DEEP LAYER-WISE NETWORKS HAVE CLOSED-FORM WEIGHTS

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We answer 2 theoretical questions about Layer-wise networks.

Abstract There is currently a debate within the neuroscience community over the likelihood of the brain performing backpropagation (BP). To better mimic the brain, training a network *one layer at a time* with only a "single forward pass" has been proposed as an alternative to bypass BP; we refer to these networks as "layer-wise" networks. We continue the work on layer-wise networks by answering two outstanding questions.

1. *do they have a closed-form weights?*
2. *how do we know when to stop adding more layers?*

This work proves that the **Kernel Mean Embedding** is the closed-form weight that automatically optimizes the network while driving them to converge towards a highly desirable kernel for classification; we call it the **Neural Indicator Kernel**.

Claim 1: If we stack the network with the HSIC objective at each layer

$$\max_{W_l} \quad \text{Tr}\left(\Gamma\left[\psi(R_{l-1}W_l)\psi^T(R_{l-1}W_l)\right]\right) \quad \text{s.t.} \quad W_l^T W_l = I, \Gamma = HYY^T H. \tag{1}$$

then, the repetitive usage the Kernel Embedding of r_{l-1} for W_l guarantees the Global Optimum of Eq. (1). The kernel embedding is defined as

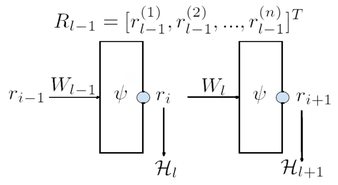


Fig. 1: Layer notation

$$W_s = \frac{1}{\sqrt{\zeta}}\left[\sum_\iota r_\iota^{(1)} \ \sum_\iota r_\iota^{(2)} \ ... \ \sum_\iota r_\iota^{(\tau)}\right] \tag{2}$$

Implication: Instead of searching to connect backpropagation to brain function, our proof suggests that very simple and repetitive patterns can also achieve equivalent training accuracy on any dataset. This strategy might be an easier path to explain the brain.

Claim 2: Let $\mathcal{S}$ be the set of pairwise samples within the same class and $\mathcal{S}^c$ its complement. By stacking the network in Fig.1, the network converges to the feature map of the following kernel:

$$\lim_{l\to\infty} \mathcal{K}(x_i, x_j)^l = \mathcal{K}^*(x_i, x_j)^l = \begin{cases} 0 & \forall i,j \in \mathcal{S}^c \\ 1 & \forall i,j \in \mathcal{S} \end{cases}. \tag{3}$$

Implication: Our construct converges to fixed kernel.

Claim 3: We define the within S_w^l and between S_b^l class scatter matrices as

$$S_w^l = \sum_{i,j\in\mathcal{S}} W_l^T(r_i - r_j)(r_i - r_j)^T W_l \quad \text{and} \quad S_b^l = \sum_{i,j\in\mathcal{S}^c} W_l^T(r_i - r_j)(r_i - r_j)^T W_l. \tag{4}$$

As the number of layers approaches ∞, the trace ratio approach 0.

$$\lim_{l\to\infty} \frac{\text{Tr}(S_w^l)}{\text{Tr}(S_b^l)} = 0 \tag{5}$$

Implication: While converging towards a kernel, the network via the HSIC objective pulls samples of the same class into a single point while pushing samples of different classes apart.

Why Maximize HSIC? What does it Accomplish?

Claim 4: We prove that maximizing HSIC Implicitly Minimizes Cross-Entropy (CE) and MSE for Classification.

Implication 1: Classification traditionally use MSE or CE. We refer to these objectives as **label-matching objectives**. We prove the HSIC is a **nonlabel-matching objective**. This implies that using our layer-wise construct for classification is equally flexible as a network trained by backpropagation.

Implication 2: This algorithm is actually learning the optimal kernel to perform kernel density estimation.

Implication 3: Simple and repetitive patterns can also achieve Universality. Perhaps we should seek to explain the brain via this path.

Claim 5: W_s is not the optimal layer-wise solution where at each layer

$$\frac{\partial}{\partial W_l}\mathcal{H}_l(W_s) \neq 0. \tag{6}$$

Implication: Unlike existing layer-wise network, obtaining the optimal solution of each layer is unnecessary.

