Periodic Spectral Ergodicity: A Complexity Measure for Deep Neural Networks and Neural Architecture Search

Mehmet Süzen ∗
MEMBER, ACM
suzen@acm.org

J. J. Cerdà
UNIVERSITAT DE LES ILLES BALEARS
jj.cerda@uib.cat

Cornelius Weber
UNIVERSITÄT HAMBURG
weber@informatik.uni-hamburg.de

Editor: na

Abstract

Establishing associations between the structure and the learning ability of deep neural networks (DNNs) is a challenging task in modern machine learning. Producing solutions to this challenge will bring progress both in the theoretical understanding of DNNs and in building new architectures efficiently. In this work, we address this challenge by developing a new simple complexity measure based on another new measure called Periodic Spectral Ergodicity (PSE) originating from quantum statistical mechanics. Based on this measure a framework is devised in quantifying the complexity of deep neural network from its learned weights and traversing network connectivity in a sequential manner, hence the term cascading PSE (cPSE) as an empirical complexity measure. Because of this cascading approach, i.e., a symmetric divergence of PSE on the consecutive layers, it is possible to use this measure in addition for Neural Architecture Search (NAS). We demonstrate the usefulness of this measure in practice on two sets of vision models, ResNet and VGG and sketch the computation of cPSE for more complex network structures.

Keywords: Generalization, Spectral Ergodicity, Deep Neural Networks, Neural Architecture Search, AutoDL, AutoML, Model Selection, Complexity

1. Introduction

Complexity measures appear in multiple fields from physics to medicine in guiding designing of artificial systems, understanding natural phenomenon and detecting signals (Pincus (1991), Shiner et al. (1999), Bandt and Pompe (2002), Zurek (2018)). One of the example systems requiring robust complexity measures appear to be machine learning systems. Their recent success in producing learning systems exceeding human ability in some tasks attributed to deep learning (LeCun et al. (2015); Mnih et al. (2015)), i.e. DNN. However, understanding complexity of DNNs both in structure and from learning theory perspective lagged behind their practical engineering success. An analogy made by LeCun (LeCun), that this situation resembles lack of theory of thermodynamics and the success of thermal machines in early industrial revolution.

∗ Corresponding author
The complex neural network architectures used in deep learning are still build by human experts who are usually highly mathematically minded. Understanding the guiding principles in such design process will help experts to increase their efficiency and for producing superior architectures. Neural Architecture Search (NAS) methods have already been proposed (Elsken et al. (2019)) in this direction. NAS methods usually operate on the search space, with a search strategy and guiding performance estimation strategy. Embedding complexity measures in both search strategy and performance estimation strategy could accelerate the NAS. Complexity measures for supervised classification were suggested (Ho and Basu (2002)). However these measures do not address specifically to deep learning architectures. Recently a complexity measure for characterising deep learning structural complexity is proposed based on topological data analysis (Rieck et al. (2019)). This can be used in NAS, It requires embedding the computation of the measure into the learning algorithm and leverage advanced mathematics.

In this work, we extent a definition of spectral ergodicity for ensemble of matrices (Süzen et al. (2017)) to handle different sized matrices within the same ensemble. This is possible by defining a periodicity on the eigenvalue vectors via a method, so called Periodic Spectral Ergodicity (PSE) on the learned weights. Our main mathematical object is defined as a complexity measure for the neural network based on PSE. This measure reflects structure of the network with a cascading computation of PSEs on the consecutive layers. This leads to a complexity of DNNs measure called cascading PSE (cPSE).

As usage of spectral properties of neural networks, i.e., learned weight matrices or Hessian matrix, is appeared recently in novel works in attempt to build strong theoretical foundation for DNNs (Pennington et al. (2017); Sagun et al. (2017); Pennington et al. (2018); Martin and Mahoney (2018, 2019a,b)) and extracting feature interaction (Tsang et al. (2017)). Our work follows a similar ethos.

2. Periodic spectral ergodicity framework

Spectral ergodicity originates from quantum statistical mechanics (Jackson et al. (2001)). In a recent inception it is attributed as a reason why deep neural networks perform in high accuracy, demonstrated on random matrix ensembles as surrogate to weight matrix ensembles (Süzen et al. (2017)). In that work, only fixed size complex matrix ensembles were used to measure the ensemble’s approach to spectral ergodicity. Changing matrix dimensions in ensembles corresponds to increasing size of a single layer, as an interpretation. Circular ensembles were used in that study as a surrogate matrices having close to unit spectral radius. In trained neural network’s weight matrices that is known to prevent gradient instability ideally have unit spectral radius. However informative, this approach was short of direct usage in real practical networks even though it has given empirical evidence of usefulness of spectral ergodicity. One short coming was how to handle different size weight matrices and the second one was how to turn complex layer structures like multi-dimensional convolutional units to a weight matrix.

