Neural networks embrace learned diversity

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Diversity conveys advantages in nature, yet homogeneous neurons typically comprise the layers of artificial neural networks. Here we construct neural networks from neurons that learn their own activation functions, quickly diversify, and subsequently outperform their homogeneous counterparts. Sub-networks instantiate the neurons, which meta-learn especially efficient sets of nonlinear responses. Such learned diversity provides examples of dynamical systems selecting diversity over uniformity and elucidates the role of diversity in natural and artificial systems.

Diversity is a hallmark of many complex systems in physics [1][2] and in physics beyond physics [3], including microscopic cell populations [4], marine and terrestrial ecosystems [5][6], financial markets [7], and social networks [8][10]. In particular, mammalian brains contain billions of neurons with diverse cell types whose complex dynamical patterns are believed responsible for the rich range of cognition, affect, and behavior [11][14]. But despite the widespread appreciation of diversity in neuroscience, researchers have just begun to explore the role of diversity and adaptability in artificial neural networks [15][17].

Motivated by the well-studied mammalian visual cortex, varying neuronal activation functions by layer is common. However, within each layer, the activations are typically identical, as in Fig. 1[1] (top). Neural networks are universal function approximators [24][25] and are often used to model hypersurfaces, either in nonlinear regression or classification. Varying the activations within a layer, as in Fig. 1[1] (center), should therefore increase the expressiveness of the network by providing diverse spanning basis functions. Furthermore, replacing the activations by neural networks, as in Fig. 1[1] (bottom), and training them for optimal results should increase the expressiveness even further. The training of the activa-

\[ a' \equiv \sigma(Wa + b), \] (1)

where the activation \( \sigma \) is typically a saturating or rectifying function and training strengthens or weakens the weights and biases \( W \) and \( b \) to minimize an error or loss function and optimize outputs.

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Figure 1. Progression from conventional artificial neural network to diverse neural network to learned diverse neural network. Line thicknesses represent weights $W$, circle thicknesses represent biases $b$, and sketches inside circles represent activation functions $\sigma$. Information flows top-to-bottom. Training adjusts the weights and biases to optimize outputs (top). Multiple activation functions enable diversity within layers (center) and increase the expressiveness of the neural network. Separate neural networks (bottom) realize these activation functions when training adjust their weights and biases (color), perhaps on a different schedule than the originals (black), to further optimize the network.

A diverse neural network can be on a different schedule than the training of the rest of the network, and the activations so obtained can be extracted from the neuronal sub-networks as interpolated functions and efficiently reused in other networks addressing different problems.

As an example of a learned diversity neural network (LDNN), construct a feed-forward classifier neural network whose neurons are sub-networks that modify base activation functions (like zero, identity, sigmoid, or sine functions). Train the classifier with many input-output pairs. Quantify the difference between the expected and correct classifications with an error or loss function. Compute the gradient of the loss function with respect to the classifier’s weights and biases, and lower the loss by shifting its weights and biases down this gradient (inner loop). Periodically compute the gradient of the loss function with respect to the sub-networks’ weights and biases, and further lower the loss by shifting their weights and biases down this gradient (outer loop). Repeat to improve accuracy.

The classifier error or loss $L(\theta, \theta_A, i)$ depends on the network weights and biases $\theta$, the sub-networks weights and biases $\theta_A$ that instantiate the activations of hidden-layer neurons, and the inputs $i$. The randomly shuffled inputs are the stochastic driver that buffets the weights and biases as they adjust to lower levels (during the meta-learning inner loop). Periodically the activation weights and biases open extra dimensions or degrees of freedom to further lower the levels (during the meta-learning outer loop), as in Fig. 2.

Here we implement [27] learned diversity neural networks with one hidden layer of 100 neurons and a cross-entropy loss function to classify the MNIST-1D data set, a minimalist variation of the classic Modified National Institute of Standard and Technology digits [28, 29]. Each neuron type in the hidden layer is further instantiated by a feed-forward neural network of 50 hidden units with hyperbolic tangent activation functions. We obtain similar results for different numbers of layers and different number of neurons per layer [30].

Figure 3 summarizes meta-learning the activation functions of neurons in the hidden layer subject to the constraint of having two functions distributed equally among the neuronal population. Figure 3(a) and (b) show the evolution of the two activation functions, with time encoded as rainbow colors from violet to red. Figure 3(c) shows violin plots demonstrating validation ac-
FIG. 3. Meta-learning 2 activations for MNIST-1D classification. (a-b) Activation functions $\sigma_n(a)$ evolve from a base sinusoid, with violet-to-red rainbow colors encoding time $t$. (c) Violin plots summarize distribution (including median, quartiles, and extent) of validation accuracy $A$ for 50 fully connected neural networks of ReLU neurons (blue), type-1 neurons (yellow), type-2 neurons (orange), and a mix of type 1 and type 2 neurons (red). The mix of 2 neuron types outperforms any single neuron type on average.

FIG. 4. Neural network MNIST-1D classification accuracy as a function of network size. Box and whiskers plots summarize accuracy distribution (including median, quartiles, extent, and outliers) for 100 initializations. Learning rate is optimized to avoid over-fitting but is the same for all network sizes. Activation functions evolved from zero (the null function) with similar results evolved from sine. Mixed networks of 2 neuron types outperform pure networks on average for all sizes and outperforms both single learned activation and traditional activations.

curacy for 50 fully connected neural networks composed of entirely $N_1$ type neurons (yellow), entirely $N_2$ type neurons (orange), and mixed type with $N_1$ and $N_2$ distributed equally among hidden layer (red). With the same training, the mixed network outperforms either pure network on average. These results are robust with respect to network size, as summarized by Fig. 4.

