Equivalence in Deep Neural Networks via Conjugate Matrix Ensembles

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A numerical approach is developed for detecting the equivalence of deep learning architectures. The method is based on generating Mixed Matrix Ensembles (MMEs) out of deep neural network weight matrices and conjugate circular ensemble matching the neural architecture topology. Following this, the empirical evidence supports the phenomenon that distance between spectral densities of neural architectures and corresponding conjugate circular ensemble are vanishing with different decay rates at long positive tail part of the spectrum i.e., cumulative Circular Spectral Distance (CSD). This finding can be used in establishing equivalences among different neural architectures via analysis of fluctuations in CSD. We investigated this phenomenon for wide range of deep learning vision architectures and with circular ensembles originating from statistical quantum mechanics. Practical implications of the proposed method for artificial and natural neural architectures discussed such as possibility of using the approach in Neural Architecture Search (NAS) and classification of biological neural networks.

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INTRODUCTION

Constructing equivalence relations among different mathematical structures are probably one of the most foundational concepts in sciences \cite{1}, a practical interest as well, beyond being a theoretical building block of many quantitative fields. This manifests in many fields of physical sciences and in practice, such as for equivalence of graph network ensembles \cite{2,5}, single-molecule experiments \cite{4,5}, Bayesian Networks \cite{6}, between ranking algorithms \cite{7} and Brain network motifs \cite{8,9}.

Recent success of deep learning \cite{10,11} in different learning tasks showing skills exceeding human capacity, specially in vision tasks brings the need for both understanding of these systems and build neural architectures in an efficient manner. In this direction, detecting equivalent deep learning architectures are not only interesting for theoretical understanding but also for finding more efficient architecture as a design principle. Neural Architecture Search (NAS) \cite{12,13} or search for smaller equivalent network, i.e., architecture compression \cite{14,15} are valuable tools in achieving this aim.

Approach in establishing equivalence between two deep learning architectures are taken here lies in the analysis of eigenvalue spectra of the trained weights, network topology and generating conjugate random matrix ensemble. There would be no dependence on the activation functions or training procedure in establishing such equivalence in the approach. This makes approach very appealing as it can be applied to wide-variety of network setting and learning procedures. The equivalence would entail components of topological structure, learning procedure and network setting. Analysis of spectral density of weights of deep learning architectures recently investigated \cite{16,19}, and we follow a similar spirit in this regard, and earlier works on investigating eigenvalue statistics in neural network learning \cite{20}.

MIXED MATRIX ENSEMBLES

In establishing equivalence of two neural networks, we have taking a route that requires a mathematical setting in the language of matrix ensembles, square matrices. Matrix ensembles especially appear in Random matrix theory \cite{21,22}. One of the prominent example is circular complex matrix ensembles \cite{23} that mimics quantum statistical mechanics systems \cite{24}. It is hinted out that decay of spectral ergodicity with increasing matrix order \textit{N} for circular matrix ensembles signifies an analogous behaviour as using deeper layers in neural networks \cite{22}, whereby circular ensembles used as a simulation tool. However, real deep learning architectures have rarely all the same order weight matrices, but the weight matrices extracted from trained deep learning architectures will have variety of different orders due to different units in layer connections and forms a Layer Matrix Ensemble, see Definition 1.

Definition 1. Layer Matrix Ensemble $\mathcal{L}^m$ \cite{19} The weights $W_l \in \mathbb{R}^{p_1 \times p_2 \times \cdots \times p_m}$ are obtained from a trained deep neural network architecture’s layer $l$ as an n-dimensional Tensor. A Layer Matrix Ensemble $\mathcal{L}^m$ is formed by transforming $m$ set of weights $W_l$ to square matrices $X_l \in \mathbb{R}^{N_l \times N_l}$, that $X_l = A_l : A_l^{T}$ and $A_l \in \mathbb{R}^{N_l \times M_l}$ is merely a stacked up version of $W_l$ where $n > 1$, $N_l = p_1$, $M_l = \prod_{j=2}^{m} p_j$ and $p_j$, \textit{n}, \textit{m}, \textit{N}_l, \textit{M}_l, \textit{j} \in \mathbb{Z}_+$. Consequently $\mathcal{L}^m$ will have $m$ potentially different $N_l$ size square matrices $X_l$ of at least size $2 \times 2$.

Circular Ensemble is formed by drawing a complex circular matrices from different size Circular Unitary Ensembles (CUEs), matching the orders, \textit{m} different orders coming from $\mathcal{L}^m$ and taking their modulus, as we are dealing with real matrices in deep learning architectures, see Definition 2.

Definition 2. Circular Unitary Mixed Ensemble $\mathcal{U}^m$ Set of matrices $A_l = \text{Mod}(U_l)$ where $U_l \in \mathbb{C}^{N_l \times N_l}$ and
A ∈ ℝ^{N_i×Ni} forms this ensemble. In component form, each U_i obeys the following construction [24, 27]: Consider a Hermitian matrix \( H \in \mathbb{C}^{N\times N} \),

\[
H_{ij} = \frac{1}{2}(a_{ij} + ib_{ij} + a_{ji} - ib_{ji}),
\]

where \( 1 \leq i, j \leq N \), and \( a_{ij}, b_{ij}, a_{ji}, b_{ji} \in \mathbb{G} \), i.e., they are elements of the set of independent identically distributed Gaussian random numbers sampled from a normal distribution and \( I \) is the imaginary number.