Having multi-dimensional connections between two consecutive layers leads to a Tensor representation of the deep neural network. For this reason, we defined a Layer Matrix Ensemble $\mathcal{L}^m$, that is coming from $m$ layer connections via mapping from multi-dimensional connections, i.e., trained weights, to two dimensional square matrices $X_l$ of size $N_l \times N_l$
Figure 1: A sample arbitrary architecture a fork. In the fork each edge represents an arbitrary DNN layer including arbitrary convolutions.

where $N_l \geq 2$, see Definition 1. In the case of linear connections, this mapping acts as a unit transformation. This would enable us to generate layer matrix ensemble or simply weight matrices of any trained deep neural network architecture.

**Definition 1** Layer Matrix Ensemble $L^m$

The weights $W_l \in \mathbb{R}^{p_1 \times p_2 \times \ldots \times p_n}$ are obtained from a trained deep neural network architecture’s layer $l$ as an $n$-dimensional Tensor. A Layer Matrix Ensemble $L^m$ is formed by transforming $m$ set of weights $W_l$ to square matrices $X_l \in \mathbb{R}^{N_l \times N_l}$, that $X_l = A_l \cdot A_l^T$ and $A_l \in \mathbb{R}^{N_l \times M_l}$ is merely a stacked up version of $W_l$ where $n > 1$, $N_l = p_1$, $M_l = \prod_{j=2}^{n} p_j$ and $p_j, n, m, N_l, M_l, j \in \mathbb{Z}_+$. Consequently $L^m$ will have $m$ potentially different $N_l$ size square matrices $X_l$ of at least size $2 \times 2$.

The original definition of spectral ergodicity for DNNs (Süzen et al. (2017)) relies on the same size squared matrices in the matrix ensemble. We proceed with applying periodic or cyclic conditions to all eigenvalue vectors, obtaining periodic eigenvalue vectors $\varepsilon^m$, see Definition 2. This preprocessing step produce a suitable dataset extracted from trained neural network weights, preserving layer order, that can be used in computing approach to spectral ergodicity.

**Definition 2** Periodic eigenvalue vectors $\varepsilon^m$

Given layer matrix ensemble $L^m$, the set of eigenvalue vectors of length $N_l$ is computed, eigenvalues of $X_l$ as $e_l$. Naturally, not all vectors will be the same length. In order to align the different size vectors, first we identify maximum length eigenvalue vector, $l_{max} = \max |e_l|$. Then we align all other eigenvalue vectors by applying cyclic boundary condition, meaning that replicating them up to length $l_{max}$, simply $N$ hereafter.

Given layer $L$ and $N$ eigenvalues, a spectral density $\rho_j$ is computed for all $j$ layers from first to the layer $L$ using periodic eigenvectors $\varepsilon^m$. Here a layer corresponds the weight matrices in the layer matrix ensemble. Spectral ergodicity at layer $L$ is defined as a distribution extracted from spectral densities,

$$
\Omega^L = \Omega^L(b_k) = \frac{1}{L \cdot N} \sum_{j=1}^{L} \left[ \rho_j(b_k) - \bar{\rho}^L(b_k) \right]^2, \quad (1)
$$
where $b_k$ are histogram bin centres, and $j$ represents layer $l \leq L$. The mean spectral density up to layer $L$ is given by

$$\rho^r(b_k) = \frac{1}{L} \sum_{j=1}^{L} \rho_j(b_k).$$

Since $\Omega^L$ alone is a distribution, in order to get an approach to spectral ergodicity over increasing depth we define a symmetric distance metric between two consecutive layers, $D_{pse}$, as follows,

$$D_{pse} = D_{pse}(N_l, N_{l+1}) = D_{KL}(\Omega^l|\Omega^{l+1}) + D_{KL}(\Omega^{l+1}|\Omega^l).$$

(2)

The terms on the right are Kullbach-Leibler divergence between consecutive layers, one backwards, and they are defined as follows, sums run over spectral density bins,

$$D_{KL}(\Omega^l|\Omega^{l+1}) = \sum_k \Omega^l \log_2 \frac{\Omega^l}{\Omega^{l+1}},$$

$$D_{KL}(\Omega^{l+1}|\Omega^l) = \sum_k \Omega^{l+1} \log_2 \frac{\Omega^{l+1}}{\Omega^l}.$$  

It is shown on circular complex matrix ensembles that increasing layer size decrease the value of $D_{pse}$. $D_{pse}$ is defined to be a distance metric for approach to spectral ergodicity for DNNs.

