The orbits of neural networks

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1 Introduction

Inspired by [10, 3, 4], consider the following question: let a training set and a trained neural network be given where the trained neural network already converged to a local minimum, meaning given a positive real number $\epsilon > 0$, then each sample X_i in the given training set, there is $N \in \mathbb{N}$ such that for the number of epoch greater than N, the model is in the epsilon ball around the local minimum of the loss surface (i.e. its parameter space or moduli space). Then, is there a way to find equivalent models of this trained model?

Definition 1. Two models are equivalent if they both give identical outputs on a fixed training set as the input.

It is necessary to ask this question so that the trained model can be understood better to a point that the distribution of its weights can be studied using random matrix theory, and if all the other equivalent models can be derived instantaneously, then this is also equivalent to apply quantum computing to find all those equivalent solutions in parallel.

If a model can be replaced by another equivalent model, then the other model might be at the different point on the loss surface, then the barrier between the local minimum to the nearest lower local minimum might have a lower height or in some better case with a negative height, meaning the model can be trained to a better model with a smaller error by using a new set of training data to descent to that lower local minimum. Hence, it is also sufficient to ask the question: how to find equivalent models of a given trained model? If the answer to this question is unknown, suppose

a trained model cannot distinguish the fake data generated by an adversary model from the true data, or if a model needs to go through a debugging process for some false classified input, then the model not only has to be retrained, but it cannot be justified it is the best solution due to the process to reach the solution is random. Thus, on the contrary, if all of its equivalent models can be found immediately, then chances are, within the set of equivalent models, there might exist a model that will not take the fake input or falsely classified a corner case, meaning a model can be replaced instantly without going through a new training process.

2 Hyperbolic-orbit Algorithm

Definition 2. Hyperbolic-orbit Algorithm is an algorithm that implements hyperbolic distance to replace matrix product.

To introduce the algorithm, it is natural to start to build up the concept and tools from the Euclidean space. In Euclidean space, equivalent models of a trained model can be obtained by redefining matrix multiplication using Euclidean distance $d_E(x,y) = |x-y|$ for all $x,y \in \mathbb{R}$. For instance, let A be in $\mathbb{R}^{n \times m}$, B be in $\mathbb{R}^{d \times m}$, and their entries are denoted by a_{ki} and b_{li} where $k \in \{1, ..., n\}$, $l \in \{1, ..., d\}$, and $i \in \{1, ..., m\}$. Then, $(AB^t)_{kl} = \sum_{i=1}^m a_{ki}b_{il}$.

Instead of using matrix multiplication, a new operation using Euclidean distance is defined in the following:

$$\left(A \odot_E B^t\right)_{kl} := \sum_{i=1}^m d_E\left(a_{ki}, b_{il}\right).$$

Now, let the above A and B be any two matrices that need to be multiplied in a given model that already converges under the above new operation \odot_E between matrices A and B. Then by adding a real number α to A and B, infinite many equivalent models can be derived, since

$$\left(\left(\alpha+A\right)\odot_{E}\left(\alpha+B^{t}\right)\right)_{kl}:=\sum_{i=1}^{m}d_{E}\left(\alpha+a_{ki},\alpha+b_{il}\right)=\sum_{i=1}^{m}d_{E}\left(a_{ki},b_{il}\right)=\left(A\odot_{E}B^{t}\right)_{kl}.$$

In other words, the original given model is unchanged. This operation results in a translation of the loss surface.

Alternatively, every entry of the matrices $A \in \mathbb{R}^{n \times m}$ and $B \in \mathbb{R}^{d \times m}$ can be embedded into

the upper half-plane \mathbb{H}^2 . That is, the entries of A and B become complex numbers with positive imaginary part: $a_{ki} \in \mathbb{H}^2$ and $b_{il} \in \mathbb{H}^2$.

The necessary condition to use hyperbolic geometry and Kleinian groups is that since that hyperbolic geometry can also reach the goal that to generate infinitely many equivalent models, and Kleinian groups are isometry group that preserved not only hyperbolic lengths, but angles which can work as the symmetric group of the space, and to act on geometric objects in the space to do rigid transformation.

Furthermore, the sufficient condition to apply hyperbolic geometry and Kleinian groups is that instead of linear transformations, linear fractional transformations (which is determined by elements in the Kleinian group) can provide non-linear and hence non-trivial feedback in back-propagation. Though it is possible to develop a similar algorithm on other Riemannian manifold that has an automrophism group and if the group elements can also preserve angles and distance, hyperbolic geometry with Kleinian groups might be the easiest example that can be computable, but give non-trivial feedback in back-propagation.

