Measuring the "size" of hypothesis spaces over $\mathbb{R}$ from the perspective of No Free Lunch

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Motivating example: symmetric functions

We want to learn, ie, use gradient descent of a neural network to approximate, a symmetric function $y = \hat{f}(\vec{x})$ satisfying the condition $\hat{f}(x_1, ...x_n) = \hat{f}(\sigma \cdot \{x_1, ...x_n\})$ where $\sigma \in \mathfrak{S}_n$ is a permutation. The **input space** is $X = \mathbb{R}^n = n$-dimensional hypercube:

(1)

Permutation symmetry implies that only one **corner** of the hypercube need be considered, this is the **fundamental domain** of the symmetry group. The **volume** of this domain over the entire hypercube shrinks exponentially as n grows, so it appears that this symmetry is very significant for efficiency consideration. We want to quantify this notion of efficiency.

As a more specific example, consider only **Boolean** functions of n variables, so the inputs are the 2^n **vertices** of the hypercube. It is well-known that the number of n-ary Boolean functions is 2^{2^n}. It can be seen this way: the 2^n vertices of the hypercube forms the entries of the **truth table**, ie, all permutations of $\top$ and $\bot$ over input variables. All we need is to assign output truth-values to these table entries; each such assignment defines a Boolean function. Thus $2^n \to \{\top, \bot\}$.

The number of **symmetric** Boolean functions $\hat{f}(x_1, ...x_n)$ does not depend on the order of its arguments. So it only depends on the **number** of 1's in the input. There could be 0, 1, ... up to n 1's in the input, which correspond to vertices of a **corner** of the n-dimension hypercube. We only need to map this corner to $\{\top, \bot\}$. The number of such functions is 2^{n+1}.

The ratio of all Boolean functions : symmetric Boolean functions $= 2^{2^n} : 2^{n+1} = 2^{2^n - (n+1)}$ of which the linear term is insignificant. This is a huge number, and this example is illustrative of the general case of functions in $\mathbb{R}^n$ because learning in high dimensions is **dominated** by the dimensions rather than the "ups and downs" along a particular direction.

One last question is that $2n + 1$ seems to be a too-small number of distinct propositions for the purpose of AGI (as each vertex represents a proposition). To be able to represent more propositions, we can increase the number of points along a single dimension, so the functions are not binary-valued but k-ary. The limit of this process is the continuum, ie $\mathbb{R}^n$ or $[0,1]^n$, the usual setting of neural networks. As we increase k, the number of distinct points in the lower corner is given by $_{k+n-1}C_n$, ie, the number of ways to choose n objects out of k objects, with replacement, and with order unimportant. Note that this number grows exponentially as k increases, so it provides many distinct points to represent propositions for AGI.

Finding the right space setting

We want to compare the **hypothesis spaces** A and B:

- A = unconstrained, fully-connected neural network with L layers and N total weights. The parameter space $A = \Theta_A = \mathbb{R}^N$.

- B = symmetric neural network with a special structure but nonetheless its parameter space is also of the form $B = \Theta_B = \mathbb{R}^M$.

My first idea is to embed the space B into space A. This will lead to "unwieldy" elements of B trying to approximate A, for example, consider if A's activation function is sigmoid but B's activation function is RELU.

