Data-driven model discovery with Kolmogorov-Arnold networks

Mohammadamin Moradi,^{1, *} Shirin Panahi,^{1, *} Erik M. Bollt,² and Ying-Cheng Lai^{1,3,[†](#page-0-1)}

 1 School of Electrical, Computer, and Energy Engineering,

Arizona State University, Tempe, AZ 85287, USA

² Department of Electrical and Computer Engineering, Clarkson Center for Complex Systems Science,

Clarkson University, Potsdam, New York 13699, USA

³Department of Physics, Arizona State University, Tempe, Arizona 85287, USA

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Data-driven model discovery of complex dynamical systems is typically done using sparse optimization, but it has a fundamental limitation: sparsity in that the underlying governing equations of the system contain only a small number of elementary mathematical terms. Examples where sparse optimization fails abound, such as the classic Ikeda or optical-cavity map in nonlinear dynamics and a large variety of ecosystems. Exploiting the recently articulated Kolmogorov-Arnold networks, we develop a general model-discovery framework for any dynamical systems including those that do not satisfy the sparsity condition. In particular, we demonstrate non-uniqueness in that a large number of approximate models of the system can be found which generate the same invariant set with the correct statistics such as the Lyapunov exponents and Kullback–Leibler divergence. An analogy to shadowing of numerical trajectories in chaotic systems is pointed out.

Discovering the model of a system from observational or measurement data has been a fundamental problem since the beginning of science. For nonlinear dynamical systems, data-driven identification, and forecasting have attracted a great deal of research in the past four decades [\[1](#page-4-0)[–37\]](#page-4-1). A diverse array of methodologies have been developed, e.g., calculating the information contained in sequential observations to deduce the deterministic equations [\[2\]](#page-4-2), approximating a nonlinear system by a large collection of linear equations [\[1,](#page-4-0) [7,](#page-4-3) [12\]](#page-4-4), fitting differential equations to chaotic data [\[9\]](#page-4-5), exploiting chaotic synchronization [\[15\]](#page-4-6) or genetic algorithms [\[17,](#page-4-7) [27\]](#page-4-8), inverse Frobenius-Perron approach to designing a dynamical system "near" the original system [\[19\]](#page-4-9), or using the least-squares best approximation for modeling [\[26\]](#page-4-10). An approach that has gained considerable interest is sparse optimization, where the system functions are assumed to have a sparse structure in that they can be represented by a small number of elementary mathematical functions, e.g., a few power- and/or Fourier-series terms. What is needed then is to estimate the coefficients associated with these terms. In a high-order series expansion, the coefficients with the vast majority of the terms are zero, except for a few. The problem of finding these nontrivial coefficients can then be naturally formulated [\[28,](#page-4-11) [38\]](#page-4-12) as a compressive-sensing problem [\[39–](#page-4-13)[43\]](#page-5-0). Under the same idea, a popular method was later developed [\[44,](#page-5-1) [45\]](#page-5-2).

The sparse-optimization approach is effective for systems whose governing equations are sufficiently simple in the sense of sparsity, such as the chaotic Lorenz [\[46\]](#page-5-3) and Rössler [\[47\]](#page-5-4) oscillators whose velocity fields contain a small number of low-order power-series terms. However, sparsity can be self-sabotage because, while it is the reason that the approach is powerful, it also presents a fundamental limitation: it works only if the system equations do in fact have a sparse structure. Dynamical systems violating the sparsity condition arise in physical and biological situations. A known example is the Ikeda map that describes the propagation of an optical pulse in a cavity with a nonlinear medium [\[48,](#page-5-5) [49\]](#page-5-6), whose functions contain an infinite number of series expansion terms. Many ecological systems and gene-regulatory circuits whose governing equations have a Holling-type of structure [\[50,](#page-5-7) [51\]](#page-5-8) also violate the sparsity condition [\[52\]](#page-5-9). For these systems, the sparse-optimization approach to model discovery fails absolutely and completely.

In this Letter, we articulate an entirely different approach to discovering the models of any dynamical systems including those that do not meet the sparsity condition. The idea exploits Kolmogorov-Arnold networks (KANs), a recent computational framework for representing sophisticated mathematical functions [\[53\]](#page-5-10) based on the classical Kolmogorov-Arnold theorem [\[54–](#page-5-11)[56\]](#page-5-12) that any multivariate mathematical function can be decomposed as a sum of single-variate functions, as illustrated in Fig. [1\(](#page-1-0)a). KANs decompose complex high-dimensional problems into simpler, more manageable univariate functions, allowing for more efficient training and better interpretability of the machine-learning model, addressing some of the limitations in traditional neural networks such as the black-box nature and computational inefficiency. As a result, KANs are rapidly gaining attention as a promising alternative in machine learning.

