Visualizing the PHATE of Neural Networks

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scottgigante/M-PHATE

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NEURAL INFORMATION PROCESSING SYSTEMS

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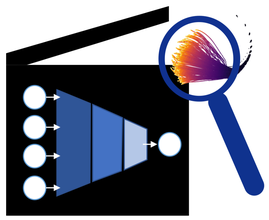
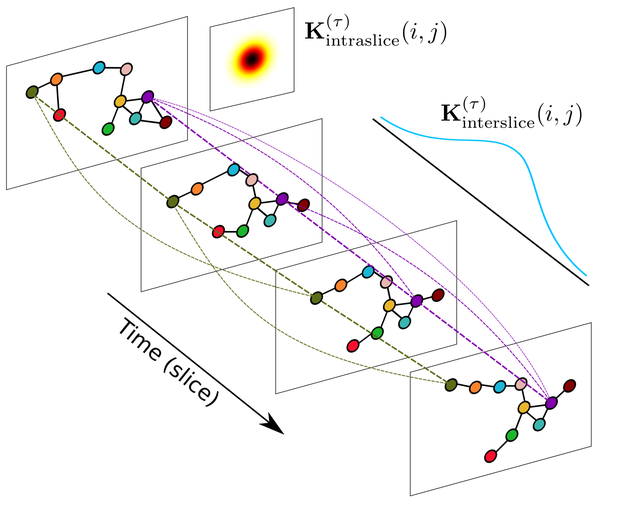
Introduction

- Grand challenge in deep learning: why and how do certain neural networks outperform others?
- Our work: Multislice PHATE (M-PHATE) for visualizing neural networks' evolution through training
- M-PHATE exposes hidden unit dynamics & structure without validation data



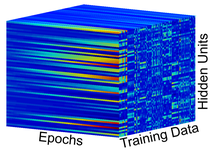
Multislice graph construction

Multislice graph represents similarities between hidden units over time



$$\mathbf{K}^{(\tau)}_{\text{intraslice}}(i,j) = \exp\left(-\|\mathbf{T}(\tau,i) - \mathbf{T}(\tau,j)\|_2^{\alpha} / \sigma^{\alpha}_{(\tau,i)}\right)$$

$$\mathbf{K}^{(i)}_{\text{interslice}}(\tau,\upsilon) = \exp\left(-\|\mathbf{T}(\tau,i) - \mathbf{T}(\upsilon,i)\|_2^{2} / \epsilon^{2}\right)$$



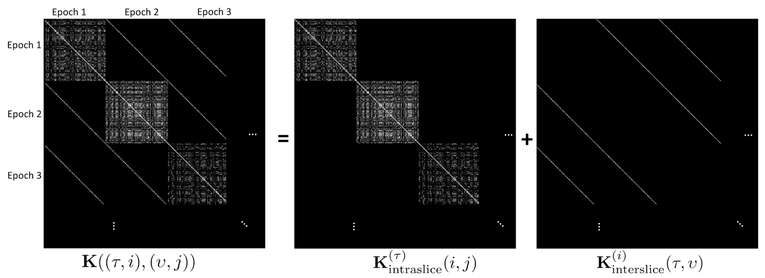
$\mathbf{T}(\tau,i)$ Activations of hidden unit i at epoch τ over a sample of the training set

$\sigma_{(\tau,i)}$ Distance of $\mathbf{T}(\tau,i)$ to its kth nearest neighbor in epoch τ

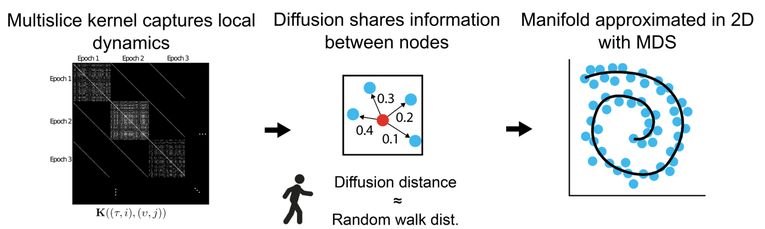
ϵ Mean distance of $\mathbf{T}(\tau,i)$ to its kth nearest neighbor in all epochs from hidden unit i

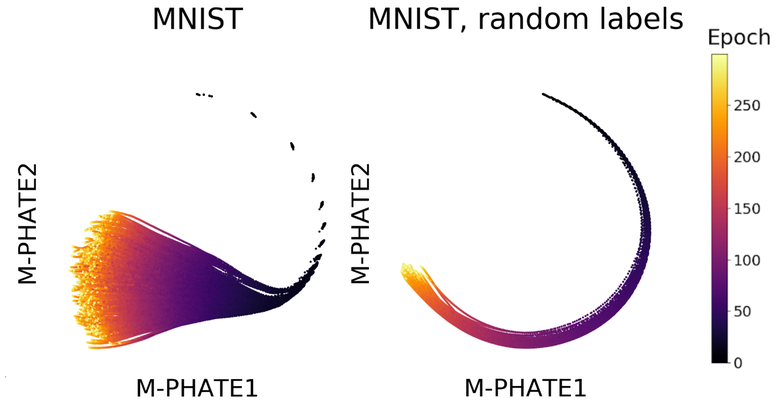
Low-dimensional embedding

Multislice kernel represents each hidden unit at each epoch as a single data point