We obtain similar results for other tasks, including nonlinear regression of the van der Pol oscillator [31], which consists of a linear restoring force and a nonlinear viscosity modeled by the differential equation

$$\ddot{x} - \mu(1-x^2)\dot{x} + x = 0,$$

where the overdots indicate time derivatives. The van der Pol oscillator can model vacuum tubes and heartbeats and was generalized by FitzHugh [32] and Nagumo [33] to model spiky neurons. For viscosity parameter $\mu = 2.7$, we trained neural networks to forecast the phase space orbit of the oscillator, as summarized by Fig. 5. On average the learned diversity neural network outperforms either of its pure components as well as a homogeneous network of neurons with sinusoidal activations.

To understand how mixed activation functions outperform homogeneous neuronal populations, we estimate the change in the dimensionality of the network activations. Start by constructing a neuronal activity data matrix $X$ with $N$ rows corresponding to $N$ neurons in the hidden layer and $M$ columns representing inputs. Each matrix element $X_{ij}$ represents the activity of the $i$th neuron at the $j$th input. Center the activity so $\langle X \rangle = 0$. Construct the neural co-variance matrix $C = M^{-1}XX^T$, which indicates how pairs of neurons vary with respect to each other, and compute the participation ratio

$$R = \frac{(\text{tr} C)^2}{\text{tr} C^2} = \frac{\left(\sum_{n=1}^{N} \lambda_n\right)^2}{\sum_{n=1}^{N} \lambda_n^2},$$

where $\lambda_n$ are the co-variance matrix eigenvalues. If all the variance is in one dimension, say $\lambda_n = \delta_{n1}$, then $R = 1$; if the variance is evenly distributed across all dimensions, so $\lambda_n = \lambda_1$, then $R = N$. Typically, $1 < R < N$, and $R$ corresponds to the number of dimensions needed to explain most of the variance [34].

The normalized participation ratio $r = R/N$.

Figure 6 plots the joint probability densities $\rho(A,r)$ for multiple realizations of the Fig. 3 Learned Diversity Neural Network and homogeneous competitors. The mix of two neurons types has the best mean accuracy $A$ and normalized participation ratio $r$, suggesting that more of its neurons are participating when the mix achieves the best MNIST-1D classification. In contrast, homogeneous networks of neurons with popular activation functions have lower accuracy and participation ratios reflecting their poorer effectiveness.

To understand the impact of learned diversity on the geometric nature of loss-function minima, we compute
FIG. 5. Meta-learning 2 activations for nonlinear regression of the van der Pol oscillator. (a-b) Activation functions $\sigma_n(a)$ evolve from a base sinusoid, with violet-to-red rainbow colors encoding time $t$. (c) Violin plots summarize distribution of neural network mean-square error or loss $L$ for 50 fully connected neural networks of sine neurons (blue), type-1 neurons (yellow), type-2 neurons (orange), and a mix of type 1 and type 2 neurons (red). The mix of 2 neuron types outperforms any single neuron type on average.

the spectrum of the Hessian matrix $H = \nabla^2 L$, which captures the curvature of the loss function. Since, $H$ is a symmetric matrix, all its eigenvalues are real. A purely convex loss function would have a positive semi-definite Hessian everywhere. However, in practice, the loss function is almost always non-convex (with multiple spurious minima) due to the presence of permutation symmetries of the hidden neurons [35]. Therefore, understanding how diversity helps training find deeper minima is crucial.

Previous work suggests that flatter minima generalizes better to the unseen data [36, 37]. For the Fig. 1 neural network meta-learning two neuronal activation functions, we find that once training has converged, the resulting minima from diverse neurons is flatter than from homogeneous ones, as measured by both the trace $\text{Tr} H$ of the Hessian and the fraction $f$ of its eigenvalues near zero: $\text{Tr} H_1 > \text{Tr} H_2 > \text{Tr} H_3$ and $f_1 < f_2 < f_3$. If steep minima are harder for gradient descent to locate, then the flatter minima engineered and discovered by learned diversity neural networks imply enhanced optimization.

Biomimetic engineering or biomimicry is design inspired by nature. Just as monoculture crops can be fragile, while diverse crops can be robust [38], heterogeneous neural networks can outperform homogeneous ones. Here, we highlight advantages of varying activation functions within each layer and learning the best variation by replacing activations by sub-networks.

Conceptually, Learned Diversity Neural Networks discover novel sets of activation functions, when most artificial neural networks use just one of a small number of conventional activations per layer. Practically, mixes of learned activations can outperform traditional activations – where even a 1% improvement can be significant – and the learned activations can be efficiently reused in diverse neural networks. Future work includes optimizing learned diversity by adjusting hyperparameters, applying learned diversity to a wider range of regression and classification problems, testing diverse neural networks for robustness [39], investigating clustering of learned activations, and applying learned diversity to different neural network architectures, such as recurrent neural networks and reservoir computers [10, 42], as well as physics-applied and physics-informed neural networks [43, 44].

Learned diversity offers neural networks sets of tailored basis functions, which enhance their expressiveness and adaptability and facilitates efficient function approximation. When given the ability to learn their neuronal activation functions, neural networks discover heterogeneous arrangements of nonlinear neuronal activations that can outperform their homogeneous counterparts with the same training. Our work provides specific examples of dynamical systems that spontaneously select diversity over uniformity, and thereby furthers our understanding of diversity and its role in strengthening natural and artificial systems.

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