Towards a Phenomenological Understanding of Neural Networks

Samuel Tovey, Sven Krippendorf, Michael Spannowsky

Konstantin Nikolaou, Christian Holm

9/11/2023

Why is this Necessary?

https://openai.com, , [1] (Sterling & Laughlin, 2015), [2] (Thorpe et al., 1996), freepik

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Parameters	175 billion
Training Time	Several months
Training Cost	~ $4.6 million

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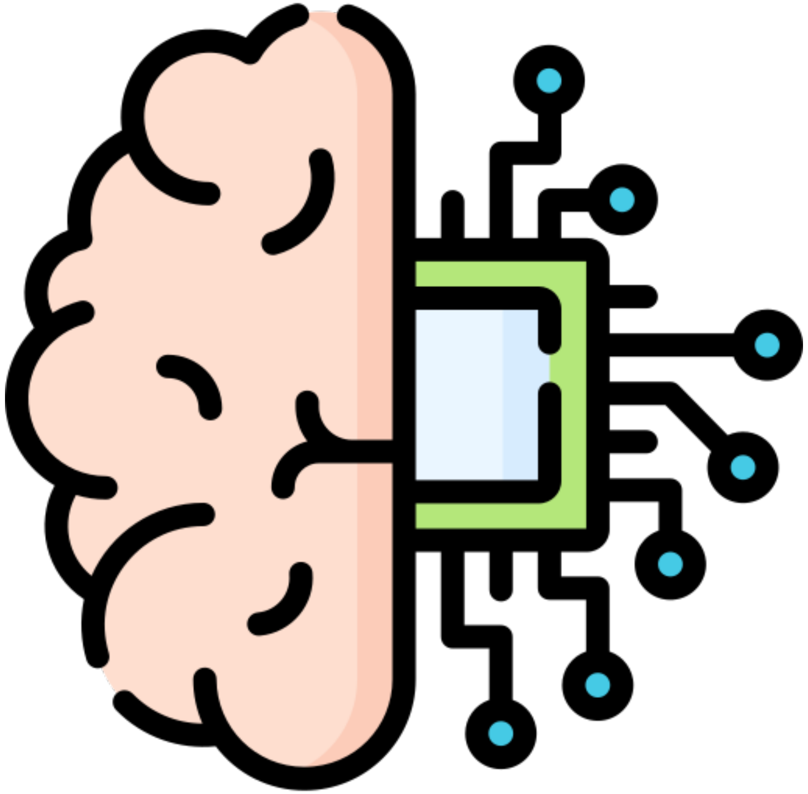

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Neurons	86 billion
Object recognition time[2]	150 ms
Energy cost[1]	< 20 W

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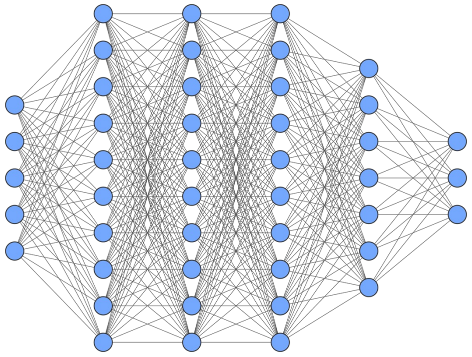
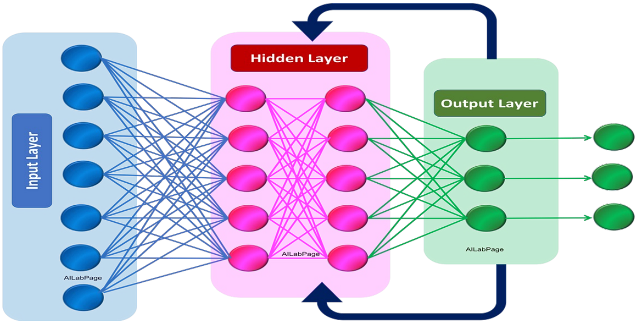
Collective Variables for Neural Networks

Entropy, trace, and more...

What is a Neural Network? (The NN Zoo)

Function fitting in a very high dimensional space.





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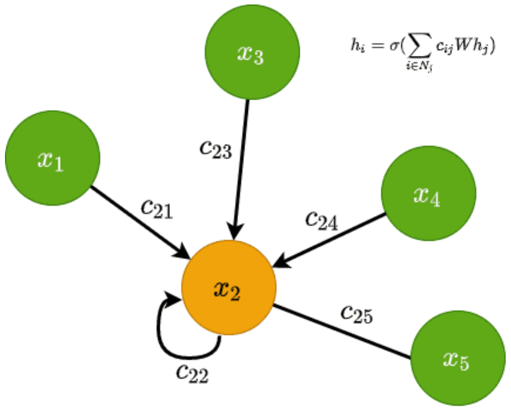

