Spectral Analysis and Stability of Deep Neural Dynamics

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Abstract

Our modern history of deep learning follows the arc of famous emergent disciplines in engineering (e.g., aero- and fluid dynamics) when theory lagged behind successful practical applications. Viewing neural networks from a dynamical systems perspective, in this work, we propose a novel characterization of deep neural networks as pointwise affine maps, making them accessible to a broader range of analysis methods to help close the gap between theory and practice. We begin by showing the equivalence of neural networks with parameter-varying affine maps parameterized by the state (feature) vector. As the paper’s main results, we provide necessary and sufficient conditions for the global stability of generic deep feedforward neural networks. Further, we identify links between the spectral properties of layer-wise weight parametrizations, different activation functions, and their effect on the overall network’s eigenvalue spectra. We analyze a range of neural networks with varying weight initializations, activation functions, bias terms, and depths. Our view of neural networks as affine parameter varying maps allows us to “crack open the black box” of global neural network dynamical behavior through visualization of stationary points, regions of attraction, state-space partitioning, eigenvalue spectra, and stability properties. Our analysis covers neural networks both as an end-to-end function and component-wise without simplifying assumptions or approximations. The methods we develop here provide tools to establish relationships between global neural dynamical properties and their constituent components which can aid in the principled design of neural networks for dynamics modeling and optimal control.

Keywords: neural networks; eigenvalues and eigenvectors; stability analysis; stability guarantees; attractor networks; structural priors

1. Introduction

Thanks to their potential to approximate arbitrary functions (Hornik et al., 1989), the availability of user-friendly and scalable implementations, and a feedback loop of favorable press acclaiming their superhuman performance for a wide range of skills emblematic of human intelligence, deep neural networks (DNN) are becoming ever more integrated into the operation of real-world systems. At the crest of this trend are safety-critical and high performance systems including robotics, autonomous driving, and process control where formal verification methods are desired to ensure safe operation. Yet the lack of guarantees on global and local behavior of DNNs still remain limiting factors for these use cases requiring robust and stable control of dynamical systems.

Our primary objective is to develop a generic eigenvalue analysis method for DNNs. To do so we demonstrate their equivalence to pointwise affine maps. Leveraging this exact linearization
allows us to compute the eigenvalues of networks with arbitrary activation functions and unlimited depth. Further, we provide necessary and sufficient conditions for global stability of feedforward DNNs by leveraging the Gelfand spectral radius theorem (Anh et al., 2020). Our eigenvalue analysis thereby represents a generic counterpart to verification methods based on over-approximations, abstract interpretation, or solution of optimization problems. We also propose methods to link the eigenvalue spectra and dynamics of a whole network with spectral properties stemming from network depth, constituent linear maps, and activation functions. In this way, our dynamical analysis enables principled design of neural networks for a range of deployed applications where deep learning is poised to come online with critical capacities for pattern recognition, predictive modeling, and optimal control. In summary, we report the following contributions:

- Proof of the equivalence of deep feedforward neural networks with pointwise affine maps.
- Eigenvalue analysis for feedforward neural networks based on exact pointwise linearizations.
- Necessary and sufficient conditions for global stability of feedforward neural networks.
- Stability analysis of commonly used activation functions.
- Case studies investigating eigenvalue spectra and dynamical properties of neural networks.

2. Related Work

Deployment of new software technology in critical settings requires a verification stage which relies on established tools such as SMT solvers. However, properties such as stochasticity, continuity, non-convexity, and inherent nonlinearity pose major challenges in DNN verification (Prabhakar and Afzal, 2019). Even simply verifying linear constraints on inputs and outputs of neural networks is an NP-hard problem (Katz et al., 2017). To overcome these obstacles a range of techniques have been proposed including output range analysis (Prabhakar and Afzal, 2019; Dutta et al., 2018), robustness analysis using reachable sets (Everett et al., 2020; Ehlers, 2017; Gehr et al., 2018; Xiang et al., 2018), and formal abstractions (Pulina and Tacchella, 2010; Sun et al., 2019; Singh et al., 2019). Verification fidelity can be improved upon for these methods by using fewer simplifying assumptions and expansion to a wider set of architectures. For an overview and comparison of different formal verification methods of neural networks we refer the reader to Huang et al. (2016); Bunel et al. (2017); Xiang et al. (2018).

The straightest path to tractable analysis of nonlinear systems is to cast them in a linear formulation. Prior to DNNs coming of age, Linear Differential Inclusions (LDI) have been used frequently in analysis of uncertain nonlinear systems (Boyd et al., 1994). Stability analysis of LDI was previously applied to neural networks for system and control design problems (Tanaka, 1996; Matusik et al., 2020; He et al., 2014; Limanond and Si, 1998) with extensions such as Polytopic Linear Differential Inclusions (Tanaka, 1995). Alternatively, in linear parameter-varying systems (LPV) (Shamma and Athans, 1990), the nonlinear model is formulated as a parameterized linear system depending on exogenous parameters. The LPV paradigm has become a standard formalism in systems and controls, with numerous efforts related to analysis (Shamma and Athans, 1991; Bruzelius et al., 2003), controller synthesis (Apkarian et al. (1995); de Souza and Trofino (2006)), and system identification of LPV models (Bamieh and Giarre, 1999; Hoffmann and Werner, 2015; Bokor and Balas, 2005). Linear analysis of neural networks has principally focused on networks with piecewise linear ReLU activations. Arora et al. (2016) prove the equivalence of deep ReLU networks with piecewise affine (PWA) maps. Hanin and Rolnick (2019a,b) provide a mathematical framework to compute the number of linear regions of ReLU DNNs. Authors in (Wang et al., 2016;
Gehr et al., 2018) interpret ReLU networks as pointwise linearizations allowing then to explore the spectral properties. Our current work provides DNN linearization for arbitrary activation functions opening linear analysis methods to a more general class of DNN architectures.

A host of works have begun to view neural networks from a dynamical systems perspective leading to new regularization objectives (Ludwig et al., 2014), architectures (Haber et al., 2019; Ciccone et al., 2018), analysis methods (Engelken et al., 2020; Vogt et al., 2020; Wang et al., 2016; Güler et al., 2019), and stability guarantees (Haber and Ruthotto, 2017). Engelken et al. (2020) calculate the Lyapunov spectrum of recurrent neural networks (RNNs), using linearization based on the Jacobian of network outputs with respect to inputs. Employing the same algorithm, Vogt et al. (2020) empirically demonstrate that quantities such as mean and maximum Lyaponov exponents can correlate with learning success. Manek and Kolter (2019) propose jointly learning a non-linear dynamics model and Lyapunov function that guarantees non-expansiveness of the dynamics. Other recent works provide eigenvalue analysis of neural network objective function Hessian (Ghorbani et al., 2019; Le Cun et al., 1991) and Gram (Goel and Klivans, 2017) matrices providing insight into the optimization dynamics which they use to develop more efficient learning algorithms. Authors in (Pennington and Worah, 2019; Louart et al., 2017; Liao and Couillet, 2018) study the eigenvalues of the data covariance matrix propagation through a single layer neural network from a perspective of random matrix theory.

