the outgoing set of weights are defined by $S(w, x)$. The two arguments, $w$ and $x$, indicate that its domain is the frequency space indexed by $w$, and range is a set of coefficients in the space indexed by $x$. For the dummy output layer of an auto-encoder, this space is essentially identical to the input layer. The deconvolution then looks like: $\hat{I}(x) = \int_{w} S(w, x)\zeta_w(I)dw$.

In short, a signal $I(X)$ is transformed into another signal $\hat{I}(X)$. Let’s denote this composite map $I \to \hat{I}$ by the symbol $\psi$, and the set of such composite maps by $\Omega$, i.e., $\Omega = \{ \psi : C_0(X, \mathbb{R}) \to C_0(X, \mathbb{R}) \}$. 
We already observed that a point in $C_0(X, \mathbb{R})$ is a figure in the intrinsic space $S = X \times \mathbb{R}$. Hence any map $\psi \in \Omega$ naturally induces the following map from the space $F(S)$ on to itself: $\psi(f) = f' \subseteq S$.

Let $\Gamma$ be the space of all deformations of this intrinsic space $S$. Then there is a map $U$ that approximates the automorphism $\psi$. But that’s not guaranteed for randomly selected $\psi, f$ and $g$.

If we can naturally extend the map to all of $S$, then we can translate the questions asked over $\Omega$ to questions over $\Gamma$. The intrinsic space being of low dimension, we can hope for easier analyses. In particular, we can examine the stabilizer subgroups over $\Gamma$ that are more tractable.

So, we now examine if a map between figures of $S$ can be effectively captured by group actions over $S$. It suffices to consider the action of $\Gamma$, one input at a time. This eliminates the conflicts arising from different inputs. Yet, $\psi(f)$ - i.e. the action of $\psi$ over a specific $f \in C_0(X, \mathbb{R})$ - is still incomplete with respect to being an automorphism of $S = X \times \mathbb{R}$ (being only defined over $f$). Can we then extend this action to the entire set $S$ consistently? It turns out - yes.

**Theorem 3.1.** Let $\psi$ be a neural network, and $f \in C_0(X, \mathbb{R})$ an input to this network. The action $\psi(f)$ can be consistly extended to an automorphism $\gamma(\psi, f) : S \rightarrow S$, i.e. $\gamma(\psi, f) \in \Gamma$.

The proof is given in the Appendix. A couple of notes. First, the input $f$ appears as a parameter for the automorphism (in addition to $\psi$), as $\psi$ alone cannot define a consistent self-map over $S$. Second, this correspondence is not necessarily unique. There’s a family of automorphisms that can correspond to the action $\psi(f)$, but we’re interested in the existence of at least one of them.

## 4 Group Actions underlying Deep Networks

### 4.1 Shadow Stabilizer-subgroups

We now search for group actions that approximate the automorphisms we established. Since such a group action is not exactly a neural network, yet can be closely mimics the latter, we will refer to these groups as Shadow groups. The existence of an underlying group action asserts that corresponding to a set of stabilizers for a figure $f$ in $\Omega$, there is a stabilizer subgroup, and lets us argue that the learnt figures actually correspond to minimal orbits, with high probability - and thus the simplest possible. The following theorem asserts this fact.

**Theorem 4.1.** Let $\psi \in \Omega$ be a neural network working over a figure $f \subseteq S$, and the corresponding self-map $\gamma(\psi, f) : S \rightarrow S$, then in fact $\gamma(\psi, f) \in \text{Homeo}(S)$, the homeomorphism group of $S$.

The above theorem (see Appendix, for a proof) shows that although neural networks may not exactly define a group, they can be approximated well by a set of group actions - that of the homeomorphism group of the intrinsic space. One can go further, and inspect the action of $\psi$ locally - i.e. in the small vicinity of each point. Our next result shows that locally, they can be approximated further by elements of $GL(S)$, which is a much simpler group to study; in fact our results from section 2.3 were really in light of the action of this group for the 2 dimensional case.

**Local resemblance to $GL(S)$**

**Theorem 4.2.** For any $\gamma(\psi, f) \in \text{Homeo}(S)$, there is a local approximation $g(\psi, f) \in GL(S)$ that approximates $\gamma(\psi, f)$. In particular, if $\gamma(\psi, f)$ is a stabilizer for $f$, so is $g(\psi, f)$.