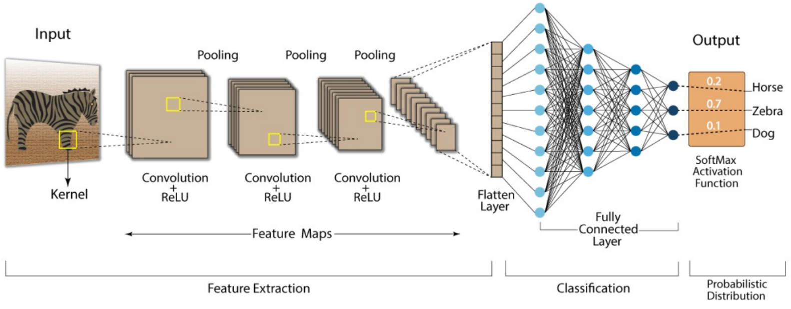

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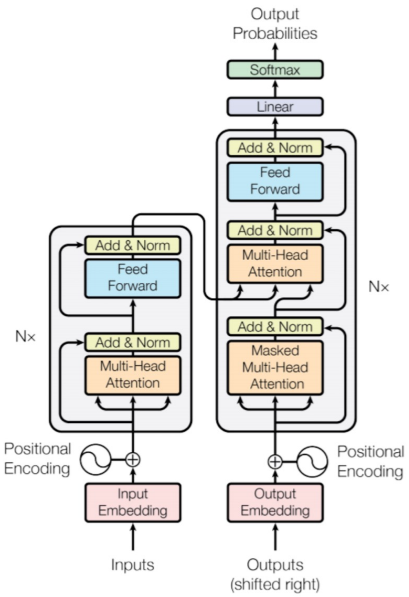

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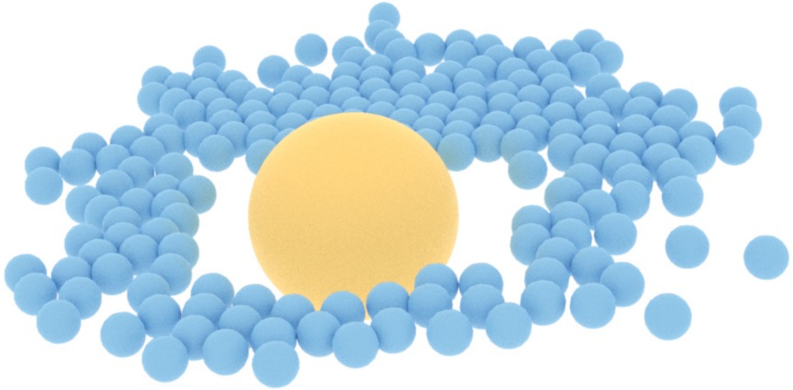

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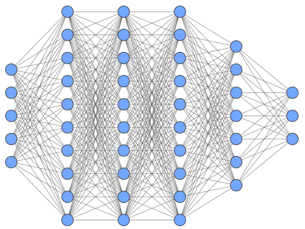

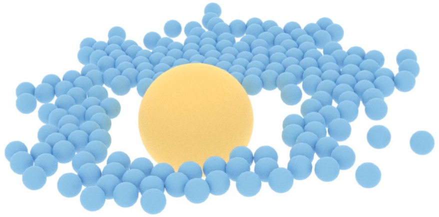

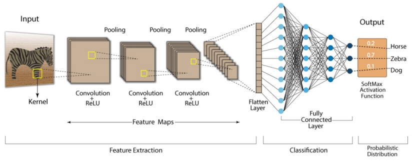

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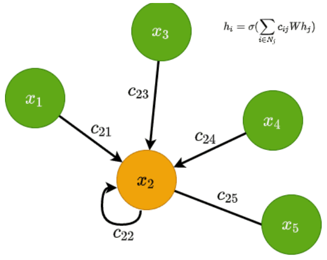

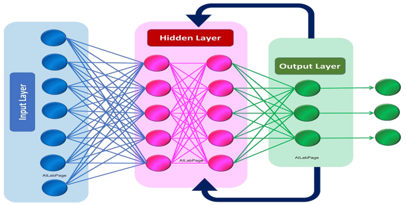

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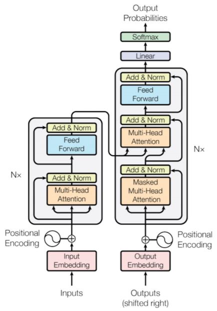

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$$f_\theta : X \rightarrow Y$$

$$\theta = \{\theta_0, \ldots, \theta_N\}$$

$$\theta_i' = \theta_i - \eta \cdot \partial_{\theta_i} \mathcal{L}(f(X), Y)$$

How do they evolve?