Claim 6: The optimal solution W^* where $\frac{\partial}{\partial W_l}\mathcal{H}_l(W_s) = 0$ is the eigenvector of the following matrix

$$\mathcal{Q}_{li} = R_{l-1}^T(\hat{\Gamma} - \text{Diag}(\hat{\Gamma}1_n))R_{l-1}, \tag{7}$$

where $\hat{\Gamma}$ is a function of W_{li} computed with $\hat{\Gamma} = \Gamma \odot K_{R_{l-1}W_{li}}$.

Implication: While W_s is interesting from a neuroscience perspective, W^* is the optimal solution to optimize the network. The matrix $\mathcal{Q}$ id $d \times d$, therefore, **it does not depend on the size of the data.**

What can we say about Generalization?

Observations:

1. W^* converges faster, requiring fewer layers.
2. W^* generalizes better?
3. W^* uses an infinitely wide network and have infinite complexity why does it generalize at all?

Claim 7: The solution yield by the eigenvector of $\mathcal{Q}$ **implicitly** regularizes the HSIC objective.

The objective can be reformulated to isolate out n functions $[D_1(W_l), ..., D_n(W_l)]$ that act as a penalty term during optimization. Let $\mathcal{S}_i$ be the set of samples that belongs to the i_{th} class and let $\mathcal{S}_i^c$ be its complement, then each function $D_i(W_l)$ is defined as

$$D_i(W_l) = \frac{1}{\sigma^2}\sum_{j\in\mathcal{S}_i}\Gamma_{i,j}\mathcal{K}_{W_l}(r_i, r_j) - \frac{1}{\sigma^2}\sum_{j\in\mathcal{S}_i^c}|\Gamma_{i,j}|\mathcal{K}_{W_l}(r_i, r_j). \tag{8}$$

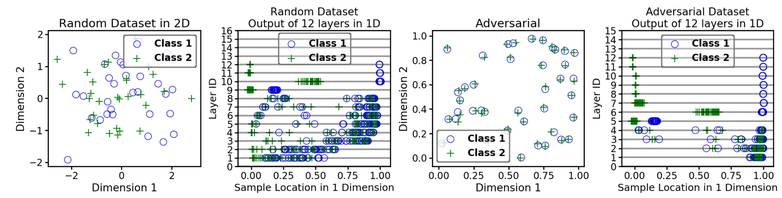
Then Eq. (1) is equivalent to

$$\max_{W_l}\sum_{i,j}\frac{\Gamma_{i,j}}{\sigma^2}e^{-\frac{(r_i-r_j)^T WW^T(r_i-r_j)}{2\sigma^2}}(r_i^T W_l W_l^T r_j) - \sum_i D_i(W_l)||W_l^T r_i||_2. \tag{9}$$

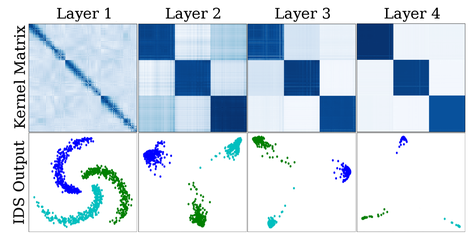
Implication: Based on this claim, $D_i(W_l)$ adds a negative variable cost to the sample norm in IDS, $||W_l^T r_i||_2$, describing how ISM implicitly regularizes HSIC. In fact, a better W_l imposes a heavier penalty on the objective where the overall HSIC value may actually decrease.

Experimental Results

Experiment 1: We designed an Adversarial and Random dataset to trick the network using W_s. It was able to achieve perfect classification on the 12th layer.



Experiment 2: Verification of Claims 2 and 3.



Experiment 3: We plot out all key metrics during training *at each layer*. Here, the objective is clearly monotonic and converging towards a global optimal of 1. Moreover, the trends for $\mathcal{T}$ and C indicate an incremental clustering of samples into separate partitions. Corresponding to low $\mathcal{T}$ and C values, the low MSE and CE errors at convergence further reinforces claim 4. This experiment indicates that the *behavior of a layer-wise MLP is predictable* via the cyclic transition model.