(2)
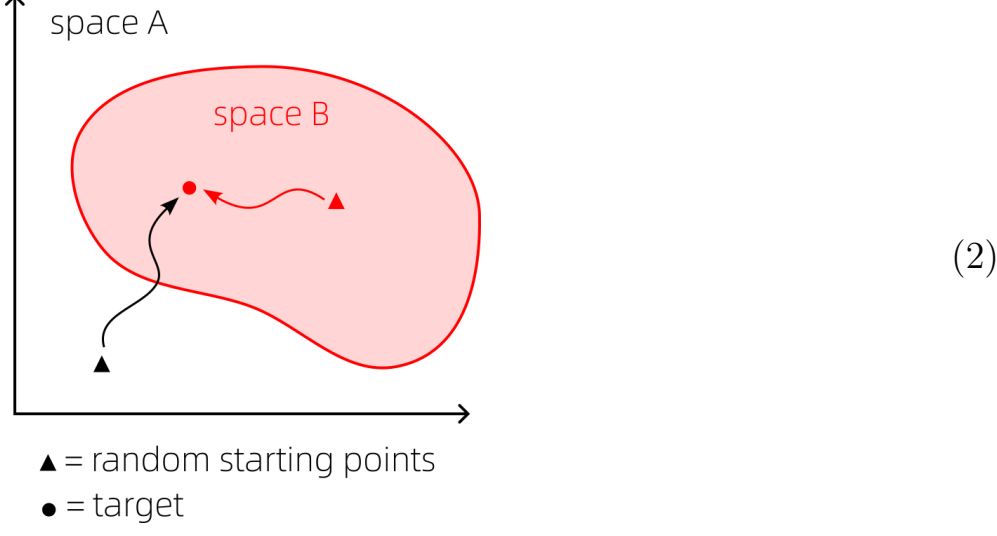
But the general idea is: If solutions are only found in space B, then limiting our search within B will lead to faster convergence as there is no need to waste time "wandering" in space A.

A better idea which is much more convenient is to consider A and B as both embedded in an ambient **function space** $\mathcal{H}$ that is "fine" enough to contain all points of A and B:

Embeddings:
$\Theta_A \hookrightarrow \mathcal{H}$
$\Theta_B \hookrightarrow \mathcal{H}$
(3)

ambient function space $\mathcal{H}$
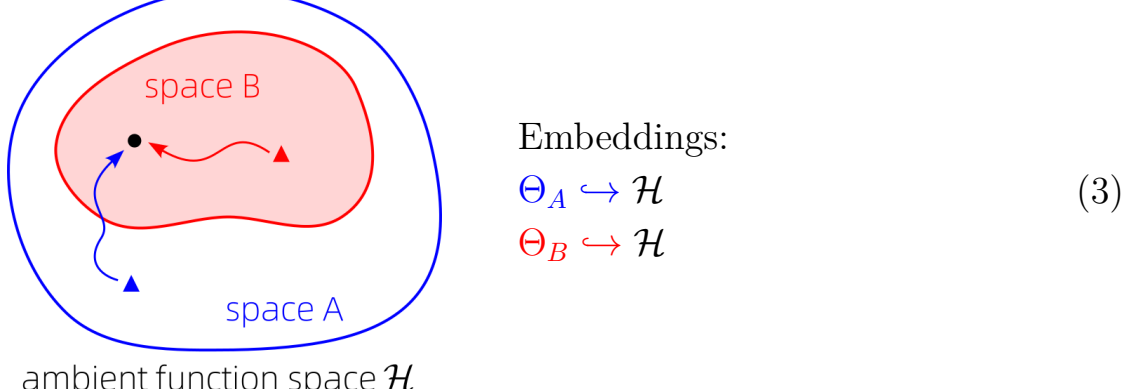
Measure roughness of landscape?

My second idea is to measure the "roughness" of the landscapes A and B in the function space $\mathcal{H}$. The objective function is usually of the form

$$\text{loss} = \sum_i d(f(x_i; \Theta), y_i) + \text{Reg}(f)$$
(4)

where d is some distance metric and Reg is a regularization function.

The models in A or B live in the parameter spaces Θ_A or Θ_B and both are embedded into the space $\mathcal{H}$. However the **paths** of gradient descent in A or B could still be different, so we have to be cautious about that.

In low-dimension space, we imagine being "trapped" in some kind of pit, so we may want to measure the roughness of the landscape by "undulations" of gradients. But our next consideration suggests that this may not be a very effective measurement...

Gradient descent in high-dimension space

It may be helpful to visualize gradient descent in high-dimension space with Fig.(5). Imagine the hypercube as having millions of vertices (as the number of weights). The "landscape" is a surface sitting "over" the hypercube but we visualize it downwards.

It is very "easy" for gradient descent to find a way "down" because there are so many dimensions to choose from.