Architecture component

$$f'_\theta(X) = f_\theta\,(x) - \underbrace{\begin{pmatrix} \nabla_\theta f_\theta(x_0)\cdot\nabla_\theta f_\theta(x_0) & \cdots & \nabla_\theta f_\theta(x_0)\cdot\nabla_\theta f_\theta(x_N) \\ \vdots & \ddots & \vdots \\ \nabla_\theta f_\theta(x_N)\cdot\nabla_\theta f_\theta(x_0) & \cdots & \nabla_\theta f_\theta(x_N)\cdot\nabla_\theta f_\theta(x_N) \end{pmatrix}}_{\Theta} \cdot \nabla_{f_\theta}\,\mathcal{L}(X)$$

Loss component

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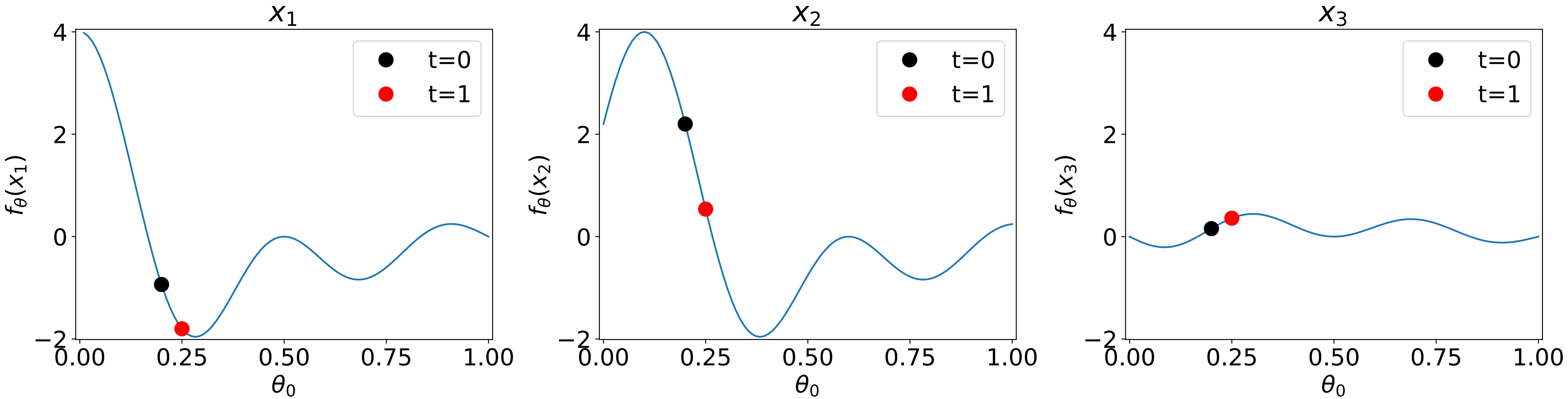

Collective Variables

Eigenvectors of the NTK matrix

$$\Theta = V\Lambda\mathrm{V}^{T}$$

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$$S = -\sum_i \lambda_i \cdot \ln \lambda_i$$

