Spectral ergodicity for explainable deep learning: A simulation approach

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Outline

1. Motivation
2. Circular ensembles
3. Spectral ergodicity
4. Simulations and results
5. Conclusions and outlook

1. Motivation: Success

- State-of-the-art performance in computer vision
  LeCun, Bengio, Hinton, Nature, 521, 436 (2015)

- No explanation so far but success is attributed to

  - *network topology,* multiple processing layers.
  - availability of *large labelled datasets*.
  - leap in *computing capacity*.

- Need a theory or quantification for explanation.

1. Motivation: Scope

- Why do we need to explain?
    - Theoretical understanding: Rethinking generalisation
      Probably Approximately Correct (PAC)
      Vapnik-Chervonenkis (VC)
      Zhang et. al. (2016)
    - Quantify how it works to better tune.
    - No black-box tools.
    - Legal issues in industry.

1. Motivation: Approaches

- Understanding spectral properties are core practice
    - Weight initialization: Dynamical Isometry.
      Pennington et. al. (2017)
    - Singularity in Hessian.
      Sagun et. al. (2016, 2017)
- Information theory: relative compressibility of layers
  Tishby et. al. (2015)

1. Motivation: Our approach

- The concept of *spectral ergodicity*
  Süzen et. al. (2017)

- How to reach to a generic conclusion independent of

  - network architecture (topology).
  - learning algorithm.
  - dataset size and type.
  - training procedure.

- Sample an ensemble of weight matrices.
  Süzen et. al. (2017)

2. Circular ensembles: Introduction

- A realistic simulation of weight matrices
  - Generate ensemble of matrices.
  - Spectral radius reflects stable learning.

- Circular ensembles
  - Spectral radius is close to 1 for *Unitary* ensemble.
  - Numerically stable and mathematically sound generation procedures.

2. Circular ensembles: Parallel Generation

Primary object to generate:
Random Gaussian Hermitian matrix $H \in \mathbb{C}^{N \times N}$

$$H_{ij} = \frac{1}{2}(a_{ij} + Ib_{ij} + a_{ji} - Ib_{ji})$$

$$1 \leq i, j \leq N$$

$a_{ij}, b_{ij}, a_{ji}, b_{ji} \in \mathbb{G}$ i.i.d. Gaussian random numbers

bristol.ensembles.Circular
https://pypi.python.org/pypi/bristol

2. Circular ensembles: Parallel Generation

Circular Unitary Ensemble (CUE) bristol.ensembles.Circular.gen_cue

$$U_{ij} = exp(\gamma_i I) \cdot v_j^i \qquad \gamma_i \in [0, 2\pi]$$

Circular Orthogonal Ensemble (COE) bristol.ensembles.Circular.gen_coe

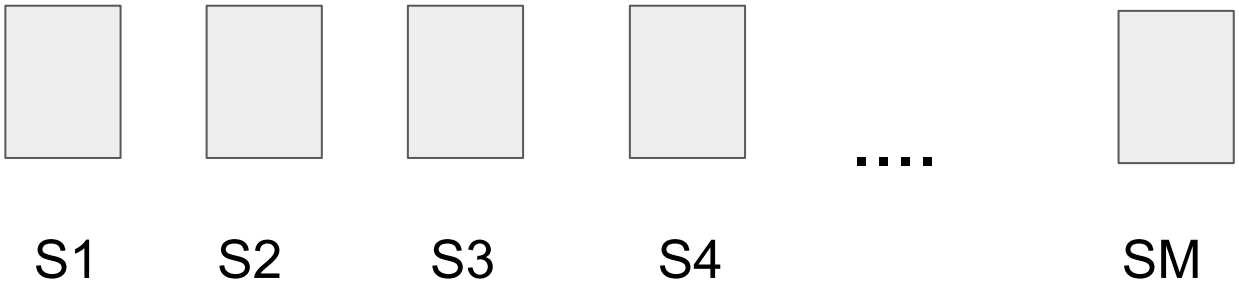
$$O = U^T U$$

Circular Symplectic Ensemble (CSE) bristol.ensembles.Circular.gen_cse

$$S \in \mathbb{C}^{2N \times 2N} \qquad S = (ZU^T Z)U$$

2. Circular ensembles: Random stream chunking

A note on reproducibility against a serial implementation



Given ensemble of size M, retain seeds vector (S1, S2, S3, S4, …, SM), so each processor/chunk gets the same random stream chunking regardless of parallel or serial execution.

bristol.ensembles.Circular.eigen_circular_ensemble

2. Circular ensembles: Interpretation

- Given network architecture:
    - Ensemble of weight matrices for different layers in feed forward networks.
    - Ensemble of weight matrices for entire network in non-sparse recurrent networks.