Stability of DNNs has been studied for several years in the context of neuro-controllers (Vrabie and Lewis, 2009; Vamvoudakis and Lewis, 2010; Vamvoudakis et al., 2015). Most notable works rely on the Lyapunov stability theorem to guarantee network weights satisfy a pre-defined function. Eigenvalues, eigenvectors and singular values prominent in linear analysis are also widely used to build stable DNN architectures. Various parametrizations and auxilliary loss terms have been proposed to restrict the eigenvalues of a neural network’s weights. Some authors use regularization to minimize eigenvalues of $WW^T$ (Ludwig et al., 2014), others use bounds on the singular values of layer weights $W$ via orthogonal (Mhammedi et al., 2017), spectral (Zhang et al., 2018), Perron-Frobenius (Tuor et al., 2020), or symplectic (Haber and Ruthotto, 2017) parametrizations. Rajan and Abbott (2006) present a family of matrices with eigenvalues constrained within a circle with arbitrary prescribed radius. Lechner et al. (2020) introduce a Gershgorin disc based regularization term to ensure negative eigenvalues on the recurrent weights and prove that this regularization ensures stability. These major accomplishments in the design of stable architectures notwithstanding, there is still limited theory on the effects of activation function choice, network depth, and weight initialization on the learned system properties. Beyond creating specialized stable DNNs by design, in this work we provide analysis methods for stability as well as other dynamic properties for a general class of feed forward neural networks that are commonly used in applications and research.

3. Methods
Our primary objective is to compute the eigenvalue spectrum of the dynamics of a deep feedforward neural network (3). We show that representing nonlinear activation functions as parameter-varying diagonal square matrices allows us to decompose the neural network’s eigenvalue problem into composition of affine maps accessible to standard methods in eigenvalue analysis. We demonstrate the equivalence of DNNs with pointwise parameter varying affine systems for arbitrary activation functions. As the main results of this section, we provide necessary and sufficient conditions for global stability of deep feedforward neural networks.
3.1. Deep Neural Networks as Parameter-varying Affine Maps

In this section we give a straightforward formulation of a deep neural network as a parameter-varying affine map. We show that our exact linearization is general for arbitrary activation functions compared to previous neural network linearizations which only apply to ReLU networks.

**Definition 1** Autonomic Ordinary Differential Equation (ODE): is given as \( \frac{d}{dt} \mathbf{x}(t) = \mathbf{f}(\mathbf{x}(t)) \), where \( \mathbf{x}(t) \in \mathbb{R}^{n_x} \) are system states. A point \( \mathbf{x} \) is called an equilibrium point if it satisfies the stationarity condition \( \mathbf{f}(\mathbf{x},t) = 0 \) for all \( t \).

**Definition 2** Linear Parameter Varying System: is a linear system with varying dynamics:

\[
\frac{d}{dt} \mathbf{x}(t) = \mathbf{A}(\mathbf{x}) (\mathbf{x}(t) - \mathbf{x})
\]

where \( \mathbf{A}(\mathbf{x}) \) is a point-wise Jacobian linearization of nonlinear system around equilibrium point \( \mathbf{x} \).

**Lemma 3** Let \( f_\theta : \mathbb{R}^m \to \mathbb{R}^n \) be a deep feedforward neural network with arbitrary activation function \( \sigma \), then there exists a parameter varying affine map \( \mathbf{A}^*(\mathbf{x}) \mathbf{x} + \mathbf{b}^*(\mathbf{x}) \) parametrized by features \( \mathbf{x} \) which satisfies the following:

\[
f_\theta(\mathbf{x}) := \mathbf{A}^*(\mathbf{x}) \mathbf{x} + \mathbf{b}^*(\mathbf{x})
\]

**Proof of Lemma 3** for Deep Neural Networks without Bias. To simplify exposition we develop the linearization for a general class of neural networks without bias. Let the so-called activation function, \( \sigma : \mathbb{R}^n \to \mathbb{R}^n \) be the elementwise application of a univariate scalar function \( \sigma : \mathbb{R} \to \mathbb{R} \) to vector elements such that \( \sigma(z) = \begin{bmatrix} \sigma(z_1) & \cdots & \sigma(z_n) \end{bmatrix}^T \). We define a deep feedforward neural network: \( f_\theta : \mathbb{R}^m \to \mathbb{R}^n \) parametrized by \( \theta = \{ \mathbf{A}_0, \ldots \mathbf{A}_L \} \) with hidden layers \( 1 \leq l \leq L \):

\[
\begin{align*}
\mathbf{f}_\theta(\mathbf{x}) &= \mathbf{A}_L \mathbf{h}_L \\
\mathbf{h}_l &= \sigma(\mathbf{A}_{l-1} \mathbf{h}_{l-1}) \\
\mathbf{h}_0 &= \mathbf{x}
\end{align*}
\]

Now observe that:

\[
\sigma(z) = \begin{bmatrix} \sigma(z_1) \\ \vdots \\ \sigma(z_n) \end{bmatrix} = \begin{bmatrix} \frac{\sigma(z_1)}{z_1} \\ \vdots \\ \frac{\sigma(z_n)}{z_n} \end{bmatrix} z = \Lambda \mathbf{z}
\]

where the final equality follows from definition of \( \Lambda \mathbf{z} \) as a compact symbol for the parameter varying map in the penultimate expression above. If we let \( \mathbf{z}_{l+1} = \mathbf{A}_l \mathbf{h}_l \), by composition, a DNN (equation 3) can now be formulated as a parameter-varying linear map \( \mathbf{A}^* \), which is a function of the input vector \( \mathbf{x} \):

\[
f_\theta(\mathbf{x}) := \mathbf{A}^*(\mathbf{x}) \mathbf{x} = \mathbf{A}_L \Lambda \mathbf{z}_L \mathbf{A}_{L-1} \ldots \mathbf{A}_1 \mathbf{A}_0 \mathbf{x}
\]

This means each input feature vector \( \mathbf{x} \) will generate a pointwise linearization \( \mathbf{A}^*(\mathbf{x}) \) of the underlying DNN \( f_\theta \).
Theorem 6
Global stability of deep feedforward neural network

Definition 5
Spectral radius: of a matrix \( A \in \mathbb{R}^{n \times n} \) is the largest absolute value of its eigenvalues:

\[
\rho(A) = \max_{i=1, \ldots, n} |\lambda_i|
\]  

Theorem 6
Global stability of deep feedforward neural network \( f_\theta(x) \):

- Necessary condition: Spectral radius (9) of \( f_\theta(x) \) is less or equal to 1 for any \( x \) in the domain of \( f_\theta(x) \), i.e. \( \rho(A^*(x)) \leq 1, \forall x \in \text{dom}(f_\theta(x)). \)

- Sufficient condition: Spectral radii (9) of all weights \( A_i \) and activation scaling matrices \( A_{z_j} \) (4) of \( f_\theta(x) \) are less or equal to 1, i.e. \( \rho(A_i) \leq 1, \rho(A_{z_j}) \leq 1, \forall j \in \mathbb{N}^L_1, \forall x \in \text{dom}(f_\theta(x)). \)

\[
\text{(9)}
\]
Proof Proof of the necessary condition for networks without bias follows directly from the exact pointwise linearizations (5) of the neural network and definition 8 of the asymptotic stability. Hence, for \( f_\theta(x) \) to be globally stable, its exact linearization \( \Lambda \sigma'(x) \) must be stable for all points in the entire domain. Proof of the sufficient condition for \( f_\theta(x) \) is based on Gelfand’s theorem of spectral radius inequality of a product of \( m \) matrices, given as follows:

\[
\rho(A_1 \ldots A_m) \leq \rho(A_1) \ldots \rho(A_m)
\]  

(10)

Notice that exact pointwise linearizations (5) of the neural network without bias is represented as a matrix product. Hence, the product of the layer-wise spectral radii yields upper bound of the spectral radius for the whole network. For the cases with bias, the dynamics of the bias recursion (7) is driven by the matrix product \( \Lambda_i \Lambda_z \). Hence, applying (10) to (7) directly expands the sufficient condition proof to neural networks with bias. For proofs of the Gelfand’s spectral radius formula (10) see (Shih et al., 1997; Bochi, 2003; Blondel and Nesterov, 2005).