Also, a "local minimum" is very rare as it requires millions of gradients to be pointing "up" at the same spot. In a model with a massive number of weights (as in the case of current LLMs), for all practical purposes, a local minimum is just as good as an acceptable solution. In this sense, *the phenomenon of "getting stuck in local minima" disappears.*

The "symmetric" parameter space

The following figure may help visualize the parameter space of our **symmetric** motivating example (but not for the AGI problem).

In our example, $\Theta_A = (u, v)$ but Θ_B is just the diagonal space $\langle u = v \rangle$. The case with 3 parameters, of which 2 are equal, is shown on the right:

hypercube

gradient descent

(5)

(6)
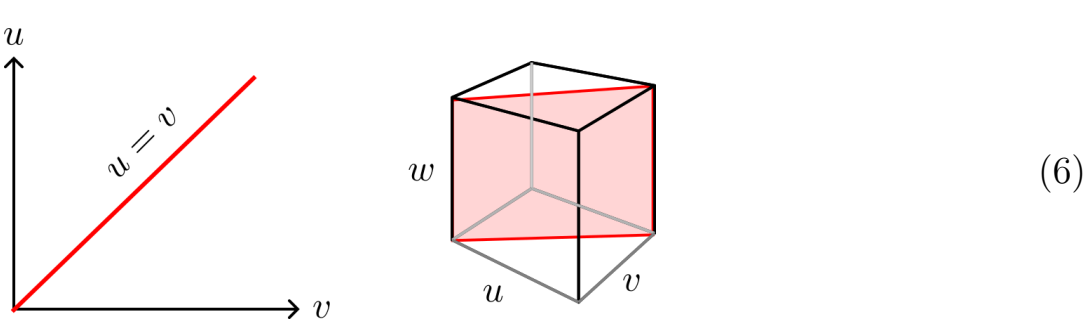
In general, multiple dimensions can collapse to one, when the weights are shared (equal).

Distribution of solution "attractors"

I find the most helpful way to visualize the AGI landscape is to imagine solution **attractors** to be more *densely* populated in the more-structured space B.

The following is a diagram I made up using a Python script and Matplotlib with randomly generated plots. One can imagine "attractors" for **gradient descent** that are distributed over the hypothesis space that lead to solutions (AGIs). I made the distribution of attractors in space B **denser** than in space A. So if an algorithm randomly starts to search, it will have a better chance of success to start within space B. The "distances" traveled by gradient descent are also different for A and B because their parameter spaces are different.

(7)
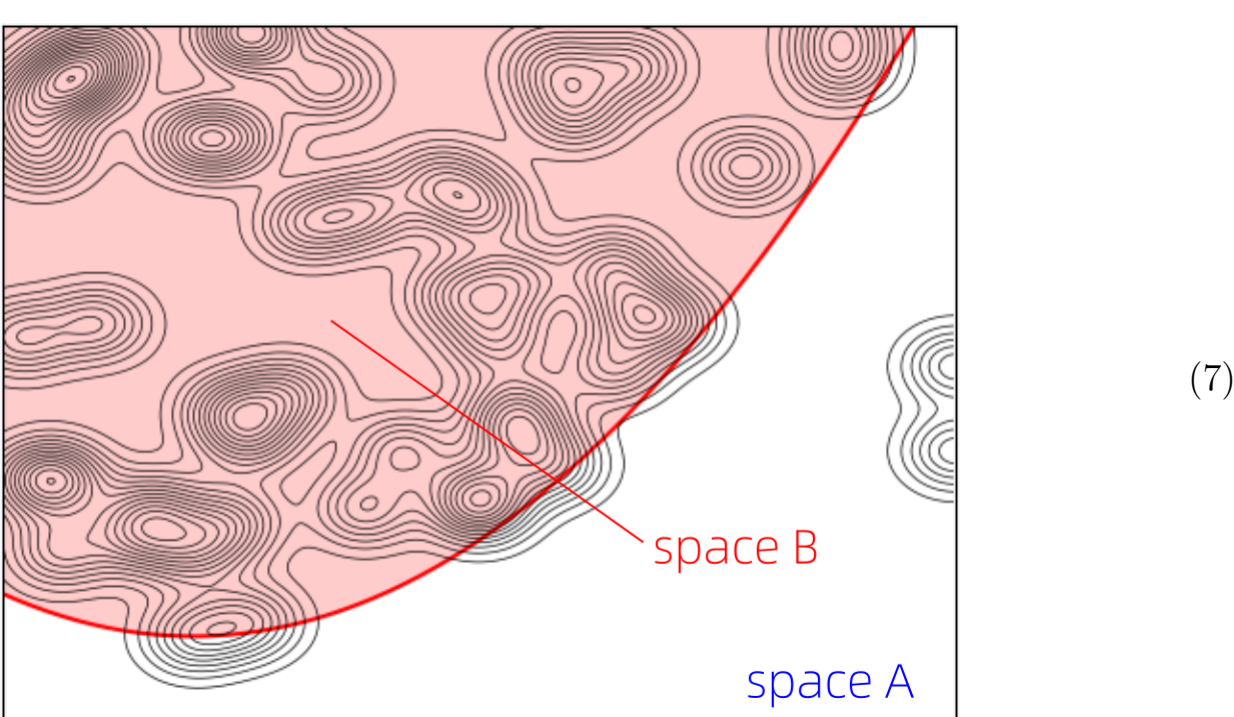
Perhaps the most crucial thing we want to prove, or at least find indirect evidence for, is whether solution attractors are *sparser* in space A than in space B. This is obviously a **problem-specific** question. In some cases, such as the learning of symmetric functions, we know *a priori* that solutions *exclusively* lie in space B. But the issue is very hard to analyze for AGI.