Ensemble matrices \( U \) is defined as

\[
U = \exp(\gamma_i I) \cdot v_i^j,
\]

\( v_i \) is the i-th eigenvector of \( H_{ij} \), where \( \gamma_i \in [0, 2\pi] \) is a uniform random number.

Both \( \mathcal{L}^m \) and \( \mathcal{M}^m \) forms a Mixed Matrix Ensembles (MMEs) as defined in Definition 3.

**Definition 3.** Mixed Matrix Ensembles (MMEs) \( \mathcal{M}^m \) are defined as set of \( m \) square matrices \( A_i \in \mathbb{R}^{N_i \times N_i}, i = 1, \ldots, m \), where by \( N_i \geq 2 \) and \( m, i, N_i \in \mathbb{Z}_+ \). Mixed here implies set of different size real square matrices forming an ensemble. In the case of all \( N_i \) having the same value makes MMEs a pure matrix ensemble. \( N_i \) is sometimes called the order of a matrix as well.

**CONJUGACY AND EQUIVALENCE**

We introduce a concept of mixed matrix conjugate ensembles inspired from statistical physics [4, 5]. Conjugacy of statistical mechanics ensembles are well founded based on Legendre Transforms [4, 5]. Here we need to follow a different approach based on core characteristic of a matrix ensembles. There is no known conjugacy rules for such ensembles and we introduce here one of the many possible conjugacy constructions.

Finding an appropriate conjugate mixed matrix ensemble given \( \mathcal{L}^m \), layer matrix ensemble coming from a trained deep learning architecture or it could be synaptic network weight matrices from Brain networks for example [6, 28] lies in pooled eigenvalues and spectra, see Definition 4.

**Definition 4.** The pooled eigenvalues and spectra of mixed matrix ensemble \( \mathcal{M}^m \) is built from the collection of eigenvalues of \( m \) square matrices \( A_i \in \mathbb{R}^{N_i \times N_i}, i = 1, \ldots, m \), denoted by \( \epsilon_{i,j}^{\text{pooled}} \) and \( j = 1, \ldots, N_i \cdot m \), with a corresponding spectral density \( \rho^{\text{pooled}}(\epsilon) \).

Now, we have well defined setting for defining conjugate ensemble and equivalence condition for MMEs. These are summarized in Definitions 5 and 6.

**Definition 5.** Conjugate MMEs

Given two mixed matrix ensembles \( \mathcal{M}_1^m \) and \( \mathcal{M}_2^m \) forms a conjugate ensembles if their respective spectral density difference approaches to zero over long positive tail part of the spectrum. Hence at \( [0, \epsilon_{\text{max}}] \), Circular Spectral Distance (CSD), \( \Delta_{\text{CSD}}(\epsilon) = \rho_1(\epsilon) - \rho_2(\epsilon) \) and with cumulative CSD defined as \( \sum_{\epsilon_{\text{max}}}^\epsilon \Delta_{\text{CSD}}(\epsilon) \) over spectral locations approaches to zero for large enough \( \epsilon_{\text{max}}, \epsilon_{\text{max}} \) being the largest eigenvalue to consider in constructing the spectral density.

**Definition 6.** Equivalence of MMEs

Given two mixed matrix ensembles \( \mathcal{M}_1^m \) and \( \mathcal{M}_2^m \) are equivalent if following two conditions met:

1. There is a third mixed matrix ensemble \( \mathcal{M}_c^m \) that is conjugate to both.
2. The Variance of Circular Spectral Distance (CSD) of them are equivalent with a small \( \delta \),

\[
\text{Var} \left( \Delta_{\text{CSD}} \right) - \text{Var} \left( \Delta_{\text{CSD}}^2 \right) = \delta
\]
EXPERIMENTS WITH VISION ARCHITECTURES

Our experiments focus on deep neural network architectures developed for vision task. Three different type of vision architectures are used: VGG [29], ResNet [30], and DenseNet [31] with different depth and batch normalisation for VGG. We generated mixed Layer Matrix Ensembles for all mentioned type networks using pretrained weights [32] and their corresponding mixed Unitary Circular Ensembles as a proposal conjugate ensembles. We used positive range for long positive tail part of the spectrum $[0, 0, 6.0]$ with 1000 equalspacing. This provides sufficiently smooth data with the given pooled eigenvalues from produced ensembles.

Computed CSDs for long positive tail part is shown for VGG, ResNet and DenseNet architectures on Figures 1, 2 and 3 respectively. We observe that different architecture’s CSDs decay in different rates. This indicates different fluctuation characteristics of each CSDs for different architectures as demonstrated on Figure 4.