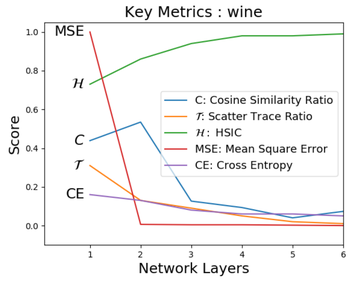


Fig. 4: Layer notation

Experiment 4: Using both W_s and W^*, we conduct 10-fold cross-validation across all 8 datasets and report their mean and the standard deviation for all key metrics. We compare our MLP against MLPs of the same size trained via SGD, where instead of HSIC, MSE and CE are used as the empirical risk.

	obj	$\sigma\uparrow$	$L\downarrow$	Train Acc ↑	Test Acc ↑	Time(s) ↓	$\mathcal{H}^*\uparrow$	MSE ↓	CE ↓	$C\downarrow$	$\mathcal{T}\downarrow$
random	ISM	0.38	3.30 ± 0.64	**1.00 ± 0.00**	0.38 ± 0.21	**0.40 ± 0.37**	**1.00 ± 0.01**	**0.00 ± 0.01**	0.05 ± 0.00	**0.00 ± 0.06**	0.02 ± 0.0
	W_s	0.15	12 ± 0.66	0.99 ± 0.01	0.45 ± 0.20	0.52 ± 0.05	0.92 ± 0.01	2.37 ± 1.23	0.06 ± 0.13	0.05 ± 0.02	0.13 ± 0.01
	CE	-	3.30 ± 0.64	**1.00 ± 0.00**	0.48 ± 0.17	25.07 ± 5.55	**1.00 ± 0.00**	10.61 ± 11.52	**0.0 ± 0.0**	**0.0 ± 0.0**	**0.0 ± 0.0**
	MSE	-	3.30 ± 0.64	0.98 ± 0.04	**0.63 ± 0.21**	23.58 ± 8.38	0.93 ± 0.12	0.02 ± 0.04	0.74 ± 0.03	0.04 ± 0.04	0.08 ± 0.1
adver	ISM	0.5	3.60 ± 0.92	**1.00 ± 0.00**	0.38 ± 0.10	**0.52 ± 0.51**	**1.00 ± 0.00**	**0.00 ± 0.00**	**0.04 ± 0.00**	**0.01 ± 0.08**	**0.01 ± 0.0**
	W_s	0.03	12.70 ± 1.50	0.90 ± 0.04	**0.42 ± 0.18**	2.82 ± 0.81	0.59 ± 0.19	15.02 ± 11.97	0.32 ± 0.15	0.30 ± 0.18	0.34 ± 0.19
	CE	-	3.60 ± 0.92	0.59 ± 0.04	0.29 ± 0.15	69.54 ± 24.14	0.10 ± 0.07	0.65 ± 0.16	0.63 ± 0.04	0.98 ± 0.03	0.92 ± 0.0
	MSE	-	3.60 ± 0.92	0.56 ± 0.02	0.32 ± 0.20	113.75 ± 21.71	0.02 ± 0.01	0.24 ± 0.01	0.70 ± 0.00	0.99 ± 0.02	0.95 ± 0.0
spiral	ISM	0.46	5.10 ± 0.30	**1.00 ± 0.00**	**1.00 ± 0.00**	**0.87 ± 0.08**	0.98 ± 0.01	0.01 ± 0.00	0.02 ± 0.01	0.04 ± 0.03	0.02 ± 0.0
	W_s	0.93	4.00 ± 1.18	0.99 ± 0.01	0.96 ± 0.02	13.54 ± 5.66	0.88 ± 0.03	38.60 ± 25.24	0.06 ± 0.02	0.08 ± 0.04	0.08 ± 0
	CE	-	5.10 ± 0.30	**1.00 ± 0**	**1.00 ± 0**	11.59 ± 5.52	**1.00 ± 0**	57.08 ± 31.25	**0 ± 0**	**0 ± 0**	**0 ± 0**
	MSE	-	5.10 ± 0.30	**1.00 ± 0**	0.99 ± 0.01	456.77 ± 78.83	**1.00 ± 0**	**0 ± 0**	1.11 ± 0.04	0.40 ± 0.01	**0 ± 0**
wine	ISM	0.47	6.10 ± 0.54	0.99 ± 0	**0.97 ± 0.05**	**0.28 ± 0.04**	0.98 ± 0.01	0.01 ± 0	0.07 ± 0.01	0.04 ± 0.03	0.02 ± 0