The above theorem (proof in Appendix) guarantees an underlying group action. But what if some large stabilizers in $\Omega$ are mapped to very small stabilizers in $GL(S)$, and vice versa? The next theorem (proof in Appendix) asserts that there is a bottom-up correspondence as well - every group symmetry over the intrinsic space has a counter-part over the set of mapping from $C_0(S, \mathbb{R})$ onto itself.

**Theorem 4.3.** Let $S$ be an intrinsic space, and $f \subseteq S$. Let $g \in GL(S)$ be a group element that stabilizes $f$. Then there is a map $U : GL(S) \rightarrow \Omega$, such that the corresponding element $U(g) = \tau \in \Omega$ that stabilizes $f$. Moreover, for $g_1, g_2 \in GL(S)$, $U(g_1) = U(g_2) \Rightarrow g_1 = g_2$. 


Summary Argument: We showed via Theorem 4.1 that any neural network action has a counterpart in the group of homeomorphisms over the intrinsic space. The presence of this shadow group lets one carry over the orbit/stabilizer principle discussed in section 2.4 to the actual neural network transforms. Which asserts that the simple features are the ones to be learned first. To analyse how these features look like, we examine them locally with the lens of $GL(S)$, an even simpler group. The Theorems 4.2 and 4.3 collectively establish this. Theorem 4.2 shows that for every neural network element there’s a nearby group element. For a large stabilizer set then, the corresponding stabilizer subgroup ought to be large, else it will be impossible to find a nearby group element everywhere. Also note that this doesn’t require a strict one-to-one correspondence; existence of some group element is enough to assert this. To see how Theorem 4.3 pushes the argument in reverse, imagine a sufficiently discrete version of $GL(S)$. In this coarse-grained picture, any small $\varepsilon$-neighbourhood of an element $g$ can be represented by $g$ itself (similar to how integrals are built up with small regions taking on uniform values). There is a corresponding neural network $U(g)$, and furthermore, for another element $f$ which is outside this neighbourhood (and thus not equal to $g$) $U(f)$ is another different network. This implies that a large volume cannot be mapped to a small volume in general - and hence true for stabilizer volumes as well.

5 Deeper Layers and Moduli-space

Now we discuss how the orbit/stabilizer interplay extends to multiple layers. At its root, lies the principle of layer-wise pre-training for the identity function. In particular, we show that this succinct step, as an algorithmic principle, is quite powerful. The principle stays the same across layers; hence every layer only learns the simplest possible objects from its own input space. Yet, a simple object at a deeper layer can represent a complex object at the input space. To understand this precisely, we first examine the critical role of the sigmoid function.

5.1 The Role of the Sigmoid Function

Let’s revisit the transfer functions from section 3.2 (convolution view of a neuron):

$$\tau_w(I) = \int_{\theta \in X} w(\theta) f(\theta) d\theta$$

$$\zeta_w(I) = \sigma(\tau_w(I))$$

Let $F_R(A)$ denote the space of real functions on any space $A$. Now, imagine a (hypothetical) space of infinite number of neurons indexed by the weight-functions $w$. Note that $w$ can also be viewed as an element of $C_0(X,R)$. Plus $\tau_w(I) \in R$. So the family $\tau = \{\tau_w\}$ induces a mapping from $C_0(X,R)$ to real functions over $C_0(X,R)$, i.e.

$$\tau: C_0(X,R) \rightarrow F_R(C_0(X,R))$$

Now, the sigmoid can be thought of composed of two steps. $\sigma_1$ turning its input to number between zero and one. And then, for most cases, an automatic thresholding happens (due to discretized representation in computer systems) creating a binarization to 0 or 1. We denote this final step by $\sigma_2$, which reduces to the output to an element of the figure space $F(C_0(X,R))$. These three steps, applying $\tau$, and then $\sigma = \sigma_1 \sigma_2$ can be viewed as

$$C_0(X,R) \xrightarrow{\tau} F_R(C_0(X,R)) \xrightarrow{\sigma_1} F_{[0,1]}(C_0(X,R)) \xrightarrow{\sigma_2} F(C_0(X,R))$$

This construction is recursive over layers, so one can envision a neural net building representations of moduli spaces over moduli spaces, hierarchically, one after another. For example, at the end of layer-1 learning, each layer-1 neuron actually learns a figure over the intrinsic space $X \times R$ (ref. equation 3). And the collective output of this layer can be thought of as a figure over $C_0(X,R)$ (ref. equation 5). These second order figures then become inputs to layer-2 neurons, which collectively end up learning a minimal-orbit figure over the space of these second-order figures, and so on.