3.3. Eigenvalues and Stability of Activation Functions

For any diagonal scaling matrix \( \Lambda_z \) (4) holds that the diagonal elements represent its eigenvalues, i.e. \( \Lambda_z = \Lambda z \). Moreover, the eigenvectors of \( \Lambda_z \) form the canonical basis of the feature space \( \mathbb{R}^n_z \). Hence, the activation functions in DNNs affect only its eigenvalues and do not change its eigenvectors. Therefore as stated in sufficient conditions of theorem 6, to guarantee the global stability of DNNs, the scaling matrices \( \Lambda_z \) generated by activation functions must yield stable eigenvalues for any \( z \). Following lemmas provide sufficient conditions this to hold.

Definition 7 Lipschitz Continuity: a function \( f : \mathbb{R} \rightarrow \mathbb{R} \) is Lipschitz continuous if there exists a positive real constant \( K \) such that, for all real \( x_1 \) and \( x_2 \), following holds:

\[
|f(x_1) - f(x_2)| \leq K|x_1 - x_2|
\]  

(11)

Lemma 8 Activation function \( \sigma(z) \) in the network \( f_\theta(x) \) is asymptotically stable over the entire domain \( \text{dom}(\sigma(z)) \) if it has trivial null space \( \sigma(0) = 0 \) and Lipschitz constant \( K < 1 \).

Proof Given the Lipschitz continuity via equation (11), it is straightforward to see that for \( x_2 = 0 \), the Lipschitz constant \( K \) for any activation function \( \sigma(x) \) is given as \( \frac{|\sigma(z_1)|}{z_1} = K \). Now observe that conditions in Lemma 8 force all diagonal entries of the activation scaling matrix \( \Lambda_z \) (4) to satisfy \( \frac{|\sigma(z_i)|}{z_i} < 1 \). And because the matrix \( \Lambda_z \) is a diagonal, its diagonal entries represent its real eigenvalues, and \( \Lambda_z \) is stable in a sense of definition 4.

Definition 9 Bounded-Input Bounded-Output (BIBO) Stability: for an ODE, every bounded input results in a bounded output:

\[
\forall \|u(t)\| < \epsilon, \ \forall t \geq 0, \ \mathbf{x}_0 = \mathbf{x} \implies \|\mathbf{x}(t) - \mathbf{x}\| < \delta, \ \forall t \geq 0
\]  

(12)

Lemma 10 Activation functions \( \sigma(z) \) in the network \( f_\theta(x) \) is BIBO stable if the eigenvalues of \( \Lambda_z \) (4) are stable on the outer regions of the domain of \( \text{dom}(\sigma(z)) \), i.e. \( \frac{|\sigma(z_i)|}{z_i} \leq 1 \), for all \( \{z_i | z_i \leq \sigma(z) \} \). Where \( [\sigma(z), \sigma(z)] \) represents bounded interval in \( \mathbb{R} \).
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**Proof** Follows directly from definition 9 of BIBO stability with $z$ being system inputs and $\sigma(z)$ being system outputs.

**Remark 11** Formula $|\frac{\sigma(z)}{z_i}| = K$ is defined for all points except $z_i = 0$. To overcome the division by zero we define this value at $z_i = 0$ as the activation function’s derivative $|\frac{\sigma(z)}{z_i}| = \sigma'(0)$.

Fig. 1 plots commonly used activation functions with guaranteed asymptotic stability\(^1\), and activations with unstable regions\(^2\). However, despite locally asymptotically unstable regions, some activations\(^3\) are BIBO stable in the sense of definition (9), and thus will not cause a gradient explosion in the DNN. In general, destabilizing properties of activation functions are non-trivial null space and Lipschitz constant $K > 1$.

![Activation functions](image)

Figure 1: Activation functions with asymptotic stability (left), with unstable regions (middle), and with BIBO stability (right), respectively. Blue areas represent stable regions covering functions with trivial null space and Lipschitz constant $K \leq 1$.

4. Case Studies

Deep neural networks are compositions of affine transformations and nonlinear activation functions with arbitrary depth. There is a range of methods analyzing layer-wise properties of DNNs. However, analyzing the dynamic and spectral properties of a network as a whole is a challenging task and remains an open problem. This section presents a first of a kind systematic investigation of the effect of different components on eigenvalue spectra and phase space dynamics of resulting DNNs. Using academic examples, we investigate and visualize individual components’ effect—namely various weight factorizations, types of activations, bias terms, and network depth—on resulting neural dynamics. We particularly focus on the relationship between a neural network’s eigenvalues spectra and its dynamical properties such as stability and regions of attractions.

1. Asymptotically stable activations: SoftExponential, BLU, PReLU, ReLU, GELU, RReLU, Hardtanh, ReLU6, Tanh, ELU, CELU, Hardshrink, LeakyReLU, Softshrink, Softsign, Tanhshrink
2. Activations with unstable regions: APLU, PELU, Sigmoid, Hardsigmoid, Hardswish, SELU, LogSigmoid, Softplus, Hardswish
3. BIBO stable activations: Sigmoid, Hardsigmoid

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Experimental Setup: In order to inspect the behavior of neural networks with specific spectral properties, we construct neural networks of various depths which use structured linear maps with spectral constraints. To observe a breadth of spectral properties and their effects on network dynamics, we chose several ranges used to constrain the eigenvalues of each linear map. We further test each factorization using various activation functions to observe how they affect dynamics, and evaluate each model with and without bias. For each configuration, we compute pointwise linearizations of the network as described in the proofs of Lemma 3 over a 2D grid ranging [-6, 6] in both dimensions to compute their eigenvalue spectra, compute spectral radii, and generate phase portraits. Additional details on the configurations used can be found in Appendix D.

Dynamical Effects of Weights: To empirically verify implications of theorem 6, we construct 2D 8-layer neural models with layer-wise eigenvalues constrained between zero and one, close to one, and greater than one. Fig. 2 demonstrates dynamical properties and associated eigenvalue spectra of DNNs with asymptotically stable\(^4\), BIBO stable\(^5\), and unstable\(^6\) dynamics, respectively. First row visualizes phase space trajectories with associated regions of attraction, while second row plots eigenvalue spectra in the complex plane. Individual plots empirically validate the necessary condition of theorem 6 linking spectral radius with stability properties.

Figure 2: DNNs with asymptotically stable (left), BIBO stable (center), and unstable dynamics (right), showing phase space trajectories, and eigenvalue spectrum of \(A^*\).