Measure of correlation in data

$$Tr(\Theta) = \sum_i \Theta_{ii}$$

Weighting of largest step direction

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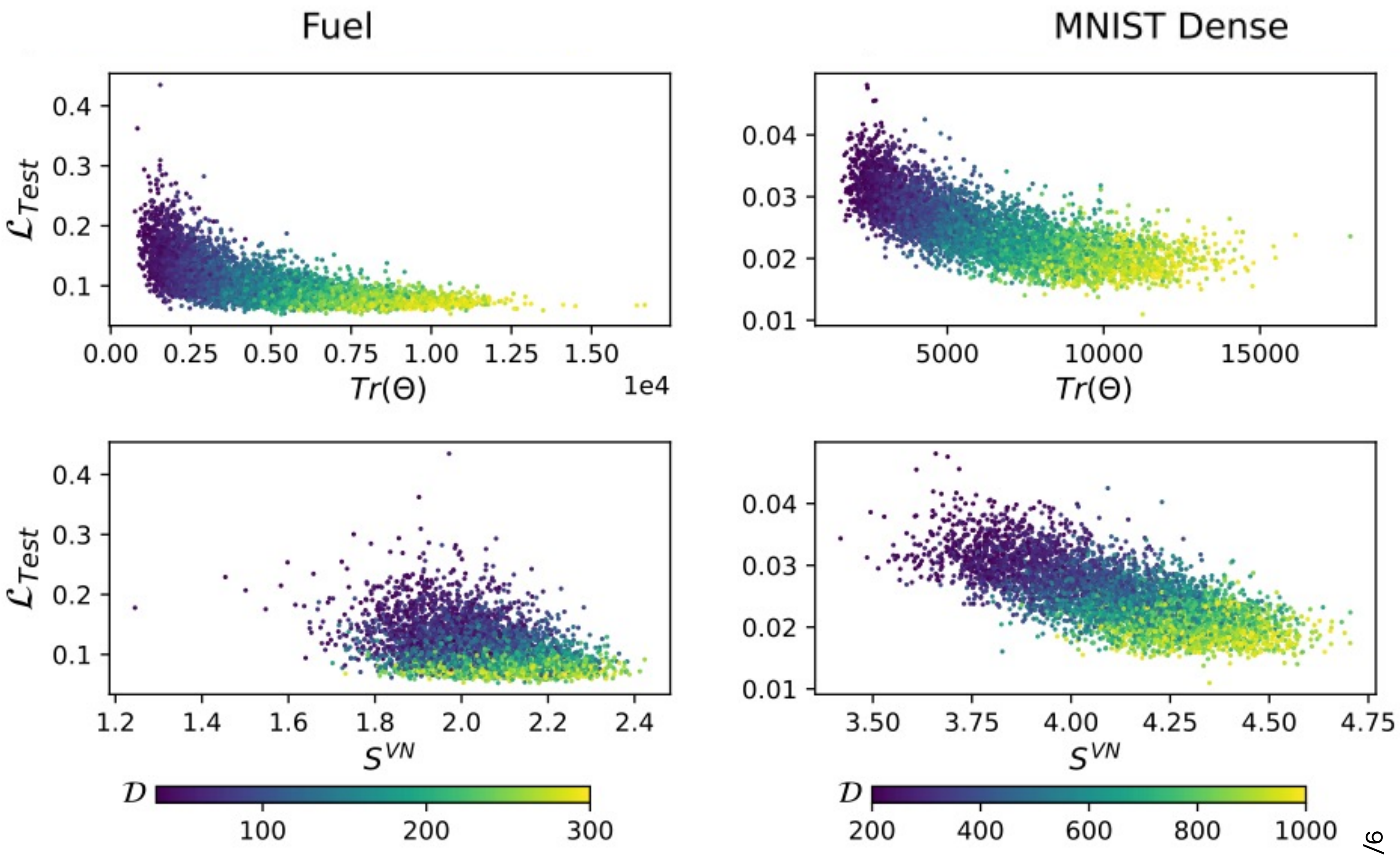

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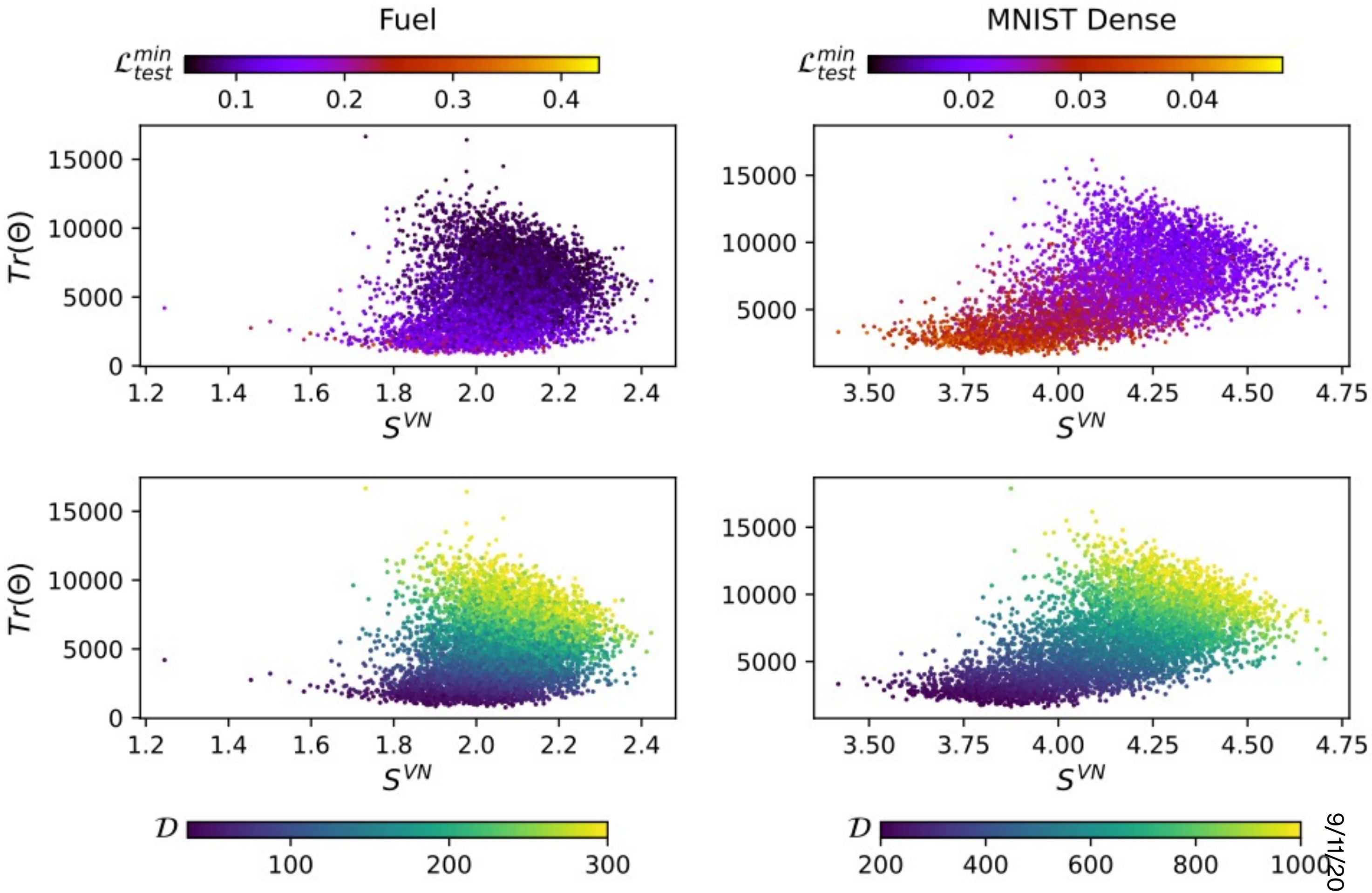