What does all this mean physically? We now show that it is the power to capture figures over moduli spaces, that gives us the ability to capture representation of features of increasing complexity.

5.2 Learning Higher Order Representations

Let’s recap. A layer of neurons collectively learn a set of figures over its own intrinsic space. This is true for any depth, and the learnt figures correspond to the largest stabilizer subgroups. In other
Every point over the space \( (M_i) \) learnt by the \( i \)-th layer corresponds to a figure over the space \( (M_{i-1}) \) learnt by the previous layer. Learning a simple shape over \( M_i \) therefore, corresponds to learning a more complex structure over \( M_{i-1} \).

(a) Moduli spaces at subsequent layers

(b) Moduli space of line segments

Figure 4: A deep network constructs higher order moduli spaces. It learns figures having increasingly smaller symmetry groups; which corresponds to increasing complexity.

words, these figures enjoy highest possible symmetry. The set of simple examples in section 2.3 revealed that for \( S = \mathbb{R}^2 \), the emerging figures are the edges.

For a layer at an arbitrary depth, and working over a very different space, the corresponding figures are clearly not physical edges. Nevertheless, we’ll refer to them as **Generalized Edges**.

Figure 4(a) captures a generic multi-layer setting. Let’s consider the neuron-layer at the \( i \)-th level, and let’s denote the embedding space of the features that it learns as \( M_i \) - i.e., this layer learns figures over the space \( M_i \). One such figure, now referred to as a **generalized edge**, is schematically shown by the geodesic segment \( P_1P_2 \) in the picture. Thinking down recursively, this space \( M_i \) is clearly a moduli-space of figures over the space \( M_{i-1} \), so each point in \( M_i \) corresponds to a generalized edge over \( M_{i-1} \). The whole segment \( P_1P_2 \) therefore corresponds to a collection of generalized edges over \( M_{i-1} \); such a collection in general can clearly have lesser symmetry than a generalized edge itself. In other words, a simple object \( P_1P_2 \) over \( M_i \) actually corresponds to a much more complex object over \( M_{i-1} \).

These moduli-spaces are determined by the underlying input-space, and the nature of training. So, doing precise calculations over them, such as defining the space of all automorphisms, or computing volumes over corresponding stabilizer sets, may be very difficult, and we are unaware of any work in this context. However, the following simple example illustrates the idea quite clearly.

5.2.1 Examples of Higher Order Representation

Consider again the intrinsic space \( \mathbb{R}^2 \). An edge on this plane is a line segment - \( \{(x_1, y_1), (x_2, y_2)\} \). The moduli-space of all such edges therefore is the entire 4-dimensional real Euclidean space sans the origin - \( \mathbb{R}^4 \setminus \{0\} \). Figure 4(b) captures this. Each point in this space \( \mathbb{R}^4 \setminus \{0\} \) corresponds to an edge over the plane \( \mathbb{R}^2 \). A generalized-edge over \( \mathbb{R}^4 \setminus \{0\} \), which is a standard line-segment in a 4-dimensional euclidean space, then corresponds to a collection of edges over the real plane. Depending on the orientation of this **generalized edge** upstairs, one can obtain many different shapes downstairs.
The Trapezoid The figure in the leftmost column of figure 4(b) shows a schematic trapezoid. This is obtained from two points $P_1, P_2 \in \mathbb{R}^4$ that correspond to two non-intersecting line-segments in $\mathbb{R}^2$.