\(^4\) Spectral radius \(\rho(A^*) \leq 1\), Tanh activation, Gershgorin disc factorized weight.
\(^5\) Spectral radius \(\rho(A^*) \approx 1\), Tanh activation, Spectral SVD factorized weight.
\(^6\) Spectral radius \(\rho(A^*) \geq 1\), Softplus activation, Gershgorin disc factorized weight.
Dynamical Effects of Activation Functions: Here we leverage the pointwise linearization $A^*$ as defined in Lemma 3 to expand the complexity analysis of linear regions of deep ReLU networks (Hanin and Rolnick, 2019a) to networks with arbitrary activation functions. To identify different regions in the network’s phase space one can apply various metrics on $A^*$ such as matrix norms, spectral density, or spectral radius. Fig. 3 displays state space regions associated with spectral radii of 4-layer DNNs with four activations: ReLU, Tanh, SELU, and Sigmoid. All weights are randomly generated to have stable eigenvalues. As expected, ReLU networks generate linear regions, while the exponential part of SELU networks make the resulting pattern of linear regions more complex. On the other hand, smooth activations Tanh and Sigmoid generate continuous gradient fields. Thanks to the asymptotic stability of ReLU and Tanh as given by Lemma 8 the whole state space is guaranteed to be stable with $\rho(A^*) \leq 1$. Because both SELU and Sigmoid activations violate the conditions of Lemma 8 the global stability of their state space is not guaranteed by design. Even though in this case, SELU network generated globally stable dynamics. On the other hand, Sigmoid network generated large unstable region surrounded by stable regions, most likely caused by its nontrivial null space. Despite this, such a state space might still be BIBO stable as the unstable region might be surrounded by stable regions on an expanded domain.

![Figure 3: Phase space regions associated with spectral radii $\rho(A^*)$ of 4-layer DNNs with different activation functions initialized with stable weights. From left to right ReLU, Tanh, SELU, and Sigmoid.](image)

Dynamical Effects of Bias Terms: If either necessary and sufficient conditions of the theorem 6 are satisfied with strict inequalities on spectral radii, it is straightforward to see that a neural network without bias is globally asymptotically stable (8) with the equilibrium point at the origin $x = 0$. In the case of non-zero biases and sufficient conditions holding with strict inequalities, the equilibrium point are uniquely defined by last layer’s bias terms $x = b_L$. This observation is implied by asymptotically stable dynamics of the bias recursion (7) as stated in the proof of theorem 6. Fig. 4 demonstrates the effect of the bias on equilibrium points $x$ of a single-layer with stable dynamics.

Therefore, we postulate that bias terms in generic DNNs do not affect the dynamical properties such as eigenvalues, stability, or convergence. Instead, biases uniquely define the centroid of attractors confined in the compact subspace of the state space. Additionally, we posit that dynamical properties are uniquely defined by the network’s weights and activation functions. Therefore a careful choice of activations and factorization of weights can lead to a pre-design of desired dynamical properties of the overall network dynamics. Additionally, this analysis reveals the significant role of the bias terms in learning stable equilbria of dynamical systems. This observation can inspire new research in the design of new, more sophisticated bias terms, for instance, using pointwise parametrizations for learning multistable dynamical systems.
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Figure 4: Dynamics of stable ReLU layer with bias $\mathbf{x} \neq 0$ (left), and without bias $\mathbf{x} = 0$ (right).

**Dynamical Effects of Network Depth:** Very deep recurrent neural networks (RNNs) are notoriously difficult to train due to the vanishing and exploding gradient problems (Pascanu et al., 2012; Kolen and Kremer, 2001). Haber and Ruthotto (2017) linked these problems with the spectral properties of RNNs. In the same spirit we leverage Lemma 3 and theorem 6 to study the eigenvalue spectra of the forward propagation of DNNs with varying depth. Please recall that as given in (5) and (6), we can equivalently cast DNNs as a matrix product of pointwise affine representations of its layers. As known, RNNs are trained by unrolling them to $L$-layer deep feedforward DNNs, where all layers share the weights and activations and hence by definition also their spectral properties. Hence by having $A_i = A_j$, $\forall (i,j) \in \mathbb{N}_L^2$ it is clear that applying Gelfand’s spectral radius formula (10) yields matrix power series. Therefore increasing the depth of RNNs with asymptotically stable layers necessarily shrinks the spectral radius with each layer. For unstable layers the opposite is true as the spectral radius expands exponentially. Therefore, theorem 6 confirms and expands the conclusions of Haber and Ruthotto (2017) saying that well-posed learning problems for arbitrarily deep networks requires spectral radius of DNNs to be close to 1, or more formally $\rho(A^*) \approx 1$.

**5. Conclusion**

This work shows the equivalence of generic deep feedforward neural networks with parameter-varying affine maps. This mapping is shown to produce the exact linearization for each data-point over the feature space. Due to their element-wise application, the nonlinear activation functions are represented linearly as parameter-varying diagonal matrices, thus contracting a multi-layer network into a series of matrix multiplications. This formulation extends prior results restricted to ReLU DNNs to networks with arbitrary activation functions. This yields a seamless way to analyze neural networks’ stability, equilibrium points, eigenvalue spectra, and regions of instability and attraction. As the paper’s main result, we proposed necessary and sufficient conditions for the global stability of generic deep neural networks. Systematic analysis of network weight eigenvalues, network depth, and choice of activation function revealed a significant impact on the final neural dynamics. We believe that the presented method based on piecewise affine representations can be a useful tool for designing and analyzing deep neural networks. The resulting visualization can help guide the network architecture design to obtain the desired dynamical behavior and properties.
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References

Pham Ky Anh, Pham Thi Linh, Do Duc Thuan, and Stephan Trenn. Stability analysis for switched discrete-time linear singular systems. *Automatica*, 119:109100, 2020. ISSN 0005-1098. doi: https://doi.org/10.1016/j.automatica.2020.109100. URL http://www.sciencedirect.com/science/article/pii/S0005109820302983.

Pierre Apkarian, Pascal Gahinet, and Greg Becker. Self-scheduled control of linear parameter-varying systems: a design example. *Automatica*, 31(9):1251–1261, 1995.

Raman Arora, Amitabh Basu, Poorya Mianjy, and Anirbit Mukherjee. Understanding deep neural networks with rectified linear units. *CoRR*, abs/1611.01491, 2016. URL http://arxiv.org/abs/1611.01491.

B. Bamieh and L. Giarré. Identification of linear parameter varying models. In *Proceedings of the 38th IEEE Conference on Decision and Control (Cat. No.99CH36304)*, volume 2, pages 1505–1510 vol.2, 1999. doi: 10.1109/CDC.1999.830205.

Julius Berner, Dennis Elbrächter, Philipp Grohs, and Arnulf Jentzen. Towards a regularity theory for relu networks–chain rule and global error estimates. In *2019 13th International conference on Sampling Theory and Applications (SampTA)*, pages 1–5. IEEE, 2019.

Vincent D. Blondel and Yurii Nesterov. Computationally efficient approximations of the joint spectral radius. *SIAM Journal on Matrix Analysis and Applications*, 27(1):256–272, 2005. doi: 10.1137/040607009. URL https://doi.org/10.1137/040607009.

Jairo Bochi. Inequalities for numerical invariants of sets of matrices. *Linear Algebra and its Applications*, 368:71 – 81, 2003. ISSN 0024-3795. doi: https://doi.org/10.1016/S0024-3795(02)00658-4. URL http://www.sciencedirect.com/science/article/pii/S0024379502006584.