Define a new binary operation between A and B using hyperbolic length on the upper-half plane $\mathbb{H}^2[2]$:

$$\left(A \odot_{\mathbb{H}^2} B^t\right)_{kl} := \sum_{i=1}^m d_{\mathbb{H}^2} \left(a_{ki}, b_{il}\right).$$

Then on the upper-half plane, the projective special linear group $PSL(2,\mathbb{R})$ is its automorphism group. Furthermore, elements of the group are conformal mapping that preserve not only angles but hyperbolic distance. Hence, $PSL(2,\mathbb{R})$ is also the isometry group of the upper-half plane.

To derive an equivalent model, take any $M \in \mathrm{PSL}(2,\mathbb{R}) \setminus \{\mathrm{id}\}$, then there exists an isomorphism to map M to a linear fractional (Möbius) map $T_M(z) = \frac{az+b}{cz+d}, a, b, c, d \in \mathbb{R}, z \in \mathbb{C}$.

Definition 3 (Hyperbolic-length product). Define the hyperbolic-length product is the following new operation:

$$\left(T_{M}(A)\odot_{\mathbb{H}^{2}}T_{M}(B^{t})\right)_{kl}:=\sum_{i=1}^{m}d_{\mathbb{H}^{2}}\left(T_{M}\left(a_{ki}\right),T_{M}\left(b_{il}\right)\right).$$

Definition 4. Let W be a neural network model and assume W converged already with the hyperbolic-length product implemented. Then with the above notations, the orbit of W of the given

weights $\{a_{ki}, b_{il}\}$ (points in the hyperbolic space) is the set:

$$\{T_M(a_{ki})\} \cup \{T_M(b_{il})\}$$

for all $M \in PSL(2,\mathbb{R})$, and for all $k \in \{1,...,n\}$, $l \in \{1,...,d\}$, and $i \in \{1,...,m\}$.

Proposition 1. With the above notations, then the newly defined product is an invariant:

$$\left(T_M(A) \odot_{\mathbb{H}^2} T_M(B^t) \right)_{kl} = \sum_{i=1}^m d_{\mathbb{H}^2} \left(T_M(a_{ki}), T_M(b_{il}) \right) = \sum_{i=1}^m d_{\mathbb{H}^2} \left(a_{ki}, b_{il} \right) = \left(A \odot_{\mathbb{H}^2} B^t \right)_{kl}.$$

Proof. This result follows immediately from the property of the Möbius mapping T_M when it is corresponding to a matrix M in the projective special linear group $PSL(2,\mathbb{R})$, then T_M is an isometry under the hyperbolic metric.

Let $\mathbb{B}^2:=\{z\in\mathbb{C}:|z|<1\}$ be the Poincare's disc and Ψ be the Cayley's transformation $\Psi:\mathbb{H}^2\to\mathbb{B}^2$. Then, $\Psi\left(T_M(z)\right)=\frac{a'z+b'}{c'z+d'}$ where $a',b',c',d'\in\mathbb{C},z\in\mathbb{C}$.

Proposition 2. With the above definition and proposition, then the value of the product has the same value when the points a_{ki} and b_{il} are sent to Poincare's disc:

$$\left(T_{M}(A)\odot_{\mathbb{H}^{2}}T_{M}(B^{t})\right)_{kl}=\sum_{i=1}^{m}d_{\mathbb{H}^{2}}\left(T_{M}\left(a_{ki}\right),T_{M}\left(b_{il}\right)\right)=\sum_{i=1}^{m}\rho_{\mathbb{B}^{2}}\left(\Psi\left(T_{M}\left(a_{ki}\right)\right),\Psi\left(T_{M}\left(b_{il}\right)\right)\right).$$

Proof. Since for each
$$z_1, z_2 \in \mathbb{H}^2$$
, $d_{\mathbb{H}^2}(z_1, z_2) = \rho_{\mathbb{B}^2}(\Psi(z_1), \Psi(z_2))$.

The 2-dimensional hyperbolic-length product can be generalized to n-dimension[5, 1, 2, 6, 7, 8], for $n \geq 3$. Let A, B be embedded into $\mathbb{H}^n, n \geq 3$.