In contrast to a standard neural network with thousands and perhaps millions of weights and biases but always fixed all the same activation functions say atan or ReLu, a KAN is a small network of say a dozen nodes but each different and carefully designed activation functions. We consider a dynamical system described by $d\mathbf{x}/dt = \mathbf{F}(\mathbf{x})$ or alternatively by $\mathbf{x}_{n+1} = \mathbf{F}(\mathbf{x}_n)$, including where $F(x)$ does not possess a sparse structure. Our goal is to find an approximation of $F(x)$, de-

[∗] The first two authors contributed equally to this work

[†] Ying-Cheng.Lai@asu.edu

noted as $\mathbf{G}(\mathbf{x})$, such that the system $d\mathbf{x}/dt = \mathbf{G}(\mathbf{x})$ or $\mathbf{x}_{n+1} = \mathbf{G}(\mathbf{x}_n)$ produces the identical dynamical behaviors as the original system (e.g., the same attractor with the same statistical and dynamical invariants to within certain numerical precision). We demonstrate, using the Ikeda map and a chaotic ecosystem as illustrative examples, that such a function $G(x)$ in an implicit form can indeed be found by the KANs.

FIG. 1. Basics of KAN. (a) Kolmogorov-Arnold theorem and neural network. (b) Schematic illustration of two different structures (blue and green) leading to two different functions $M(x)$ and $L(x)$ that generate the same dynamics as $x_{n+1} =$ **in the relevant phase-space domain.**

The interpretability of the KAN structure lies in its accessibility to the internal mechanisms of the model, such as the activation functions $F_i(\mathbf{x})$, $G_i(\mathbf{x})$, and $K_i(\mathbf{x})$ in Fig. [1\(](#page-1-0)b). Unlike the conventional machine-learning methods, which often operate as "black boxes," KANs provide a more transparent view of how inputs are transformed into outputs. This transparency allows for a better understanding of the underlying dynamics and how each function influences the system's behavior, thereby making them more interpretable than conventional methods. Figure [1\(](#page-1-0)b) presents two different KAN structures highlighted in blue and green. The blue KAN has two inputs and two outputs without any hidden nodes, where the functions $M_1 = F_1(\mathbf{x}_n) + F_3(\mathbf{y}_n)$ and $M_2 = F_2(\mathbf{x}_n) + F_4(\mathbf{y}_n)$ are linear combinations of the activation functions F_i for $i = 1, \dots, 4$. The green structure has two extra hidden nodes where $L_1 =$ $K_1(G_1(\mathbf{x_n}) + G_3(\mathbf{y_n})) + K_3(G_2(\mathbf{x_n}) + G_4(\mathbf{y_n}))$ and $L_2 =$ $K_2(G_1(\mathbf{x_n}) + G_3(\mathbf{y_n})) + K_4(G_2(\mathbf{x_n}) + G_4(\mathbf{y_n})).$ Both structures produce the same dynamics in the relevant

phase-space domain (yellow shaded area), where the dynamics outside of this domain can be different. This concept will be elucidated below with a concrete example.

From the standpoint of data-driven model discovery, the Ikeda map represents perhaps the most difficult kind of system - so far there has been no success with any sparse optimization method. The two-dimensional map is given by [\[48,](#page-5-5) [49\]](#page-5-6) $x_{n+1} = 1 + \mu (x_n \cos(\phi_n) - y_n \sin(\phi_n))$ and $y_{n+1} = \mu(x_n \sin(\phi_n) + y_n \cos(\phi_n))$, where $\phi_n =$ $0.4 - 6(1 + x_n^2 + y_n^2)^{-1}$ and μ is a bifurcation parameter. (We fix $\mu = 0.9$, so that the map generates a chaotic attractor in the phase-space domain $(x \in [-1,2], y \in$ [−2.5, 1]). Sparse optimization fails spectacularly for this system because in either the power- or the Fourier-series expansions or a combination of both, an infinite number of terms are required to represent each map function - see Supplementary Information (SI) for more details [\[57\]](#page-5-13).

FIG. 2. KANs applied to the Ikeda map. (a) A KAN structure with 2 input, 4 hidden, and 2 output nodes. (b) Training (red) and testing (black dashed) loss curves. (c) Chaotic attractor during the training phase (blue - ground truth; orange - KAN produced). (d,e) Time series during the training. The blue and orange traces overlap well, signifying a high training accuracy. (f) Chaotic attractor during testing (blue - ground truth; orange - KAN produced). (g,h) The corresponding time series. While the predicted time series diverges from the ground truth after a few iterations due to chaos, the KAN generates the correct attractor in the pertinent phase-space domain. The true Lyapunov exponents of the chaotic attractor are [0.5025, −0.7263]. The KAN predicted model gives the values of the two exponents as $[0.5075, -0.7182]$, agreeing with the ground truth.