József Bokor and Gary Balas. Linear parameter varying systems: A geometric theory and applications. *IFAC Proceedings Volumes*, 38(1):12 – 22, 2005. ISSN 1474-6670. doi: https://doi.org/10.3182/20050703-6-CZ-1902.00003. URL http://www.sciencedirect.com/science/article/pii/S1474667016360153. 16th IFAC World Congress.

Stephen Boyd, Laurent El Ghaoui, Eric Feron, and Venkataramanan Balakrishnan. *4. Linear Differential Inclusions*, pages 51–59. 1994. doi: 10.1137/1.9781611970777.ch4. URL https://epubs.siam.org/doi/abs/10.1137/1.9781611970777.ch4.

F. Bruzelius, S. Pettersson, and C. Breitholtz. Region of attraction estimates for lpv-gain scheduled control systems. In *2003 European Control Conference (ECC)*, pages 892–897, 2003. doi: 10.23919/ECC.2003.7085071.
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Rudy Bunel, Ilker Turkaslan, Philip H. S. Torr, Pushmeet Kohli, and M. Pawan Kumar. Piecewise linear neural network verification: A comparative study. *CoRR*, abs/1711.00455, 2017. URL http://arxiv.org/abs/1711.00455.

Marco Ciccone, Marco Gallieri, Jonathan Masci, Christian Osendorfer, and Faustino J. Gomez. Nais-net: Stable deep networks from non-autonomous differential equations. *CoRR*, abs/1804.07209, 2018. URL http://arxiv.org/abs/1804.07209.

Carlos E de Souza and Alexandre Trofino. Gain-scheduled h2 controller synthesis for linear parameter varying systems via parameter-dependent lyapunov functions. *International Journal of Robust and Nonlinear Control: IFAC-Affiliated Journal*, 16(5):243–257, 2006.

Souradeep Dutta, Susmit Jha, Sriram Sankaranarayanan, and Ashish Tiwari. Output range analysis for deep feedforward neural networks. In Aaron Dutle, César Muñoz, and Anthony Narkawicz, editors, *NASA Formal Methods*, pages 121–138, Cham, 2018. Springer International Publishing. ISBN 978-3-319-77935-5.

Rüdiger Ehlers. Formal verification of piece-wise linear feed-forward neural networks. *CoRR*, abs/1705.01320, 2017. URL http://arxiv.org/abs/1705.01320.

C. Eliasmith. Attractor network. *Scholarpedia*, 2(10):1380, 2007. doi: 10.4249/scholarpedia.1380. revision #91016.

Rainer Engelken, Fred Wolf, and LF Abbott. Lyapunov spectra of chaotic recurrent neural networks. *arXiv preprint arXiv:2006.02427*, 2020.

Michael Everett, Golnaz Habibi, and Jonathan P. How. Robustness analysis of neural networks via efficient partitioning: Theory and applications in control systems, 2020.

Timon Gehr, Matthew Mirman, Dana Drachsler-Cohen, Petar Tsankov, Swarat Chaudhuri, and Martin Vechev. Ai2: Safety and robustness certification of neural networks with abstract interpretation. In *2018 IEEE Symposium on Security and Privacy (SP)*, pages 3–18. IEEE, 2018.

Behrooz Ghorbani, Shankar Krishnan, and Ying Xiao. An investigation into neural net optimization via hessian eigenvalue density. *arXiv preprint arXiv:1901.10159*, 2019.

Surbhi Goel and Adam Klivans. Eigenvalue decay implies polynomial-time learnability for neural networks. In *Advances in Neural Information Processing Systems*, pages 2192–2202, 2017.

Batuhan Güler, Alexis Laignelet, and Panos Parpas. Towards robust and stable deep learning algorithms for forward backward stochastic differential equations, 2019.

Eldad Haber and Lars Ruthotto. Stable architectures for deep neural networks. *Inverse Problems*, 34(1):014004, 2017. URL http://arxiv.org/abs/1705.03341.

Eldad Haber, Keegan Lensink, Eran Treister, and Lars Ruthotto. Imxnet: A forward stable deep neural network. *CoRR*, abs/1903.02639, 2019. URL http://arxiv.org/abs/1903.02639.
SPECTRAL ANALYSIS AND STABILITY OF DEEP NEURAL DYNAMICS

Boris Hanin and David Rolnick. Complexity of linear regions in deep networks. volume 97 of Proceedings of Machine Learning Research, pages 2596–2604, Long Beach, California, USA, 09–15 Jun 2019a. PMLR. URL http://proceedings.mlr.press/v97/hanin19a.html.

Boris Hanin and David Rolnick. Deep relu networks have surprisingly few activation patterns. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d’Alché-Buc, E. Fox, and R. Garnett, editors, Advances in Neural Information Processing Systems 32, pages 361–370. Curran Associates, Inc., 2019b. URL http://papers.nips.cc/paper/8328-deep-relu-networks-have-surprisingly-few-activation-patterns.pdf.

X. He, C. Li, T. Huang, C. Li, and J. Huang. A recurrent neural network for solving bilevel linear programming problem. IEEE Transactions on Neural Networks and Learning Systems, 25(4):824–830, 2014. doi: 10.1109/TNNLS.2013.2280905.

C. Hoffmann and H. Werner. A survey of linear parameter-varying control applications validated by experiments or high-fidelity simulations. IEEE Transactions on Control Systems Technology, 23(2):416–433, 2015. doi: 10.1109/TCST.2014.2327584.

Kurt Hornik, Maxwell Stinchcombe, Halbert White, et al. Multilayer feedforward networks are universal approximators. Neural networks, 2(5):359–366, 1989.

Xiaowei Huang, Marta Kwiatkowska, Sen Wang, and Min Wu. Safety verification of deep neural networks. CoRR, abs/1610.06940, 2016. URL http://arxiv.org/abs/1610.06940.

Guy Katz, Clark Barrett, David L Dill, Kyle Julian, and Mykel J Kochenderfer. Reluplex: An efficient smt solver for verifying deep neural networks. In International Conference on Computer Aided Verification, pages 97–117. Springer, 2017.

J. F. Kolen and S. C. Kremer. Gradient Flow in Recurrent Nets: The Difficulty of Learning LongTerm Dependencies, pages 237–243. 2001.

Yann Le Cun, Ido Kanter, and Sara A Solla. Eigenvalues of covariance matrices: Application to neural-network learning. Physical Review Letters, 66(18):2396, 1991.

Mathias Lechner, Ramin Hasani, Daniela Rus, and Radu Grosu. Gershgorin loss stabilizes the recurrent neural network compartment of an end-to-end robot learning scheme. In 2020 International Conference on Robotics and Automation (ICRA). IEEE, 2020.

Zhenyu Liao and Romain Couillet. The dynamics of learning: A random matrix approach, 2018.

S. Limanond and J. Si. Neural network-based control design: an lmi approach. IEEE Transactions on Neural Networks, 9(6):1422–1429, 1998. doi: 10.1109/72.728392.

Cosme Louart, Zhenyu Liao, and Romain Couillet. A random matrix approach to neural networks, 2017.

Oswaldo Ludwig, Urbano Nunes, and Rui Araujo. Eigenvalue decay: A new method for neural network regularization. Neurocomputing, 124:33–42, 2014.
Spectral Analysis and Stability of Deep Neural Dynamics

Gaurav Manek and J. Zico Kolter. Learning stable deep dynamics models. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d’Alché-Buc, E. Fox, and R. Garnett, editors, Advances in Neural Information Processing Systems 32, pages 11126–11134. Curran Associates, Inc., 2019. URL http://papers.nips.cc/paper/9292-learning-stable-deep-dynamics-models.pdf.