2.1 Cascading PSE for feed forward networks

Complexity of entire feed forward neural network, possibly having many complicated connections as in convolution units, can be identified with the cumulative of approach to spectral ergodicity for given $L$ layered network,

$$\phi^L = \frac{1}{L} \sum_{i=1}^{L-1} \log_{10} D_{pse}(N_i, N_{i+1}),$$

(3)
which is identified as cascading PSE (cPSE) due to fact that approach to spectral ergodicity of consecutive layers are summed up in a cascading manner.

**Theorem 3** Decreasing cPSE for feedforward networks

Given $L$ layered DNN and corresponding complexity cPSE $\mathcal{C}^L$, adding one more layer to the DNN almost certainly will not increase the complexity measure cPSE, $\mathcal{C}^L \geq \mathcal{C}^{L+1}$. This implies lower the cPSE higher the complexity.

The assertion that increasing number of layers will decrease the complexity measure $\mathcal{C}^L$ is given in Theorem 3. Interpretation of this assertion follows a reverse effect. This means increasingly complex deep network will have a smaller $\mathcal{C}^L$ value. However, this assertion is closely related to the learning performance too. Decreasing value of $\mathcal{C}^L$ follows performance improvement, i.e., complexity measure is directly correlated to learning performance. Once a network reached to periodic spectral ergodicity, very small $D_{pse}$ values, the designed network’s performance will not increase. This is a consequence of the Theorem 4.

**Theorem 4** Performance and cPSE

Given $L$ layered DNN, corresponding complexity cPSE $\mathcal{C}^L$ and generalisation performance measure $\mathcal{P}^L$. Given set of ordered series $\mathcal{S}^C = (L, \mathcal{C}^L)$ and $\mathcal{S}^P = (L, \mathcal{P}^L)$ and for large enough set of values of $L$, $\mathcal{S}^C$ and $\mathcal{S}^P$ are almost perfectly correlated.

It is observed that adding many more layers to DNN degrade the performance after certain depth (Paszke et al. (2017)). We asserted that this discrepancy is a characteristics of training and numerical difficulty, rather than a generalised theoretical property of correspondence between learning and the architectures. Performance should not degrade just to due to depth, everything else fixed, as a logical inference from Theorem 4.

2.2 Cascading PSE for arbitrary architectures

The extension of feedforward complexity $\mathcal{C}^L$ to any type of connectionist architecture lies in how to treat branching connections, i.e., a layer connecting to multiple layers. A basic
| Architecture | Top-1 error | Top-5 error | cPSE |
|--------------|-------------|-------------|------|
| vgg11        | 30.98       | 11.37       | 0.04 |
| vgg13        | 30.07       | 10.75       | 0.41 |
| vgg16        | 28.41       | 9.63        | 0.14 |
| vgg19        | 27.62       | 9.12        | -0.10|
| vgg11bn      | 29.62       | 10.19       | 0.38 |
| vgg13bn      | 28.45       | 9.63        | 0.36 |
| vgg16bn      | 26.63       | 8.50        | 0.18 |
| vgg19bn      | 25.76       | 8.15        | -0.07|
| resnet18     | 30.24       | 10.92       | -0.19|
| resnet34     | 26.70       | 8.58        | -0.74|
| resnet50     | 23.85       | 7.13        | -1.03|
| resnet101    | 22.63       | 6.44        | -1.77|
| resnet152    | 21.69       | 5.94        | -2.29|

Table 1: Classification performance and cPSE of investigated architectures. The correlation between both classification performances and cPSE for ResNet ($\rho = 0.94$) for VGG ($\rho = 0.44$ and $\rho_{bn} = 0.93$ with batch normalisation).

rule to treat branches, compute complexity up to a branching point and also up to end of the branch, the difference of the value would give the branch complexity. By this rule one could compute cPSE for entire arbitrary architectures.

We demonstrate the computation of cPSE for arbitrary architecture with a dummy example. The fork shaped architecture is identified with 15 layers, branching out at layer 3 to 3 different branches, see Figure 1. Using layer ranges as subscripts to indicate cPSE computation in between those layers, total cPSE for the fork architecture reads,

$$ C^L = C^{L}_{1-7} + C^{L}_{1-11} + C^{L}_{1-15} - 2 \cdot C^{L}_{1-3}. $$

Automation of this branching rule might require efficient graph algorithms for more complex architectures in detecting branches. For recurrent networks, a transformed version of the architecture to non-recurrent topology is needed to compute cPSE.

3. Experiments

We tested our assertions and framework on real-life feed forward architectures designed for vision tasks: ResNet and VGG variants. Pre-trained weights (Paszke et al. (2017)) are used to build Layer Matrix Ensembles to compute $D_{pse}$ over increasing layer depth within the architecture variant. Overall network complexity $C^L$ is computed via mean $\log_N D_{pse}$ values and show to be decreasing with the depth.