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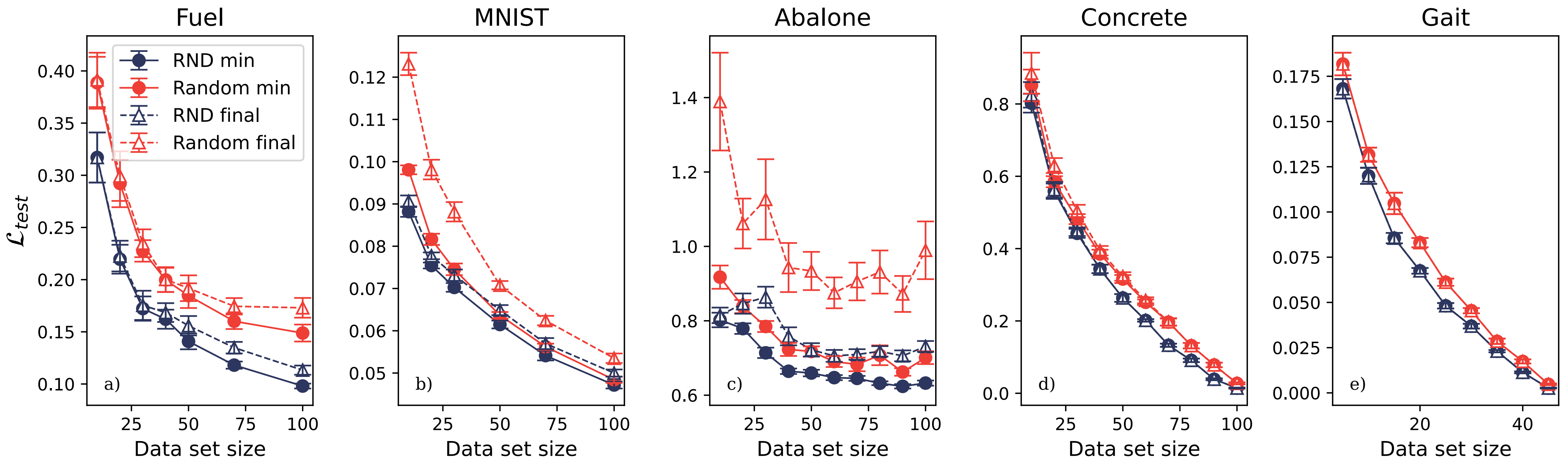
Datasets	5
Optimizer	ADAM(0.001)
Loss Function	MSE or CE
Architectures	5
Epochs	200