Radosław Matusik, Andrzej Nowakowski, Sławomir Plaskacz, and Andrzej Rogowski. Finite-time stability for differential inclusions with applications to neural networks. SIAM Journal on Control and Optimization, 58(5):2854–2870, 2020. doi: 10.1137/19M1250078.

Zakaria Mhammedi, Andrew Hellicar, Ashfaqur Rahman, and James Bailey. Efficient orthogonal parametrisation of recurrent neural networks using householder reflections. In International Conference on Machine Learning, pages 2401–2409. PMLR, 2017.

Razvan Pascanu, Tomas Mikolov, and Yoshua Bengio. Understanding the exploding gradient problem. CoRR, abs/1211.5063, 2012. URL http://arxiv.org/abs/1211.5063.

Jeffrey Pennington and Pratik Worah. Nonlinear random matrix theory for deep learning. Journal of Statistical Mechanics: Theory and Experiment, 2019. doi: 10.1088/1742-5468/ab3bc3.

Pavithra Prabhakar and Zahra Rahimi Afzal. Abstraction based output range analysis for neural networks. In Advances in Neural Information Processing Systems, volume 32, pages 15788–15798. Curran Associates, Inc., 2019. URL https://proceedings.neurips.cc/paper/2019/file/5df0385cbe256a135be596dbe28fa7aa-Paper.pdf.

Luca Pulina and Armando Tacchella. An abstraction-refinement approach to verification of artificial neural networks. In Tayssir Touili, Byron Cook, and Paul Jackson, editors, Computer Aided Verification, pages 243–257, Berlin, Heidelberg, 2010. Springer Berlin Heidelberg. ISBN 978-3-642-14295-6.

Kanaka Rajan and L. F. Abbott. Eigenvalue spectra of random matrices for neural networks. Phys. Rev. Lett., 97:188104, Nov 2006. doi: 10.1103/PhysRevLett.97.188104. URL https://link.aps.org/doi/10.1103/PhysRevLett.97.188104.

Bodo Rueckauer and Shih-Chii Liu. Linear approximation of deep neural networks for efficient inference on video data. In 2019 27th European Signal Processing Conference (EUSIPCO), pages 1–5. IEEE, 2019.

J. S. Shamma and M. Athans. Analysis of gain scheduled control for nonlinear plants. IEEE Transactions on Automatic Control, 35(8):898–907, 1990. doi: 10.1109/9.58498.

Jeff S. Shamma and Michael Athans. Guaranteed properties of gain scheduled control for linear parameter-varying plants. Automatica, 27(3):559 – 564, 1991. ISSN 0005-1098. doi: https://doi.org/10.1016/0005-1098(91)90116-J. URL http://www.sciencedirect.com/science/article/pii/000510989190116J.

Mau-Hsiang Shih, Jinn-Wen Wu, and Chin-Tzong Pang. Asymptotic stability and generalized gelfand spectral radius formula. Linear Algebra and its Applications, 252(1):61 – 70, 1997. ISSN 0024-3795. doi: https://doi.org/10.1016/0024-3795(95)00592-7. URL http://www.sciencedirect.com/science/article/pii/0024379595005927.
Gagandeep Singh, Timon Gehr, Markus Püschel, and Martin Vechev. An abstract domain for certifying neural networks. *Proc. ACM Program. Lang.*, 3(POPL), January 2019. doi: 10.1145/3290354. URL https://doi.org/10.1145/3290354.

Xiaowu Sun, Haitham Khedr, and Yasser Shoukry. Formal verification of neural network controlled autonomous systems. In *Proceedings of the 22nd ACM International Conference on Hybrid Systems: Computation and Control*, HSCC ’19, page 147–156, New York, NY, USA, 2019. Association for Computing Machinery. ISBN 9781450362825. doi: 10.1145/3302504.3311802. URL https://doi.org/10.1145/3302504.3311802.

K. Tanaka. Stability analysis of neural networks via lyapunov approach. In *Proceedings of ICNN’95 - International Conference on Neural Networks*, volume 6, pages 3192–3197 vol.6, 1995. doi: 10.1109/ICNN.1995.487296.

K. Tanaka. An approach to stability criteria of neural-network control systems. *IEEE Transactions on Neural Networks*, 7(3):629–642, 1996. doi: 10.1109/72.501721.

Aaron Tuor, Jan Drgona, and Draguna Vrabie. Constrained neural ordinary differential equations with stability guarantees. *arXiv preprint arXiv:2004.10883*, 2020.

K. G. Vamvoudakis, F.L. Lewis, and Shuzhi Sam Ge. *Neural Networks in Feedback Control Systems*, chapter 23, pages 1–52. American Cancer Society, 2015. ISBN 9781118985960. doi: https://doi.org/10.1002/9781118985960.meh223. URL https://onlinelibrary.wiley.com/doi/abs/10.1002/9781118985960.meh223.

Kyriakos G. Vamvoudakis and Frank L. Lewis. Online actor–critic algorithm to solve the continuous-time infinite horizon optimal control problem. *Automatica*, 46(5):878 – 888, 2010. ISSN 0005-1098. doi: https://doi.org/10.1016/j.automatica.2010.02.018. URL http://www.sciencedirect.com/science/article/pii/S0005109810000907.

Richard Varga. *Geršgorin and His Circles*, volume 36. Springer, Berlin, Heidelberg, 01 2004. doi: 10.1007/978-3-642-17798-9.

Ryan Vogt, Maximilian Puelma Touzel, Eli Shlizerman, and Guillaume Lajoie. On lyapunov exponents for rnns: Understanding information propagation using dynamical systems tools. *arXiv preprint arXiv:2006.14123*, 2020.

Draguna Vrabie and Frank Lewis. Neural network approach to continuous-time direct adaptive optimal control for partially unknown nonlinear systems. *Neural Networks*, 22(3):237–246, 2009.

Shengjie Wang, Abdel rahman Mohamed, Rich Caruana, Jeff A. Bilmes, Matthai Philipose, Matthew Richardson, Krzysztof Geras, Gregor Urban, and Özlem Aslan. Analysis of deep neural networks with extended data jacobian matrix. In *ICML*, pages 718–726, 2016. URL http://proceedings.mlr.press/v48/wanga16.html.

W. Xiang, H. Tran, and T. T. Johnson. Output reachable set estimation and verification for multilayer neural networks. *IEEE Transactions on Neural Networks and Learning Systems*, 29(11):5777–5783, 2018. doi: 10.1109/TNNLS.2018.2808470.
Appendix A: Equivalence with Other Linearization Methods

**Proposition 12** For ReLU networks, where \( \sigma(x) = \max(0, x) \), the pointwise linearization \( A^*(x) \) of the underlying deep neural network \( f_\theta \) is equivalent to its first-order Taylor approximation.