A Triangle The middle column shows an example where the starting point of the two line segments are the same - the connecting generalized edge between the two points in $\mathbb{R}^4$ is a line parallel to two coordinate axes (and perpendicular to the other two). A middle point $P_m$ maps to a line-segment that’s intermediate between the starting lines (see the coordinate values in the figure). Stabilizing $P_1P_2$ upstairs effectively stabilizes the triangular area over the plane.

A Butterfly The third column shows yet another pattern, drawn by two edges that intersect with each other. Plotting the intermediate points of the generalized edge over the plane as lines, a butterfly-like area is swept out. Again, stabilizing the generalized edge $P_1P_2$ effectively stabilizes the butterfly over the plane, that would otherwise take a long time to be found and stabilized by the first layer.

More general constructions We can also imagine even more generic shapes that can be learnt this way. Consider a polygon in $\mathbb{R}^2$. This can be thought of as a collection of triangles (via triangulation), and each composing triangle would correspond to a generalized edge in layer-2. As a result, the whole polygon can be effectively learnt by a network with two hidden layers.

In a nutshell - the mechanism of finding out maximal stabilizers over the moduli-space of figures works uniformly across layers. At each layer, the figures with the largest stabilizers are learnt as the candidate features. These figures correspond to more complex shapes over the space learnt by the earlier layers. By adding deeper layers, it then becomes possible to make a network learn increasingly complex objects over its original input-space.

6 RELATED WORK
This starting influence for this paper were the key steps described by Hinton & Salakhutdinov (2006), where the authors first introduced the idea of layer-by-layer pre-training through autoencoders. The same principles, but over Restricted Boltzmann machines (RBM), were applied for image recognition in a later work (see Salakhutdinov & Hinton (2009)). Lee et al. (2009) showed, perhaps for the first time, how a deep network builds up increasingly complex representations across its depth. Since then, several variants of autoencoders, as well as RBMs have taken the center stage of the deep learning research. Bengio et al. (in preparation) and Bengio (2013) provide a comprehensive coverage on almost every aspect of DL techniques. Although we chose to analyse auto-encoders in this paper, we believe that the same principle should extend to RBMs as well, especially in the context of a recent work by Kamyshanska & Memisevic (2014), that reveals seemingly an equivalence between autoencoders and RBMs. They define an energy function for autoencoders that corresponds to the free energy of an RBM. They also point out how the energy function imposes a regularization in the space. The hypothesis about an implicit regularization mechanism was also made earlier by Erhan et al. (2010). Although we haven’t investigated any direct connection between symmetry-stabilization and regularization, there are evidences that they may be connected in subtle ways (for example, see Shah & Chandrasekaran (2012)).

Recently Anselmi et al. (2013) proposed a theory for visual-cortex that’s heavily inspired by the principles of group actions: although there is do direct connection with layer-wise pre-training in that context, Bouvrie et al. (2009) studied invariance properties of layered network in a group-theoretic framework and showed how to derive precise conditions that must be met in order to achieve invariance - this is very close to our work in terms of the machineries used, but not about how a unsupervised learning algorithm learns representations. Mehta & Schwab (2014) recently showed an intriguing connection between Renormalization group flow and deep-learning. They constructed an explicit mapping from a renormalization group over a block-spin Ising model (as proposed by Kadanoff et al. (1976)), to a DL architecture. On the face of it, this result is complementary to ours, albeit in a slightly different settings. Renormalization is a process of coarse-graining a system by first throwing away small details from its model, and then examining the new system under the simplified model (see Cardy (1996)). In that sense the orbit-stabilizer principle is a re-normalizable theory - it allows for the exact same coarse-graining operation at every layer - namely, keeping only minimal orbit shapes and then passing them as new parameters for the next layer - and the theory remains unchanged at every scale.

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This subject is widely studied in many areas of physics, such as quantum field theory, statistical mechanics and so on.
While generally good at many recognition tasks, DL networks have been shown to fail in surprising ways. Szegedy et al. (2013) showed that the mapping that a DL network learns could have sudden discontinuities. For example, sometimes it can misclassify an image that is derived by applying only a tiny perturbation to an image that it actually classifies correctly. Even the reverse was also reported (see Nguyen et al. (2014)) - here, a DL network was tested on grossly perturbed versions of already learnt images - perturbed to the extent that humans cannot recognize them for the original any more - and they were still classified as their originals. Szegedy et al. (2013) made a related observation: random linear combination of high-level units in a deep network also serve as good representations. They concluded - it is the space, rather than the individual units, that contain the semantic information in the high layers of a DL network. We don’t see any specific conflicts of any of these observations with the orbit-stabilizer principle, and view the possible explanations of these phenomena in the clear scope a future work.