Definition 5 (Hyperbolic-length product). Define n-dime the hyperbolic-length product is the following new operation:

$$\left(T_{M}(A)\odot_{\mathbb{H}^{n}}T_{M}(B^{t})\right)_{kl}:=\sum_{i=1}^{m}d_{\mathbb{H}^{n}}\left(T_{M}\left(a_{ki}\right),T_{M}\left(b_{il}\right)\right).$$

This n-dimension result could be useful for applying the hyperbolic-orbit algorithm to any

trained models that were trained without implementing the hyperbolic-length product during the training. Likewise, for higher dimensions, the hyperbolic-length product is also an invariant:

Proposition 3. With the above notations, then the newly defined product is an invariant:

$$(T_{M}(A) \odot_{\mathbb{H}^{n}} T_{M}(B^{t}))_{kl} = \sum_{i=1}^{m} d_{\mathbb{H}^{n}} (T_{M}(a_{ki}), T_{M}(b_{il})) = \sum_{i=1}^{m} d_{\mathbb{H}^{n}} (a_{ki}, b_{il}) = (A \odot_{\mathbb{H}^{n}} B^{t})_{kl}.$$

The question that aimed to solve by using this algorithm was mentioned in the first section. The goal is to replace matrix multiplication with a caveat that the situation mostly does not include finding inverses.

In summary, there are two cases to apply hyperbolic-orbit algorithm. Let a model W and a training set X be given.

- Case 1 W was trained. The goal is to find an auxiliary matrix C and instead of applying hyperbolicorbit algorithm on A times B, applying it to M times C, M is defined in step 1, i.e. make ABbecome invertible and find an auxiliary matrix C such that the solution of the embedding coordinates of entries $(M)_{ki}$ and $(C)_{il}$ exists. That is, entries of matrix M and C can be mapped to \mathbb{H}^3 such that the hyperbolic length between $(M)_{ki}$ and $(C)_{il}$ is preserved by the hyperbolic-length product.
 - Step 1 If AB is not invertible, then extend it to a $2n \times 2n$ matrix which is invertible: $\begin{pmatrix} AB & I \\ I & 0 \end{pmatrix}$.

 If AB is invertible, then denote it by M := AB, if not then denote $M := \begin{pmatrix} AB & I \\ I & 0 \end{pmatrix}$.
 - Step 2 To embed each k-th column of C parallel to y_3 -axis in \mathbb{H}^3 . So, design each hyperbolic length between $(M)_{ki}$ and $(C)_{il}$ in a matrix called M', e.g. let each $(M)_{ki}$ to be linked with $(C)_{il}$ symmetrically, although at this step $(C)_{il}$ is still unknown. But, just because of this reason, all hyperbolic lengths can be designed symmetrically such that the solution exists.
 - Step 3 Now, what remains is to find the matrix C. Since M is invertible, and M' is known, it suffices to solve the matrix equation MC = M'. Thus, $C = M^{-1}M'$.

(i) If
$$C$$
 is not invertible, then extend C to $C':=\begin{pmatrix} C & I \\ I & 0 \end{pmatrix}$, M to $M_I:=\begin{pmatrix} M & I \\ I & 0 \end{pmatrix}$, M' to $M'_I:=\begin{pmatrix} M' & I \\ I & 0 \end{pmatrix}$.

(ii) If C is invertible, rename C to C', M to M_I , and M' to M'_I .

Case 2 W was not trained.

Method 1 Treat W as trained and reduce it to either case 1.

Method 2 Train W without using hyperbolic-length product till it converges, then treat it as trained, i.e. again, apply methods of case 1.

Method 3 Implement the hyperbolic-length product into W directly.

- Step 1 The selected matrices A and B can be embedded freely to hyperbolic space as long as the hyperbolic-length product can work properly in the usual training process.
- Step 2 The dimension of hyperbolic space could start with two dimension to optimize the memory usage. If there is no restriction on the use of memory, then the easiest way is starting with dimension $n \times d$, where \times is the scalar product in \mathbb{N} .

In Case 1, since each step from step 1 to step 3 is invertible, after these operations, hyperbolic-length product can be applied to M'_I and C', then apply all the inverses and restrictions to back to AB, so the output is also unchanged, but the orbit of the neural network can be found using the above hyperbolic-orbit algorithm.