**Proof** The first order Taylor approximation of the learned function \( f_\theta(x) \) about a point \( a \) is:

\[
 f(x) \approx f(a) + \frac{\partial f(a)}{\partial x} (x - a)
\]  

(13)

We take the limit as \( a \to 0 \) since the derivative of ReLU is not defined at 0. We observe that \( \operatorname{sign}(a_i) = \operatorname{sign}(x_i) \). Taking the limit as \( a \) goes to 0:

\[
\lim_{a \to 0} \left( f(a) + \frac{\partial f(a)}{\partial x} (x - a) \right) = \lim_{a \to 0} f(a) + \lim_{a \to 0} \frac{\partial f(a)}{\partial x} (x - a) = \lim_{a \to 0} \frac{\partial f(a)}{\partial x} x = \frac{\partial f(x)}{\partial x} x
\]  

(14)

The final equivalence follows from the fact that the derivative of \( f \) only depends on the sign of the input vector elements. Now let \( a_l(h) = A_l h \). We have

\[
\frac{\partial f}{\partial x} = \frac{\partial}{\partial x} \left( a_L \circ \sigma \circ a_{L-1} \circ \sigma \circ \ldots \circ \sigma \circ a_0 \right)
\]  

(15)

\[
= \frac{\partial A_L h_L}{\partial h_L} \frac{\partial \sigma(A_{L-1} h_{L-1})}{\partial A_{L-1} h_{L-1}} \frac{\partial A_{L-1} h_{L-1}}{\partial h_{L-1}} \ldots \frac{\partial \sigma(A_0 a)}{\partial A_0 a} \frac{\partial A_0 a}{\partial a} = A_L \sigma'_L A_{L-1} \ldots \sigma'_1 A_0
\]  

(16)

where

\[
\sigma'_{k+1} = \begin{bmatrix} \sigma'((A_k h_k)_1) & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \sigma'((A_k h_k)_n) \end{bmatrix}
\]  

(18)

Now

\[
\sigma'(x_i) = \begin{cases} 1 & x_i > 0 \\ 0 & x_i < 0 \end{cases} = \frac{\operatorname{ReLU}(x_i)}{x_i}
\]  

(19)

And so \( \sigma'_k = A z_k \) and therefore in the special case of ReLU we have the equivalence to the first order Taylor approximation:

\[
f(x) = A_L \sigma'_L A_{L-1} \ldots \sigma'_1 A_0 x = A_L A_{z_L} A_{L-1} \ldots A_{z_1} A_0 x = A^*(x) x
\]  

(20)
We pay special mind to the fact that for \( x \in \{ x : \exists i \text{ s.t. } x_i = 0 \} \), \( A^*(x) \) is undefined. For ReLU networks, this is in fact an issue for the first order Taylor approximation as well, since the derivative of ReLU is not defined for \( x = 0 \). In practice, deep learning libraries such as Pytorch and Tensorflow, which have shown great success in many applications using ReLU networks set \( \text{ReLU}'(0) = 0 \). Berner et al. (2019) provide arguments motivated by regularity theory to justify this as a reasonable practice. However, in this work we skirt the issue entirely. In the case of ReLU networks, as shown in the arguments above, our formulation is equivalent to the exact linearization independently presented in several recent works (Rueckauer and Liu, 2019; Berner et al., 2019; Wang et al., 2016; Gehr et al., 2018). However, our formulation generalizes the exact linearization to an extended class of neural networks. In practice, the set of unsupported points does not inhibit our subsequent analysis—the probability of randomly sampling from the set excluded from the support of \( A^* \) is actually 0 since the points do not form a volume in \( \mathbb{R}^n \).

Appendix B: Eigenvalue Constraints and Regularizations of Weight Matrices

As given in sufficient conditions of theorem 6, all weight matrices \( A_i, i \in \mathbb{N}_0 \) must have stable eigenvalues to guarantee the global stability of deep neural network \( f_\theta \). Following paragraphs summarize a set of methods for constraining the eigenvalues of the weights in deep neural networks via matrix factorizations and regularizations.

**Perron-Frobenius Weights:** This factorization introduced by Tuor et al. (2020) leverages the Perron-Frobenius theorem, which states that the row-wise minimum and maximum of any positive square matrix defines its dominant eigenvalue’s lower and upper bound, respectively. Based on this theorem, we construct a state transition matrix \( \tilde{A} \) with bounded eigenvalues:

\[
M = \lambda_{\text{max}} - (\lambda_{\text{max}} - \lambda_{\text{min}})\sigma(M')
\]

\[
\tilde{A}_{i,j} = \frac{\exp(A'_{ij})}{\sum_{k=1}^{\lambda_{\text{max}}} \exp(A'_{ik})} M_{i,j}
\]

where matrix \( M \) represents damping parameterized by the matrix \( M' \in \mathbb{R}^{n_x \times n_x} \). We apply a row-wise softmax to another parameter matrix \( A' \in \mathbb{R}^{n_x \times n_x} \), then elementwise multiply by \( M \) to obtain the stable weight \( \tilde{A} \) with eigenvalues lower and upper bounds \( \lambda_{\text{min}} \) and \( \lambda_{\text{max}} \).

**Spectral Weights:** This method parametrizes a weight matrix as a factorization via singular value decomposition (SVD). The weight is defined as two unitary matrices \( U \) and \( V \) initialized as orthogonal matrices, and singular values \( \Sigma \) initialized randomly. During optimization, \( U \) and \( V \) are constrained via regularization terms such that they remain orthogonal:

\[
\mathcal{L}_U = ||I - UU^T||_2 + ||I - U^TU||_2
\]

\[
\mathcal{L}_V = ||I - VV^T||_2 + ||I - V^TV||_2
\]

\[
\mathcal{L}_{\text{reg}} = \mathcal{L}_U + \mathcal{L}_V
\]
Similar to Perron-Frobenius weights, this regularization also enforces boundary constraints on the singular values $\Sigma$, and its eigenvalues by extension. This is achieved by clamping and scaling $\Sigma$:

$$\tilde{\Sigma} = \text{diag}(\lambda_{\text{max}} - (\lambda_{\text{max}} - \lambda_{\text{min}}) \cdot \sigma(\Sigma))$$  \hspace{1cm} (23a)

$$\tilde{A} = U\tilde{\Sigma}V$$  \hspace{1cm} (23b)

where $\lambda_{\text{min}}$ and $\lambda_{\text{max}}$ are the lower and upper singular value bounds, respectively. Instead of regularization terms (22c) for enforcing orthogonal structure, Zhang et al. (2018) used Householder reflectors to represent unitary matrices $U$ and $V$ by design. However, the disadvantage of using Householder reflectors is increased computational requirements compared to using (22c).

**Skew-symmetric Weights:** Skew-symmetric (or antisymmetric) matrix $\tilde{A}$ is a square matrix whose transpose equals its negative $\tilde{A} = -\tilde{A}^T$. The implementation is straightforwardly given as:

$$\tilde{A} = L - L^T - \gamma I$$ \hspace{1cm} (24)

Where $L$ represents lower triangular parameter matrix, $I$ is an identity matrix, and $\gamma$ is a damping factor. This factorization was introduced in Haber and Ruthotto (2017).

**Hamiltonian Weights:** This method introduces symmetry by encoding weight $\tilde{A}$ as symplectic matrix:

$$\tilde{A} = \begin{bmatrix} 0 & A \\ -A^T & 0 \end{bmatrix}$$ \hspace{1cm} (25)

The proposed factorization is intrinsically stable by design regardless of the spectrum of parameter matrix $A$, see Haber and Ruthotto (2017) for details. This factorization generates system with energy conversion property and no dissipativeness. Hence, the dominant eigenvalue $\lambda_{\text{max}} = 1$.