7 Conclusions and Future Work
In a nutshell, this paper builds a theoretical framework for unsupervised DL that is primarily inspired by the key principle of finding a generative model of the input samples first. The framework is based on orbit-stabilizer interplay in group actions. We assumed layer-wise pre-training, since it is conceptually clean, yet, in theory, even if many layers were being learnt simultaneously (in an unsupervised way, and still based on reconstructing the input signal) the orbit-stabilizer phenomena should still apply. We also analysed how higher order representations emerge as the networks get deeper.

Today, DL expanded well beyond the principles P1 and P2 (ref. introduction). Several factors such as the size of the datasets, increased computational power, improved optimization methods, domain specific tuning, all contribute to its success. Clearly, this theory is not all-encompassing. In particular, when large enough labeled datasets are available, training them in fully supervised mode yielded great results. The orbit-stabilizer principle cannot be readily extended to a supervised case; in the absence of a self-map (input reconstruction) it is hard to establish a underlying group action. But we believe and hope that a principled study of how representations form will eventually put the two under a single theory.

8 Appendix
This section involves elementary concepts from different areas of mathematics. For functional analysis see Bollobás. For elementary ideas on groups, Lie groups, and representation theory, we recommend Artin, Fulton & Harris. The relevant ideas in topology can be looked up in Munkres or Hatcher.

Lemma 8.1. The group of invertible square matrices are dense in the set of square matrices.

Proof - This is a well known result, but we provide a proof for the sake of completeness. Let \( A \) be \( n \times n \) matrix, that is square, and not necessarily invertible. We show that there is a non-singular matrix nearby. To see this, consider an arbitrary non-singular matrix \( B \), i.e. \( \det(B) \neq 0 \), and consider the following polynomial parametrized by a real number \( t \),

\[
    r(t) = \det((1-t)A + tB)
\]

Since \( r \) is finite degree polynomial, and it is certainly not identically zero, as \( r(1) = \det(B) \neq 0 \), it can only vanish at a finite number of points. So, even if \( p(0) = 0 \), there must be a \( t' \) arbitrarily close to 0 such that \( r(t') \neq 0 \). So the corresponding new matrix \( M = (1-t')A + t'B \) is arbitrarily close to \( A \), yet non-singular, as \( \det(M) = r(t') \) does not identically vanish. □

Lemma 8.2. The action of a neural network can be approximated by a network that’s completely invertible.

Proof - A three layer neural network can be represented as \( W_2 \sigma W_1 \), where \( \sigma \) is the sigmoid function, and \( W_1 \) and \( W_2 \) are linear transforms. \( \sigma \) is already invertible, so we only need to show existence of invertible approximations of the linear components.

Let \( W_1 \) be a \( \mathbb{R}^{m \times n} \) matrix. Then \( W_2 \) is a matrix of dimension \( \mathbb{R}^{n \times m} \). Consider first the case where \( m > n \). The map \( W_1 \) however can be lifted to a \( \mathbb{R}^{m \times m} \) transform, with additional \( (m-n) \) columns set to zeros. Let’s call this map \( W_1' \). But then, by Lemma 8.1, it is possible to obtain a square invertible
transform $W_1'$ that serves as a good approximation for $W_1'$, and hence for $W_1$. One can obtain a similar invertible approximation $W_2$ of $W_2$ in the same way, and thus the composite map $W_2 \sigma W_1'$ is the required approximation that’s completely invertible. The other case where $m < n$ is easier; it follows from the same logic without the need for adding columns. □

**Lemma 8.3.** Let the action of a neural network $\psi$ over a figure $f$ be $\psi(f) = f'$ where $f, f' \subseteq S$, the intrinsic space. The action then induces a continuous mapping of the sets $f \xrightarrow{\psi} f'$.