Furthermore, the isometry group of \mathbb{H}^n is a group of Möbius mapping, hence its group elements preserve not only hyperbolic length but angles, thus the information of the sign of each $a_{ki}b_{il}$ could be preserved.

3 Examples

3.1 Self-attention mechanism in any transformer-based models with the hyperbolic-length product implemented before training

All layers of a given neural network model can be implemented with the above hyperbolic-orbit algorithm. The following is an example when the hyperbolic-orbit algorithm is applied to the self-attention mechanism, i.e. transformer-based models. Let $A = Q \in \mathbb{C}^{n \times d_q}$ and $B = K^t \in \mathbb{C}^{d_k \times n}$ in self-attention mechanism[9] using dynamic scaling factor β (defined in our another work in progress), and by convention let $d_q = d_k$.

4 Discussion

Furthermore, with the hyperbolic-orbit algorithm, it is possible to find an appropriate Möbius mapping that is corresponding to $M \in \mathrm{PSL}(2,\mathbb{R})$ such that training a 3-node neural network become not necessarily NP-hard in [3]. Further, if every layer of a given neural network is implemented with the hyperbolic-orbit algorithm introduced in this paper, by combining with perturbations and parallel computing, the steepest descent path toward the global minimum could be designed. The algorithm introduced by the paper can help to save training time for parallel computing in the ensemble method, that is, instead of starting over from the beginning to train N' models in parallel, $N' \in \mathbb{N}$, the training can start with N' models that are equivalent to a trained model that already has an error that cannot be reduced by using the old training set—but on the orbits of the trained model, each equivalent model on the orbit can be kept training with a new training set by updating the weight matrices using back-propagation with the gradient descent algorithm. Then, in each epoch, the best model could be selected and instantaneously its N' equivalent models could be obtained using the hyperbolic-orbit algorithm.

5 Limitation

The hyperbolic-orbit algorithm has a limitation when it is applied to case 2 if the model was trained. To show the limitation, consider an example where there are two points a_1 , and a_2 from A, and two points b_1 and b_2 in B. In \mathbb{H}^n , $n \geq 3$, suppose the hyperbolic length between b_1 to a_1 and b_2 to a_1 are both zero, and the hyperbolic length between b_1 and a_2 is L. But, for b_2 , the hyperbolic length between b_2 and a_2 is 2L. If this happens, it might be possible to find an auxiliary invertible matrix C and instead of applying hyperbolic-orbit algorithm on A times B, applying it to AB times C and multiply the final result with C inverse such that the matrix product ABC is positive and does not have any case like the one mentioned in this section. This is the starting point of designing case 1 in the algorithm

References

- Lars V. Ahlfors, Möbius transformations in several dimensions, Ordway Professorship Lectures in Mathematics, University of Minnesota, School of Mathematics, Minneapolis, Minn., 1981. MR 725161
- [2] Alan F. Beardon, The geometry of discrete groups, Graduate Texts in Mathematics, vol. 91, Springer-Verlag, New York, 1995, Corrected reprint of the 1983 original. MR 1393195
- [3] Avrim Blum and Ronald Rivest, Training a 3-node neural network is np-complete, Advances in neural information processing systems 1 (1988).
- [4] J Stephen Judd, Neural network design and the complexity of learning, MIT press, 1990.
- [5] M. È. Kapovich and L. D. Potyagaĭlo, On the absence of finiteness theorems of Ahlfors and Sullivan for Kleinian groups in higher dimensions, Sibirsk. Mat. Zh. 32 (1991), no. 2, 61–73, 212. MR 1138441
- [6] Michael Kapovich, Kleinian groups in higher dimensions, Geometry and dynamics of groups and spaces, Progr. Math., vol. 265, Birkhäuser, Basel, 2008, pp. 487–564. MR 2402415

- [7] John G. Ratcliffe, Foundations of hyperbolic manifolds, Graduate Texts in Mathematics, vol. 149, Springer, Cham, [2019] ©2019, Third edition [of 1299730]. MR 4221225
- [8] José Seade and Alberto Verjovsky, Higher dimensional complex Kleinian groups, Math. Ann.
 322 (2002), no. 2, 279–300. MR 1893917
- [9] Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin, Attention is all you need, Advances in neural information processing systems 30 (2017).
- [10] Chulhee Yun, Suvrit Sra, and Ali Jadbabaie, Global optimality conditions for deep neural networks, arXiv preprint arXiv:1707.02444 (2017).