Data

Levelling the playing field

Data Selection in Neural Networks



RND selected data-sets outperform random selection

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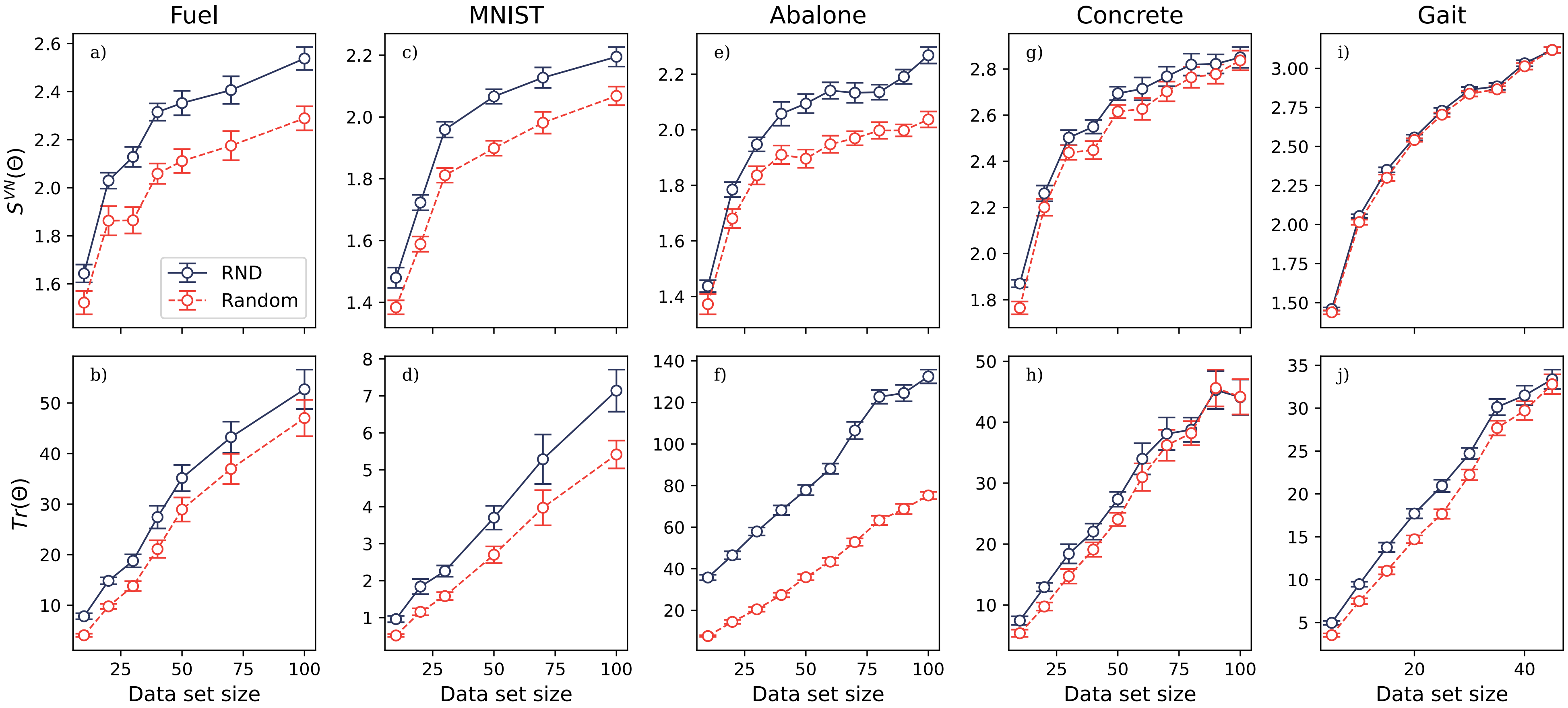
What do the collective variables say?



Datasets with larger trace / entropy perform better!

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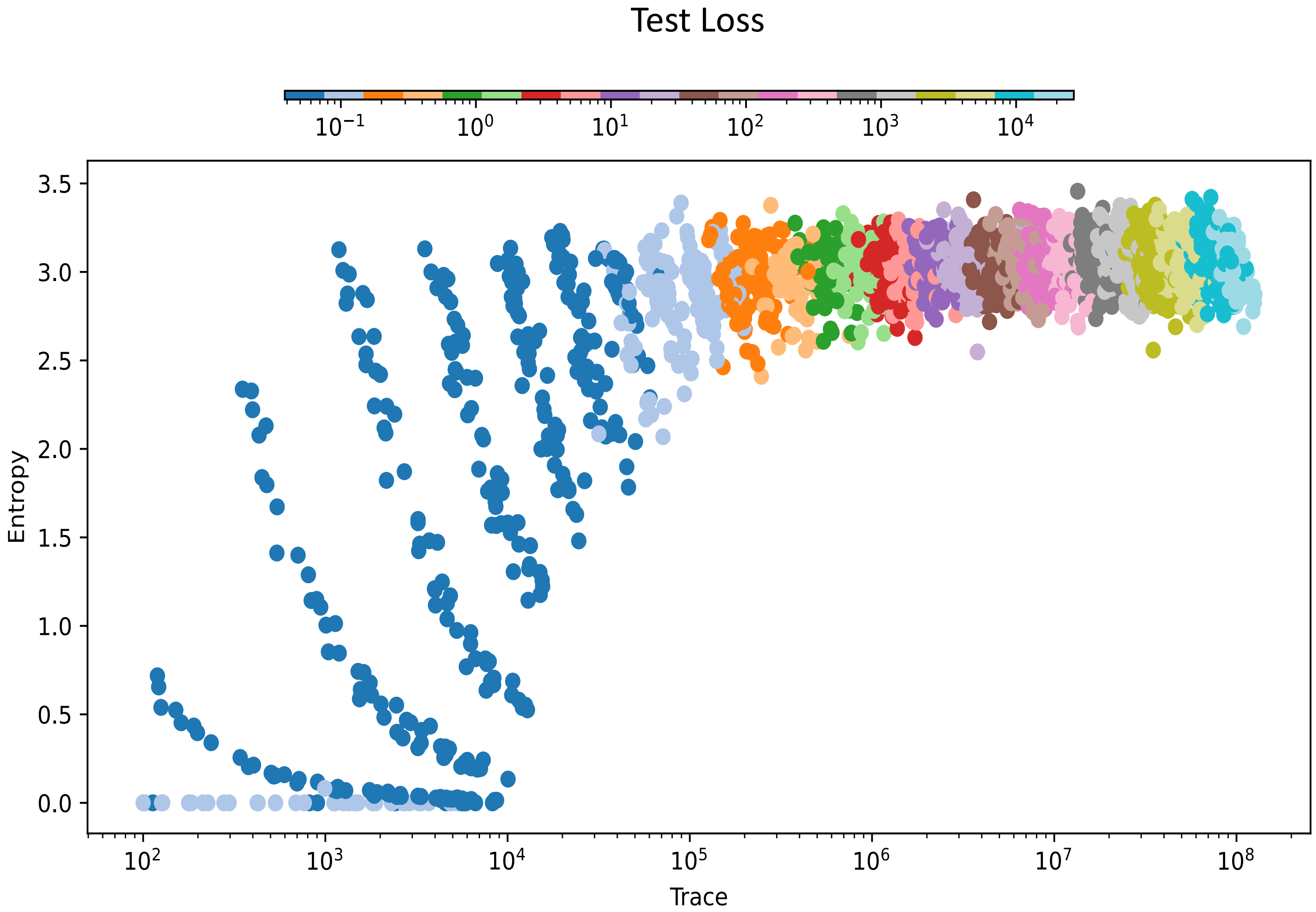
Next Steps: Initialization