Variance of all CSDs for all investigated architectures are summarized in Table I. We clearly see that each architecture type clearly seperated by Variance of CSDs. We see the equivalence of all VGG architectures implying the reported performance metrics are not too far apart in reality, VGG with batch normalisation architectures forms the subset, this is also observed in cumulative CSDs in Figure 1. However the equivalence goes away very quickly with increasing depth, this is observed between resnet18 and resnet152, similarly between densenet121 and densenet201. Equivalence between densenet169 and densenet201 could also be accepted.

CONCLUSIONS

We have developed a mathematically well defined approach to detect equivalance between deep learning architectures. The method relies on building conjugate matrix ensembles and investigating their spectral difference over the long positive tail part. This approach can also be used in detecting Brain motifs if synaptic weights are known.

The method is very practical and can be used in designing new artificial neural architectures via Neural Architecture Search (NAS) or compression of the existing known architecture by systematic or random reduction of the network size and computing variance of CSD as proposed in this work.

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SUPPLEMENTARY MATERIAL

A Python code notebook with functions to reproduce the data and results is provided with this manuscript, deep_Dyon_networks.ipynb.

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[1] J. B. Rosser, Logic for Mathematicians (Courier Dover Publications, 2008).
[2] J. Barré and B. Gonçalves, Physica A: Statistical Mechanics and its Applications 386, 212 (2007).
[3] F. den Hollander, M. Mandjes, A. Roccaverde, N. Starreveld, et al., Electronic Journal of Probability 23 (2018).
[4] M. Costeniuc, R. S. Ellis, and H. Touchette, Journal of Mathematical physics 46, 063301 (2005).
[5] M. Súzen, M. Sega, and C. Holm, Physical Review E 79, 051118 (2009).
[6] D. M. Chickering, Journal of Machine Learning Research 2, 445 (2002).
[7] Ş. Ertekin and C. Rudin, Journal of Machine Learning Research 12, 2905 (2011).
[8] O. Sporns and R. Kötter, PLoS biology 2 (2004).
[9] E. Bullmore and O. Sporns, Nature reviews neuroscience 10, 186 (2009).
[10] J. Schmidhuber, Neural networks 61, 85 (2015).
[11] Y. LeCun, Y. Bengio, and G. Hinton, Nature 521, 436 (2015).
[12] T. Elsken, J. H. Metzen, and F. Hutter, Journal of Machine Learning Research 20, 1 (2019).
[13] P. Ren, Y. Xiao, X. Chang, P.-Y. Huang, Z. Li, X. Chen, and X. Wang, arXiv preprint arXiv:2006.02903 (2020).
[14] A. Kumar, T. Serra, and S. Ramalingam, arXiv preprint arXiv:1905.11428 (2019).
[15] T. Serra, A. Kumar, and S. Ramalingam, arXiv preprint arXiv:2001.00218 (2020).
[16] J. Pennington, S. S. Schoenholz, and S. Ganguli, arXiv preprint arXiv:1802.09979 (2018).
[17] L. Sagun, U. Evcı, V. U. Güney, Y. Dauphin, and L. Bottou, arXiv preprint arXiv:1706.04454 (2017).
[18] C. H. Martin and M. W. Mahoney, arXiv preprint arXiv:1901.08276 (2019).
[19] M. Súzen, J. J. Cerdà, and C. Weber, arXiv e-prints, arXiv:1911.07831 (2019), [arXiv:1911.07831 [cs.LG]]
[20] Y. Le Cun, I. Kanter, and S. A. Solla, Physical Review Letters 66, 2396 (1991).
[21] M. L. Mehta, Random Matrices (Elsevier, 2004).
[22] E. P. Wigner, SIAM Review 9, 1 (1967).
[23] F. J. Dyson, Journal of Mathematical Physics 3, 1199 (1962).
[24] F. Haake, Quantum Signatures of Chaos, Vol. 54 (Springer Science & Business Media, 2013).
[25] M. Súzen, C. Weber, and J. J. Cerdà, arXiv preprint arXiv:1704.08303 (2017).
[26] F. Mezzadri, Notices of AMS 54, 592 (2006).
[27] M. Berry and P. Shukla, New Journal of Physics 15, 013026 (2013).
[28] K. Rajan and L. Abbott, Physical Review Letters 97, 188104 (2006).
[29] K. Simonyan and A. Zisserman, arXiv preprint arXiv:1409.1556 (2014).
[30] K. He, X. Zhang, S. Ren, and J. Sun, in Proceedings of the IEEE conference on computer vision and pattern recognition (2016) pp. 770–778.
[31] G. Huang, Z. Liu, L. Van Der Maaten, and K. Q. Weinberger, in Proceedings of the IEEE conference on computer vision and pattern recognition (2017) pp. 4700–4708.
[32] A. Paszke, S. Gross, F. Massa, A. Lerer, J. Bradbury, G. Chanan, T. Killeen, Z. Lin, N. Gimelshein, L. Antiga, A. Desmaison, A. Kopf, E. Yang, Z. DeVito, M. Raison, A. Tejani, S. Chilamkurthy, B. Steiner, L. Fang, J. Bai, and S. Chintala, in NeurIPS 32, pp. 8024–8035.