3.1 VGG architectures

The convolutional network depth investigated for visual image classification (Simonyan and Zisserman (2014)), so called VGG architectures. We have used pre-trained variants of in computing
$D_{pse}$, approach to PSE over layers and single $cPSE$ measure per variant. Results summarized in Figure 2. We observe the decreasing $D_{pse}$ values increasing depth. The VGG variants and their corresponding batched normalised versions: vgg11, vgg13, vgg16 and vgg19. We observed that vgg11’s cPSE did not obey the monotonicity of cPSE. However batched normalised vgg11 did obey.

3.2 ResNet architectures

A residual neural network (ResNet) brings state-of-the-art results in visual object classification tasks by introducing layer skip procedures in training (He et al. (2015)). We have used pre-trained variants of ResNet: resnet18, resnet34, resnet50, resnet101 and resnet152 in computing $D_{pse}$, approach to PSE over layers and single $cPSE$ measure per variant.

4. Empirical evidence for Theorem 4

We have compared cPSE values for each architecture from our ResNet and VGG variants against their misclassification errors. We found very strong correlation between classification performance and cPSE for ResNet and VGG. Correlations remain the same for both top-1 and top-5 errors. We attribute the drop in correlation for VGG poorer training approach and the effect of batch normalisation. The summary is given in Table 1, classification performance and cPSE of investigated architectures. The correlation between both classification performances and cPSE for ResNet $\rho = 0.94$ for VGG $\rho = 0.44$ and $\rho_{bn} = 0.93$ with batch normalisation. Results shown an empirical evidence supporting Theorem 3, higher the depth smaller the cPSE complexity measure.

5. Conclusion

We developed a complexity measure for arbitrary neural network architectures based on spectral ergodicity defined on learned weights among layers so called cPSE measure. This measure has given consistent numerical results on ResNet and VGG architectures. We also sketch how to compute cPSE with branched networks, i.e. arbitrary architectures. cPSE provided a quantitative connection between architecture and learning performance in our test. Moreover, we provided mathematical properties of cPSE, such as monotonicity.

In this work, we explain the success of deeper neural networks via theoretically founded structural complexity measure. Going beyond theoretical understanding, proposed complexity measure for DNNs is simple to implement and it can be directly used in practice with a minimal effort. Usage of our complexity measure can also be embedded into NAS methods. For this reason, we sketch how to compute cPSE for arbitarily branched networks. A search strategies can use cPSE in deciding how to grow a network or in genetic algorithms settings how to mutate to a new structure.

Acknowledgements

We would like to express our gratitute to Charles Martin for pointing us out the usage of pre-trained weights form pytorchvision and pytorch core team for bundling these datasets neatly.
Appendix A: Code Supplement

We have provided a Python notebook, periodic_spectral_ergodicity.ipynb that contains prototype implementation of cPSE, our experiments with ResNet and VGG architectures. We used bristol python package for spectral ergodicity core computations (Süzen et al. (2017)) and leverage pytorch and numpy ecosystem where needed.

Appendix B: Proof of Theorem 3

We present a proof of Theorem 3 by contradiction.

The approach to ergodicity requires decreasing values in distance metric $\log_{10} D_{pse}$ for well behaved spectra. Given

$$D_{l, l+1} = \log_{10} D_{pse}(N_l, N_{l+1})$$

than it follows

$$D_{l, 2} > D_{l, 3} > D_{l, 4} > ... > D_{l, l-1} > D_{l, l+1}, ...$$

because of the fact that increasing ensemble size $\Omega_L$ should approach to zero monotonically, leading to decreasing symmetric distance on consecutive layers. This implies $D_{l, 2} >> D_{l, L-1}.$

Now, let’s say $c^{L+1} > c^L$ contradicting the theorem, this yields to

$$\frac{1}{L} \sum_{l=1}^{L-1} D_{l, l+1} < \frac{1}{L+1} \sum_{l=1}^{L} D_{l, l+1}$$

$$\frac{L}{L^2 + L} \sum_{l=1}^{L-1} D_{l, l+1} < D_{L, L+1}$$

$$\lambda < D_{L, L+1}$$

is a contradiction as $L$ is very large both $D_{L, L+1}$ and $\lambda$ approaches to zero. So $D_{L, L+1}$ can not be greater than $\lambda$ for large $L$. Hence, the value of cPSE by adding one layer should not increase, $c^{L+1} \leq c^L.$

q.e.d.

Appendix D: Declaration of not practicing HARK

We did not practice so called HARKing in this work: HARK issues in machine learning research (Gencoglu et al. (2019)). The theorems are asserted first, if there is a connection between cPSE and the performance. The following questions were set before initiating any data analysis of weight structure and computing cPSE:

1. Are there any relationship between network predictive performance and cPSE?
2. Can we say anything about cPSE causing better architecture?
3. How can we use cPSE in Neural Architecture Search (NAS)?

We generated the data to address these questions as much as possible and this work was hypothesis first driven exercise.
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