Fibration as symmetry

Plan of attack: The fibration is a topological structure. Remember Felix Klein's Erlangen programme in which **geometric structures** are equated with their respective **isometry groups of invariance**. Similarly, we can express a fibration (a topological structure) as an invariance under some appropriate transformation group G. Next, we define a class of functions (supposed to be the neural networks we wish to build) which are invariant under the same group G. By the logic of the Erlangen programme, this is equivalent to saying that these functions are defined over the topological structure of fibrations, which is our goal.

Definition of a fiber bundle

A quadruple $\xi = (X, p, B, F)$ is a **fiber bundle** if:

(i) X is a topological space called the **total space**

(ii) B is a topological space called the **base space**

(iii) F is a topological space called the **fiber** of ξ

(iv) $p : X \to B$ is a continuous surjective map called the **fiber bundle projection**

(v) the inverse image $p^{-1}(b) = F_b$ is **homeomorphic** to F, $\forall b \in B$

(vi) B has an open covering $\{U_i\}_{i \in I}$ such that $\forall i$, $p^{-1}(U_i)$ is **homeomorphic** to $U_i \times F$, with the projection p yielding the first factor U_i.

We may use the symbol $\cong$ to denote homeomorphism, eg: $p^{-1}(b) \cong F$.

Definition of a bundle morphism

If $\begin{smallmatrix} X \\ \downarrow p \\ B \end{smallmatrix}$ and $\begin{smallmatrix} Y \\ \downarrow q \\ A \end{smallmatrix}$ are fiber bundles, then the double map $\sigma = (c, \gamma)$ is a **bundle morphism** if the following diagram commutes:

$$
\begin{array}{ccc}
X & \xrightarrow{\ c\ } & Y \\
\downarrow{\scriptstyle p} & & \downarrow{\scriptstyle q} \\
B & \xrightarrow{\ \gamma\ } & A
\end{array}
\tag{8}
$$

The group G of such morphisms $\sigma \in G$ is the **transformation group** we're looking for. We can turn around the definition of a fiber bundle, using the idea of **invariance** under G, as follows:

Alternative definition of a fiber bundle (using invariance)

If $\begin{smallmatrix} X \\ \downarrow p \\ B \end{smallmatrix}$ is any projection, and if under any morphism $\sigma = (c, \gamma)$ such that diagram (8) commutes, and if the following invariance hold:

(i) $\forall b \in B, \exists a \in A. \quad p^{-1}(b) \cong q^{-1}(a)$

(ii) $\forall i \in I, \exists j \in J. \quad p^{-1}(U_i) \cong q^{-1}(U_j)$

then $\begin{smallmatrix} X \\ \downarrow p \\ B \end{smallmatrix}$ is a fiber bundle.