**Proof** Let’s consider an infinitely small subset $\varepsilon_a \subset f$. Let $f_a = f \setminus \varepsilon_a$. The map $\psi(f)$ can be described as $\psi(f) = \psi(\{f_a \cup \varepsilon_a\}) = f'$. Now let’s imagine an infinitesimal deformation of the figure $f$ - by continuously deforming $\varepsilon_a$ to a new set $\varepsilon_b$. Since the change is infinitesimal, and $\psi$ is continuous, the new output, let’s call it $f''$, differs from $f'$ only infinitesimally. That means there’s a subset $\varepsilon_b' \subset f''$ that got deformed into a new subset $\varepsilon_b'' \subset f''$ to give rise to $f''$. This must be true as Lemma 8.2 allows us to assume an invertible mapping $\psi$ - so that a change in the input is detectable at the output. Thus $\psi$ induces a mapping between the infinitesimal sets $\varepsilon_a \rightarrow \varepsilon_a'$ and $\varepsilon_a' \rightarrow \varepsilon_a''$. Now, we can split an input figure into infinitesimal parts and thereby obtain a set-correspondence between the input and output. □

**Proof of Theorem 3.1**

We assume that a neural network implements a differentiable map $\psi$ between its input and output. That means the set $\Omega \subset \text{Diff}(C_0(X, \mathbb{R}))$ - i.e. the set of diffeomorphisms of $C_0(X, \mathbb{R})$. This set admits a smooth structure (see [Hajiyev 1997]). Moreover, being parametrized by the neural-network parameters, the set is connected as well, so it makes sense to think of a curve over this space. Let’s denote the identity transform in this space by $I$. Consider a curve $\eta(t) : [0, 1] \rightarrow \text{Diff}(C_0(X, \mathbb{R}))$, such that $\eta(0) = I$ and $\eta(1) = \psi$. By Lemma 8.3, $\eta(t)$ defines a continuous map between $f$ and $\eta(t)(f)$. In other words, $\eta(t)$ induces a partial homotopy on $S = X \times \mathbb{R}$. Mathematically, $\eta(0) = 1(f) = f$ and $\eta(1) = \psi(f) = f'$. In other words, the curve $\eta$ induces a continuous family of deformations of $f$ to $f'$. Refer to figure 5 for a visual representation of this correspondence. In the language of topology such a family of deformations is known as a homotopy. Let us denote this homotopy by $\Phi_t : f \rightarrow f'$. Now, it is easy to check (and we state without proof) that for a $f \in C_0(X, \mathbb{R})$, the pair $(X \times \mathbb{R}, f)$ satisfies Homotopy Extension property. In addition, there exists an initial mapping $\Phi_0 : S \rightarrow S$ such that $\Phi_0(f) = f_0$. This is nothing but the identity mapping. The well known Homotopy Extension Theorem (see [Hatcher]) then asserts that it is possible to lift the
same homotopy defined by $\eta$ from $f$ to the entire set $X \times \mathbb{R}$. In other words, there exists a map $\Phi_t : X \times \mathbb{R} \rightarrow X \times \mathbb{R}$, such that the restriction $\Phi_t|_f = \phi_t$ for all $t$. Clearly then, $\Phi_{t=1}$ is our intended automorphism on $S = X \times \mathbb{R}$, that agrees with the action $\psi(f)$. We denote this automorphism by $\eta \psi, f)$, and this is an element of $\Gamma$, the set of all automorphisms of $S$. □

**Proof of Theorem 4.1**

Note that lemma 8.2 already guarantees invertible mapping between $f$ and $f' = \psi(f)$. Which means in the context of theorem 3.1 there is an inverse homotopy, that can be extended in the opposite direction. This means $\eta \psi, f)$ is actually a homeomorphism, i.e. a continuous invertible mapping from $S$ to itself. The set Homeo($S$) is a group by definition. □