- Sample ensemble of circular matrices M times,
  number of hidden layers with different sizes N,
  depth in the given layer.

3. Spectral Ergodicity: Definition

- Sample ensemble of circular matrices `M` times, with different sizes `N` and given bin size `b`.
  - Time-averaged eigenvalue-spectra: Compute eigenvalue spectra for `j-th` realization

    $\rho_j(b_k)$
  - Ensemble-averaged eigenvalue-spectra: Compute average spectra over M realisation.

    $$\bar{\rho}(b_k) = \frac{1}{M} \sum_{j=1}^{M} \rho_j(b_k)$$

3. Spectral Ergodicity: Definition

- Approach to spectral ergodicity for given weight matrix size, corresponds to depth of a given layer.

$$\Omega_k^N \equiv \Omega^N(b_k) = \frac{1}{M \cdot N} \sum_{j=1}^{M} \left[\rho_j(b_k) - \bar{\rho}(b_k)\right]^2$$

- Inspired from physical definition of ergodicity, Süzen (2014) recall diffusion coefficient over time.

3. Spectral Ergodicity: Definition

- How far would *spectral ergodicity* drift with an additional depth? A *distance metric*

$$D_{se}(N_a, N_b) = D_{KL}(\Omega^{N_a} || \Omega^{N_b}) + D_{KL}(\Omega^{N_b} || \Omega^{N_a})$$

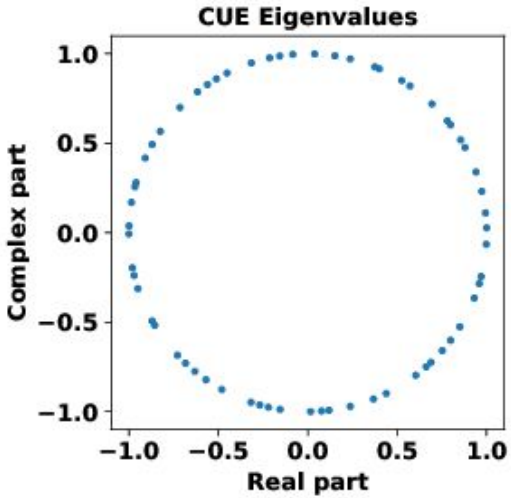
$$D_{KL}(\Omega^{N_a} || \Omega^{N_b}) = \sum_{k=1}^{K} \Omega_k^{N_a} \log_2(\Omega_k^{N_a} / \Omega_k^{N_b})$$