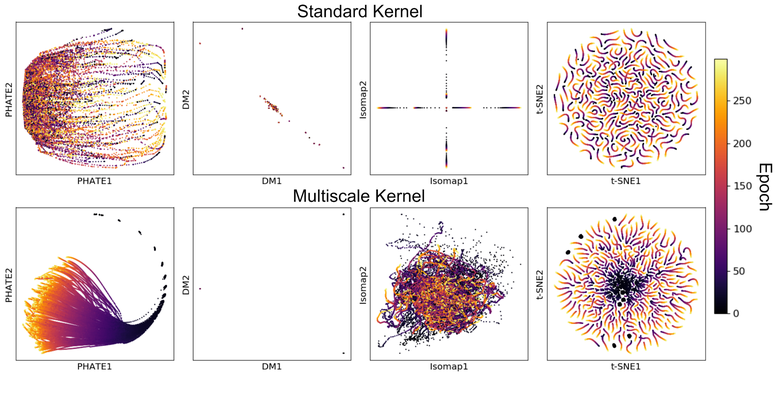


PHATE[3] embeds diffusion distances in low dimensions



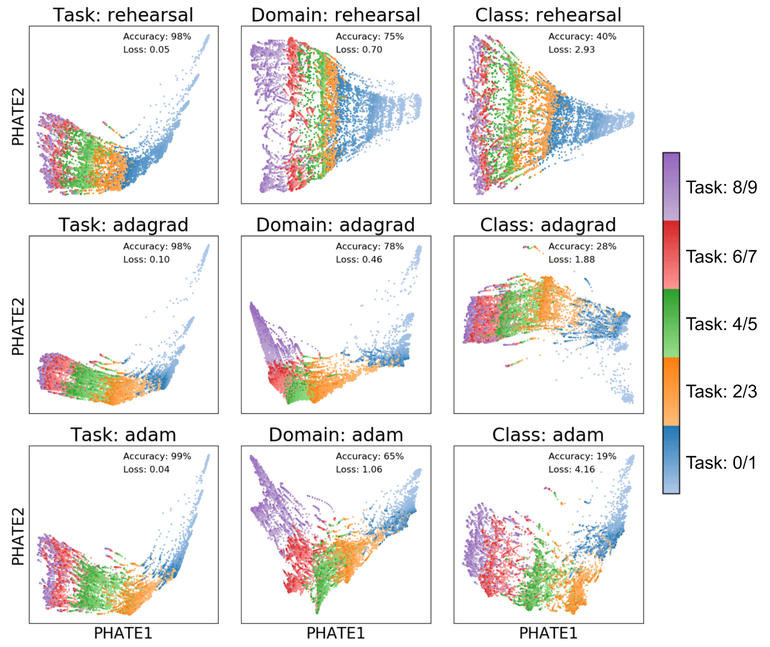


M-PHATE provides unique insight into network's evolution

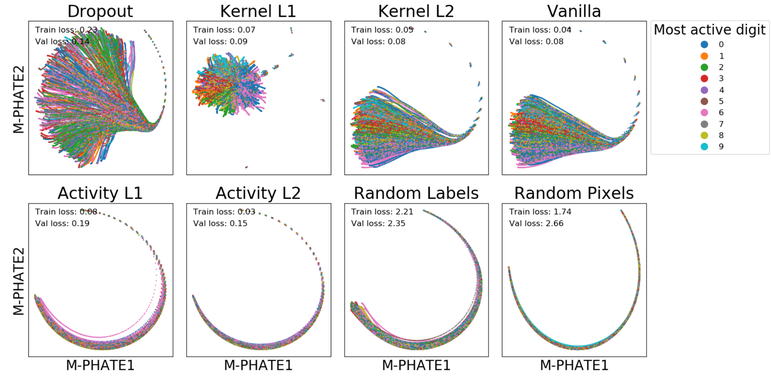


Applications

Continual learning: performance of task-switching networks[2] trained on MNIST is predicted by retention of structure in M-PHATE



Generalization: discrepancy between training and validation loss in classifiers corresponds to complexity of M-PHATE visualization



Conclusion

- M-PHATE allows us to visually understand a network's performance without requiring access to validation data
- Networks with higher entropy and contiguity in M-PHATE perform better in generalization and continual learning

References

1. Gigante, Charles, Krishnaswamy and Mishne. *Visualizing the PHATE of Neural Networks.* NeurIPS 2019.
2. Hsu, Liu and Kira. *Re-evaluating Continual Learning Scenarios: A Categorization and Case for Strong Baselines.* Continual learning workshop, NeurIPS 2018. arXiv:1810.12488.
3. Moon, van Dijk, Wang, Gigante, et al. *Visualizing structure and transitions in high-dimensional biological data.* Nature Biotechnology, doi:10.1038/s41587-019-0336-3.

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