**Proof of Theorem 4.2**

Let $\psi(f)$ be the neural network action under consideration. By Theorem 3.1, there is a corresponding homomorphism $\eta \psi, f) \in \Gamma(S)$. This is an operator acting $S \rightarrow S$, and although not necessarily differentiable everywhere, the operator (by its construction) is differentiable on $f$. This means it can be locally (in small vicinity of points near $f$) approximated by its Fréchet derivative (analogue of derivatives over Banach space) near $f$; however, in finite dimension this is nothing but the Jacobian of the transformation, which can be represented by a finite dimensional matrix. So we have a linear approximation of this deformation $\eta \psi, f) = J(\eta \psi, f) = \hat{\gamma}$. But then since this is a homeomorphism, by the inverse function theorem, $\hat{\gamma}^{-1}$ exists. Therefore $\hat{\gamma}$ really represents an element $g \in GL(S)$. □

**Proof of Theorem 4.3**

Let $S$ be the intrinsic space over an input vector space $X$, i.e. $S = X \times \mathbb{R}$, and $g \in GL(S)$ a stabilizer of a figure $f \in C_0(X, \mathbb{R})$. Define a function $\chi \in F(S) \rightarrow F(S)$

$$\chi(h) = \bigcup_{s \in h} g(s) = h'$$

It is easy to see that $\chi$ so defined stabilizes $f$. However there is the possibility that $h' \notin C_0(X, \mathbb{R})$; although $h'$ is a figure in $S$, it may not be a well-defined function over $X$. To avoid such a pathological case, we make one more assumption - that the set of functions under considerations are all bounded. That means - there exists an upper bound $B$, such that every $f \in C_0(X, \mathbb{R})$ under consideration is bounded in sup norm - $|f|_{sup} < B^6$. Define an auxiliary function $\zeta : X \rightarrow \mathbb{R}$ as follows.

$$\zeta(x) = B \quad \forall x \in sup(f)$$

$$\zeta(x) = 0 \quad \text{otherwise}$$

Now, one can always construct a continuous approximation of $\zeta$ - let $\zeta \in C_0(X, \mathbb{R})$ be such an approximation. We are now ready to define the neural network $U(g) = \tau$. Essentially it is the collection of mappings between figures (in $C_0(X, \mathbb{R})$) defined as follows:

$$\tau(f)(h) = \chi(f)(h) \quad \text{whenever} \quad \chi(f)(h) \in C_0(X, \mathbb{R})$$

$$\tau(f)(h) = \zeta \quad \text{otherwise}$$

To see why the second part of the theorem holds, observe that since $U(g_1)$ and $U(g_2)$ essentially reflect group actions over the intrinsic space, their action is really defined point-wise. In other words, if $p, q \subseteq S$ are figures, and $r = p \cap q$, then the following restriction map holds.

$$U(g_1)(p)|_r = U(g_1)(q)|_r$$

Now, further observe that given a group element $g_1$, and a point $x \in S$, one can always construct a family of figures containing $x$ all of which are valid functions in $C_0(X, \mathbb{R})$, and that under the action

^6 This is not a restrictive assumption, in fact it is quite common to assume that all signals have finite energy, which implies that the signals are bounded in sup norm.
of $g_1$ they remain valid functions in $C_0(X, \mathbb{R})$. Let $f_1, f_2$ be two such figures such that $f_1 \cap f_2 = x$. Now consider $x' = U(g_1)(f_1) \cap U(g_1)(f_2)$. However, the collection of mapping $\{x \rightarrow x'\}$ uniquely defines the action of $g_1$. So, if $g_2$ is another group element for which $U(g_2)$ agrees with $U(g_1)$ on every figure, that agreement can be translated to point-wise equality over $S$, asserting $g_1 = g_2$. □

8.1 A Note on the Thresholding Function

In section 5.1 we primarily based our discussion around the sigmoid function that can be thought of as a mechanism for binarization, and thereby produces figures over a moduli space. This moduli space then becomes an intrinsic space for the next layer. However, the theory extends to other types of thresholding functions as well, only the intrinsic spaces would vary based on the nature of thresholding. For example, using a linear rectification unit, one would get a mapping into the space $\mathcal{F}_{[0,\infty]}(C_0(X,\mathbb{R}))$. The elements of this set are functions over $C_0(X,\mathbb{R})$ taking values in the range $[0,\infty]$. So, the new intrinsic space for the next level will then be $S = [0,\infty] \times C_0(X,\mathbb{R})$, and the output can be thought of as a figure in this intrinsic space allowing the rest of the theory to carry over.

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