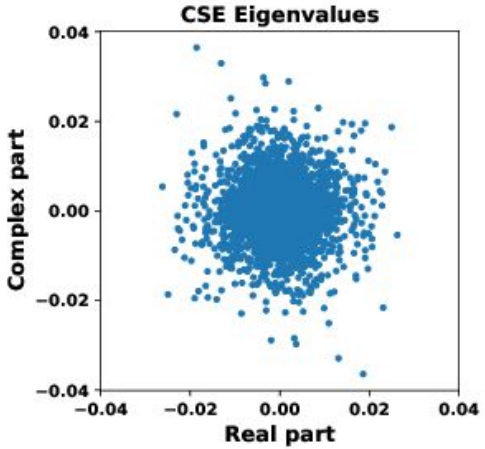
4. Simulations and Results: Summary

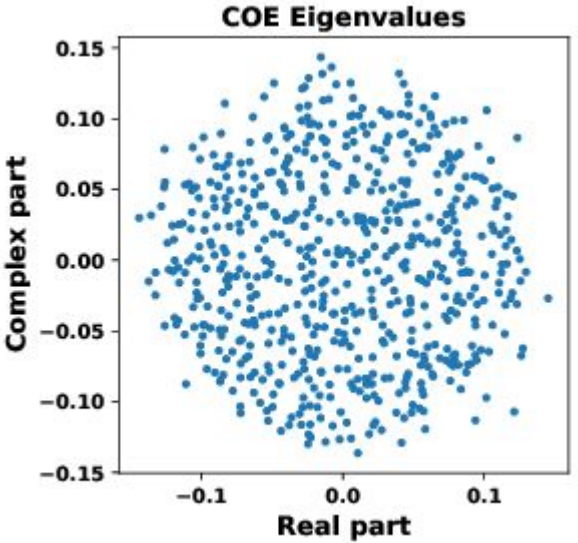
- Ensemble size, M=40, recall, number of hidden layers.
- Weight matrix sizes, N=64, 128, 256, 512, 768, 1024, recall, layer depth.
- Generate all matrices.
- Generate eigenvalues, data available publicly. https://zenodo.org/record/822411#.WmX1AHWnHqM
- Compute the distance metric for increasing depth transitions.
  - 64-128, 128-256, 256-512, 512-768, 768-1024
  - Jupyter Notebook, available publicly. https://github.com/msuzen/bristol/blob/v0.2.2/works/spectralErgodicity/02_ergodicity_random_matrix.ipynb

4. Simulations and Results: Eigenvalues

- Sample of eigenvalues for different ensembles.

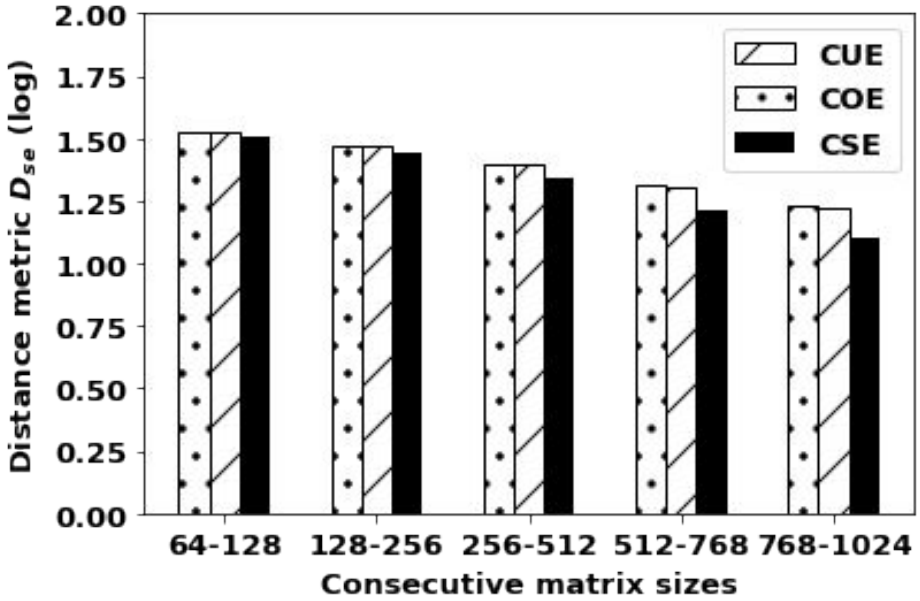






4. Simulations and Results: Spectral ergodicity

- Distance metric.



5. Conclusions and outlook

- We attribute the success of deep learning to spectral ergodicity of a given topology and learning algorithm using surrogate random matrices.
- Interpretation of ensemble can be different layers or entire network.
- The work can be extended to synaptic matrices in the context of spiking neurons.

Thank you
Q & A

Spectral Ergodicity in Deep Learning Architectures via Surrogate Random Matrices
Mehmet Süzen, Cornelius Weber, Joan J. Cerdà
arXiv preprint arXiv:1704.08303 (2017)
dataset zenodo doi: 10.5281/zenodo.822411
code zenodo doi: 10.5281/zenodo.579642

Python package:
https://pypi.python.org/pypi/bristol