**Gershgorin Discs Weights:** This factorization is based on Gershgorin Circle Theorem. We define parameter matrix $M \in \mathbb{R}^{n \times n}$ with $m_{i,j} \sim \mathcal{U}(0, 1)$, except $m_{i,i} = 0$. We divide each row’s elements by it’s sum and multiply by a radius $r$, finally adding a diagonal matrix of values where the layer eigenvalues should be centered. For layer weights $\tilde{A}$ and $s_j = \sum_{i \neq j} m_{i,j}$ we have:

$$\tilde{A} = \text{diag} \left( \frac{r}{s_1}, \ldots, \frac{r}{s_n} \right) M + \text{diag} \left( \lambda, \ldots, \lambda \right)$$ \hspace{1cm} (26)

So, by the Gershgorin Circle Theorem (Varga, 2004), all eigenvalues $\lambda_i$ will be bounded in a circle in the complex plane with center $\lambda$ and radius $r$.

**Appendix C: Spectral Properties and Attractors of Deep Neural Networks**

**Spectral Properties of Networks with Varying Depth:** Fig. 5 displays a visualization of the spectral plots with increasing depth in deep neural network as discussed in the last paragraph of section 4.

**Attractors of Deep Neural Networks:** Understanding dynamical effects of individual components of deep neural networks allow us to analyze neural dynamics with different attractors. In neuroscience, different types of attractor networks have been associated with different brain functions (Eliasmith, 2007). We believe that insights in neural dynamics and connections with neuroscience can inspire new advances theory of learning deep neural networks. Example could be
enforcing desired dynamical properties associated with the learning task. For instance, it is known that cyclic attractors can describe repetitive behaviors such as walking, line attractors have been linked with oculomotor control and integrators in control theory, while point attractors have been linked with associative memory, pattern completion, noise reduction, and classification tasks (Eliasmith, 2007). Fig. 6 demonstrates the expressive capabilities of deep neural networks to model six prominent attractor types: single equilibrium, multiple equilibria, line attractor, limit cycle, chaotic attractor, unstable attractor. Figs. 7 and 8 further show the spectral radii of $A^*$ across the feature space and their eigenvalue spectra, respectively.

Figure 5: Real eigenvalue spectra of neural networks with varying depth using GELU layers with asymptotically stable (first row), on the edge of stability (second row), and unstable dynamics (third row), respectively. Single-layer (left), 4-layer (center), 8-layer (right).
Figure 6: Different attractor types generated by deep neural networks. From left to right: single point, multiple points, line attractor, limit cycle, chaotic attractor, unstable dynamics.
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Figure 7: A∗ regions represented by spectral radii at each point of the feature space corresponding to the phase portraits in Fig. 6.

Appendix D: Details on Experimental Setup

As a holistic analysis of the dynamics and stability of neural networks, we employ a grid search to compare across the axes of structured linear maps, eigenvalue constraints, activation functions, network depths, and biases. For each combination of factorization, spectral constraints, and network depths, we swap out activation functions and toggle bias usage while keeping model parameters fixed to control for the effects of initializations when comparing how these latter two hyperparameters affect network dynamics and stability.

Linear Map Factorizations and Constraints (λ_{min}, λ_{max}):

- Gershgorin Disc, real eigenvalues: (−1.50, −1.10), (0.00, 1.00), (0.99, 1.00), (0.99, 1.01), (0.99, 1.10), (1.00, 1.01), (1.10, 1.50)
- Gershgorin Disc, complex eigenvalues: (−1.50, −1.10), (0.00, 1.00), (0.99, 1.00), (0.99, 1.01), (0.99, 1.10), (1.00, 1.01), (1.10, 1.50)
- Spectral: (−1.50, −1.10), (0.00, 1.00), (0.99, 1.00), (0.99, 1.01), (0.99, 1.10), (1.00, 1.01), (1.10, 1.50)
- Perron-Frobenius: (1.00, 1.00)
- Unstructured: no spectral constraints

Network Depth: 1, 4, 8 layers
Figure 8: Eigenvalue spectra associated with different attractor types generated by deep neural networks, with corresponding phase fields displayed in Fig. 6 and $A^*$ spectral radii displayed in Fig. 7. From left to right: single point, multiple points, line attractor, limit cycle, chaotic attractor, unstable dynamics.
**Activation Functions:** ReLU, SELU, GELU, Tanh, logistic sigmoid, Softplus

**Bias:** Enabled, disabled

Overall, we generated 828 different models for examination. From this sampling, we then selected the models which were most relevant to our analysis based on their dynamical behavior. Table 1 outlines the hyperparameters of each of the curated examples shown in the figures.

| Figure   | Factorization | Activation | N. Layers | Eigenvalue Range | Bias |
|----------|---------------|------------|-----------|------------------|------|
| Fig. 2   | Gershgorin, Real | Tanh       | 8         | (0.99, 1.00)     | N    |
|          | Spectral      | Tanh       | 8         | (0.99, 1.10)     | N    |
|          | Gershgorin, Real | Softplus  | 8         | (1.00, 1.01)     | Y    |
| Fig. 3   | Gershgorin, Complex | ReLU     | 4         | (0.00, 1.00)     | N    |
|          | Gershgorin, Real | Tanh       | 4         | (0.00, 1.00)     | N    |
|          | Gershgorin, Real | Sigmoid    | 4         | (0.00, 1.00)     | N    |
|          | Spectral      | SELU       | 4         | (0.00, 1.00)     | N    |
| Fig. 4   | Gershgorin, Complex | ReLU     | 1         | (0.00, 1.00)     | Y    |
|          | Gershgorin, Complex | ReLU     | 1         | (0.00, 1.00)     | N    |
| Fig. 5   | Gershgorin, Complex | GELU     | 1         | (0.00, 1.00)     | N    |
|          | Gershgorin, Complex | GELU     | 4         | (0.00, 1.00)     | N    |
|          | Gershgorin, Complex | GELU     | 8         | (0.00, 1.00)     | N    |
|          | Gershgorin, Complex | GELU     | 1         | (0.99, 1.00)     | N    |
|          | Gershgorin, Complex | GELU     | 4         | (0.99, 1.00)     | N    |
|          | Gershgorin, Complex | GELU     | 8         | (0.99, 1.00)     | N    |
|          | Gershgorin, Real | GELU       | 1         | (0.99, 1.10)     | Y    |
|          | Gershgorin, Real | GELU       | 4         | (0.99, 1.10)     | Y    |
|          | Gershgorin, Real | GELU       | 8         | (0.99, 1.10)     | Y    |
| Figs. 6, 7, 8 | Gershgorin, Real | ReLU     | 1         | (0.00, 1.00)     | N    |
|          | Gershgorin, Real | SELU       | 1         | (-1.50, -1.10)   | Y    |
|          | Perron-Frobenius | ReLU      | 1         | (1.00, 1.00)     | N    |
|          | Spectral      | Tanh       | 8         | (0.99, 1.10)     | N    |
|          | Spectral      | SELU       | 8         | (0.99, 1.10)     | N    |
|          | Gershgorin, Complex | Softplus | 1         | (0.99, 1.10)     | N    |

Table 1: Layer factorizations, activation functions, network depths, spectral constraints, and bias usage of the models depicted in each figure.