Want. F is defined on a structure which is a bundle.

Have. $F(x) = F(\sigma \cdot x) \quad \forall \sigma \in G$. F is invariant under a certain transformation group G. Bundle ξ is defined by an invariance under group G. F is defined over what kind of **space**? The invariance of F perhaps delineates a fundamental domain and that is the fibration structure?

A symmetry is an invariance. An invariance defines a transformation group that leaves something unchanged. A transformation group defines a geometric structure which is the fundamental domain. But a transformation group also defines a geometry *a la* Klein's Erlangen programme. So we have the invariance of $f(x)$ versus the invariance of shapes. $f(x) = f(\sigma \cdot x)$ versus shape $= \sigma \cdot$ shape. Shape $=$ set of points $= \{x_i\}$. Thus $\{x_i\} = \{\sigma \cdot x_i\}$.

What does the fundamental domain signify in this analogy? $f(x)$ can be evaluated once in $\mathcal{F}$ and be duplicated for the entire domain. But what does $\mathcal{F}$ mean in transformational geometry?
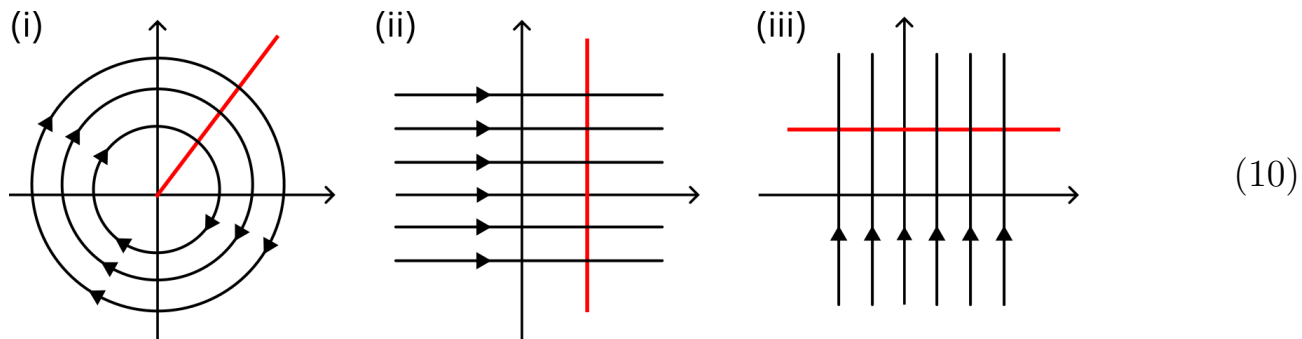
Fundamental domains

The paper *Group-invariant machine learning by fundamental domain projections* [Aslan, Platt, Sheard 2022], by a team of researchers from London, is very inspiring to us. They study the problem of machine learning over data sets that have group-invariant structure. One of the simplest such examples is permutation invariance. There is a way to build neural networks that are *intrinsically* invariant under permutation of input variables. They are expressed as sums of single-variable functions, which can be shown to be a universal form of all permutation-invariant functions; its proof involves the Kolmogorov-Arnold representation theorem.

But instead of building such *intrinsic* invariant neural networks, the authors of the paper proposed a novel approach based on **projections to fundamental domains**. This can be explained by the following diagram, where $\beta : X \to Y$ is the

$$
\begin{array}{ccc}
X & \xrightarrow{\ \beta\ } & Y \\
\pi \downarrow & \nearrow_{\overline{\beta}} & \\
\overline{\mathcal{F}} & &
\end{array}
\tag{9}
$$

Some examples of fundamental domains

The following are examples I created to get an intuitive understanding of fundamental domains for **continuous groups**:

$$\tag{10}$$

(i) If the group $G = \{$ rotations about the origin at various radii $\}$, then the fundamental domain is any ray from the origin

(ii) If $G = \{$ horizontal translations at various heights $\}$, then the fundamental domain is any vertical straight line

(iii) Similar to (ii), for vertical translations

(iv) If G is the group of (ii) and (iii) combined, then the fundamental domain is just any point, and the function is a constant function.

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