Dataset	MNIST (1000)
Optimizer	ADAM(0.001)
Architecture	$\mathcal{D}^{128} r \mathcal{D}^{128} r \mathcal{D}^{10}$
Weight std	0.0 – 1.0
Bias std	0.0 - 1.0



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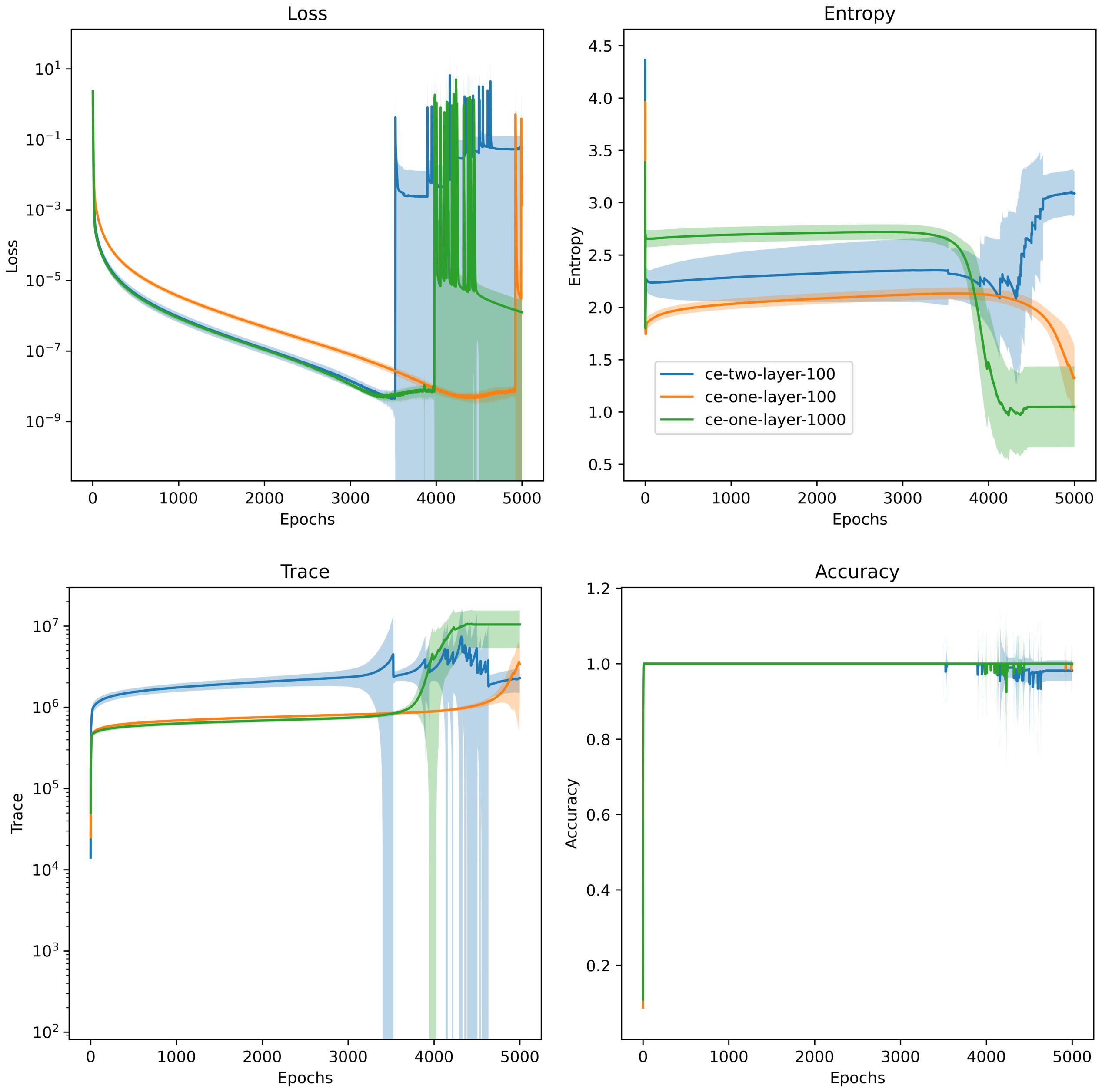
Next Steps: Dynamics