	W_s	0.98	3.00 ± 0	0.98 ± 0.01	0.92 ± 0.04	0.78 ± 0.09	0.93 ± 0.01	2.47 ± 0.26	0.06 ± 0.01	0.05 ± 0.01	0.08 ± 0.01
	CE	-	6.10 ± 0.54	**1.00 ± 0.00**	0.94 ± 0.06	3.30 ± 1.24	**1.00 ± 0.00**	40.33 ± 35.5	**0 ± 0**	**0 ± 0**	**0 ± 0**
	MSE	-	6.10 ± 0.54	**1.00 ± 0**	0.89 ± 0.17	77.45 ± 45.40	**1.00 ± 0**	**0 ± 0**	1.15 ± 0.07	0.49 ± 0.02	**0 ± 0**
cancer	ISM	0.39	8.10 ± 0.83	0.99 ± 0	**0.97 ± 0.02**	**2.58 ± 1.07**	0.96 ± 0.01	0.02 ± 0.01	0.04 ± 0.01	0.02 ± 0.04	0.04 ± 0.0
	W_s	2.33	1.30 ± 0.46	0.98 ± 0.01	0.96 ± 0.03	6.21 ± 0.36	0.88 ± 0.01	41.31 ± 56.17	0.09 ± 0.01	0.09 ± 0.02	0.16 ± 0.03
	CE	-	8.10 ± 0.83	**1.00 ± 0**	**0.97 ± 0.01**	82.03 ± 35.15	**1.00 ± 0**	2330 ± 2915	**0 ± 0**	**0 ± 0**	**0 ± 0**
	MSE	-	8.10 ± 0.83	**1.00 ± 0.00**	**0.97 ± 0.03**	151.81 ± 27.27	**1.00 ± 0**	**0 ± 0**	0.66 ± 0.06	**0 ± 0**	**0 ± 0**
car	ISM	0.23	4.90 ± 0.30	**1.00 ± 0**	**1.00 ± 0.01**	**1.51 ± 0.35**	0.99 ± 0	**0 ± 0**	0.01 ± 0.00	0.04 ± 0.03	0.01 ± 0
	W_s	1.56	2.70 ± 0.46	1.00 ± 0	1.00 ± 0	5.15 ± 1.07	0.93 ± 0.02	12.89 ± 2.05	0 ± 0	0.06 ± 0.02	0.08 ± 0.02
	CE	-	4.90 ± 0.30	**1.00 ± 0**	**1.00 ± 0**	25.79 ± 18.86	**1.00 ± 0**	225.11 ± 253	**0 ± 0**	**0 ± 0**	**0 ± 0**
	MSE	-	4.90 ± 0.30	**1.00 ± 0**	**1.00 ± 0**	504 ± 116.6	**1.00 ± 0**	**0 ± 0**	1.12 ± 0.07	0.40 ± 0	**0 ± 0**
face	ISM	0.44	4.00 ± 0	**1.00 ± 0**	**0.99 ± 0.01**	**0.78 ± 0.08**	0.97 ± 0	**0 ± 0**	0.17 ± 0	0.01 ± 0	**0 ± 0**
	W_s	0.05	3.40 ± 0.66	0.97 ± 0.01	0.80 ± 0.26	11.12 ± 3.05	0.86 ± 0.04	2.07 ± 1.04	0.28 ± 0.51	0.04 ± 0.01	0.01 ± 0
	CE	-	4.00 ± 0	**1.00 ± 0**	0.79 ± 0.31	23.70 ± 8.85	**1.00 ± 0**	16099 ± 16330	**0 ± 0**	**0 ± 0**	**0 ± 0**
	MSE	-	4.00 ± 0	0.92 ± 0.10	0.52 ± 0.26	745.2 ± 282	0.94 ± 0.07	0.11 ± 0.12	3.50 ± 0.28	0.72 ± 0.01	**0 ± 0**
divorce	ISM	0.41	4.10 ± 0.54	0.99 ± 0.01	0.98 ± 0.02	**0.71 ± 0.41**	0.99 ± 0.01	0.01 ± 0.01	0.03 ± 0	**0 ± 0.05**	0.02 ± 0
	W_s	2.10	2.30 ± 0.64	0.99 ± 0	0.95 ± 0.06	1.54 ± 0.13	0.91 ± 0.01	60.17 ± 70.64	0.04 ± 0.01	0.05 ± 0.01	0.08 ± 0
	CE	-	4.10 ± 0.54	**1.00 ± 0**	**0.99 ± 0.02**	2.62 ± 1.21	**1.00 ± 0**	14.11 ± 12.32	**0 ± 0**	**0 ± 0**	**0 ± 0**
	MSE	-	4.10 ± 0.54	**1.00 ± 0**	0.97 ± 0.03	47.89 ± 24.31	**1.00 ± 0**	**0 ± 0**	0.73 ± 0.07	**0 ± 0.01**	0.01 ± 0