- Compute CVs at all epochs
- Search for universal behaviour
- Interesting long-time behaviour

Dataset	MNIST (1000)
Loss Function	Cross-entropy
Optimizer	SGD(0.01)
Architectures	3



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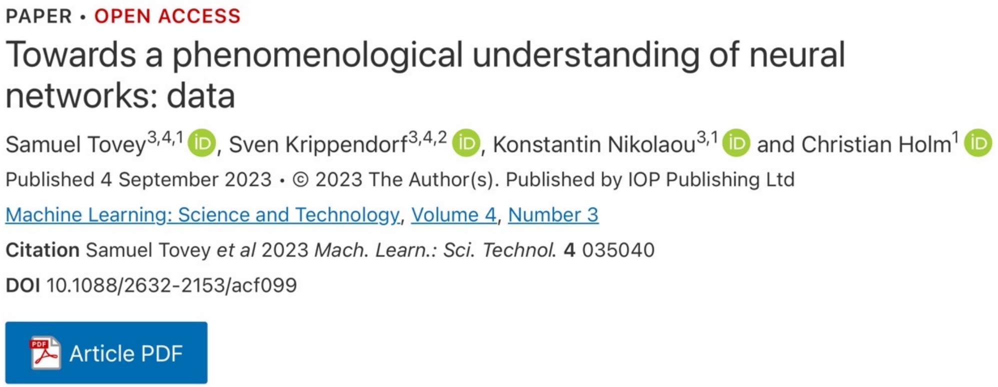
Wrapping Up: ZnNL



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Towards a phenomenological understanding of neural networks: data

Samuel Tovey[3,4,1], Sven Krippendorf[3,4,2], Konstantin Nikolaou[3,1] and Christian Holm[1]

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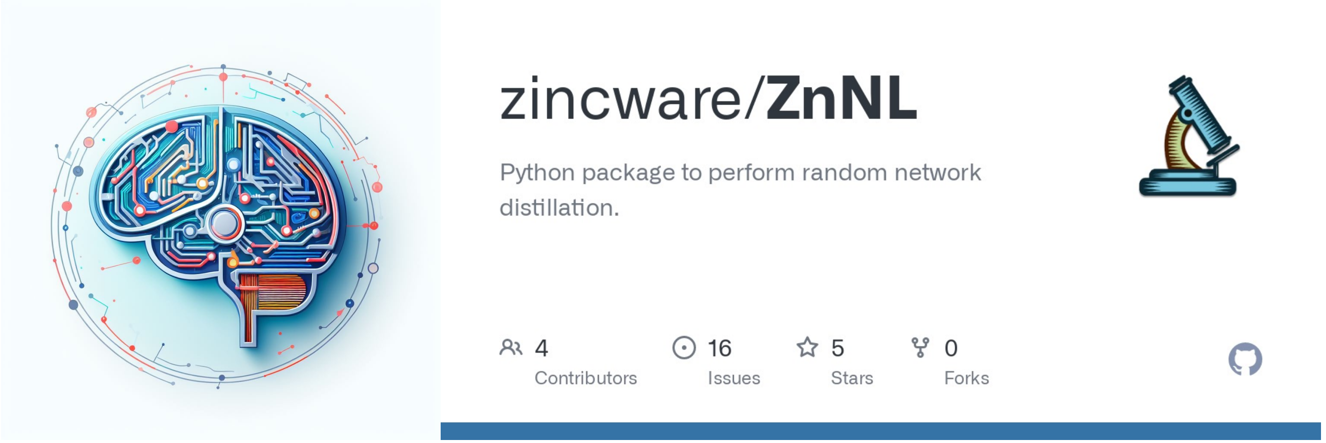

zincware/**ZnNL**

Python package to perform random network distillation.

https://github.com/zincware/ZnNL

DALL . E 3

- Tools of physics can help us understand neural networks
  - Statistical Physics
  - Quantum Mechanics

- We can leverage this understanding
  - Data Selection
  - Initialization
  - Optimization and dynamics