We first use a [2, 4, 2] KAN structure, as shown in Fig. $2(a)$, which has 2 input, 4 hidden, and 2 output nodes. The time-series data contain 10^4 points, with 80% allocated for training and the remaining 20% for testing. The training process contains 50 iterations with the following hyperparameter values: $k = 3$ (cubic B-splines), grid size $G = 10$ for the splines, regularization parameters $\lambda = 0$ and $\lambda_{entropy} = 10$, learning rate 0.1, and a zero initial random seed. (see SI [\[57\]](#page-5-13) for a detailed description of these hyperparameters). Training is administered in a feedforward process in which the KAN is trained to minimize the difference between the input and output so as to predict the evolution of the Ikeda map into the future with the input of the dynamical variables from the past. The training loss as a function of time is shown as the red curve in Fig. [2\(](#page-1-1)b), and the KAN-produced attractor and time series during the training phase in comparison with the ground truth are shown in Figs. $2(c-e)$, respectively. The training loss decreases rapidly to zero, indicating high training accuracy and efficiency with skill. For the testing phase, we use the same set of parameter values but replace the original input data point with the output of the KAN at each iteration. The testing loss is shown in Fig. [2\(](#page-1-1)b) as the black dashed curve, and the KAN predicted attractor and time series are shown in Figs. [2\(](#page-1-1)f-h), respectively. While the KAN-predicted time series diverges from the ground truth after a few iterations due to chaos, the predicted attractor agrees with the ground truth well, indicating that the KAN has generated the correct model of the Ikeda map.

To demonstrate that a KAN can be readily modified to generate a different representation of the Ikeda map but with the same chaotic attractor, we construct a more sophisticated architecture than the one in Fig. $2(a)$, as shown in Fig. $3(a)$. The training and prediction results are shown in Figs. [3\(](#page-2-0)b-h).

For generality, we now present results from a continuous-time system, a chaotic ecosystem [\[58\]](#page-5-14) of three dynamical variables: $\dot{N} = N (1 - N/K) - x_p y_p N P / (N +$ N_0 , $\dot{P} = x_p P (y_p N/(N + N_0) - 1) - x_q y_q P Q / (P + P_0)$, and $\dot{Q} = x_q Q (y_q P/(P + P_0) - 1)$, where N, P, and Q are the populations of the primary producer, the herbivore, and the carnivore, respectively, and the bifurcation parameter K is the carrying capacity. For $K = 0.98$ and other parameters set as $x_p = 0.4$, $y_p = 2.009$, $x_q = 0.08$, $y_q = 2.876$, $N_0 = 0.16129$, and $P_0 = 0.5$, the system exhibits a chaotic attractor [\[58\]](#page-5-14). A power-series expansion of the velocity field contains an infinite number of terms, violating the sparsity condition - see SI for more details [\[57\]](#page-5-13).

Our KAN architecture has a [3, 3] structure (3 input and 3 output nodes, no hidden nodes), as illustrated in Fig. [4\(](#page-3-0)a). The neural network was trained using 10,000 data points of sampling interval $\delta t = 0.5$ (corresponding to about 1,155 cycles of oscillation), with 90% of the data allocated for training and the remaining 10% for testing. The training process involved 100 iterations for the following hyperparameter values: cubic B-spline $(K = 3)$, grid size $G = 3$, $\lambda = 0$, $\lambda_{entropy} = 10$, learning rate 0.5, and a zero initial random seed. Figure [4\(](#page-3-0)b) shows the rapid decrease in the training and testing loss with increasing epochs. The KAN generated attractor and the corresponding time series during the training phase

FIG. 3. A KAN configuration generating a different representation of the Ikeda map but with the same chaotic attractor. The KAN has 2 input, 10 hidden, and 2 output nodes. Legends are the same as those in Fig. [2.](#page-1-1) The two Lyapunov exponents of the KAN predicted model are [0.5033, −0.7311], which again agrees with the true exponents.

are shown in Figs. $4(c-f)$, where a comparison with the ground truth indicates successful training. The KAN attractor and the time series generated during the testing phase are shown in Figs. $4(g-j)$, demonstrating the KAN's forecasting power. The Lyapunov exponents of the attractor are consistent with the true values. (Detailed comparative results for the power spectra, correlation dimension and three types of distance divergences are provided in SI [\[57\]](#page-5-13).)

To gain insights into the meaning of the interpretability of the KAN-discovered models, we offer a mathematical scheme to interpret machine-learning modeling errors of as representing the true underlying system. The issue of considering models that produce realistic data, even with orbital errors, is general. In our case, the KAN model G is said to produce identical behavior as the true system ${\bf F}$ if numerically computed orbits of ${\bf G}$ shadow some true orbits of F, at least for the observed finite time of the data set. For maps, if a true orbit of **F** is a sequence $Orbit_{\mathbf{F}}(\mathbf{x}_0) = {\mathbf{x}_0, \mathbf{F}(\mathbf{x}_0), \mathbf{F}^2(\mathbf{x}_0)...}$ \equiv ${x_0, x_1, x_2, \ldots}$, it is unreasonable to expect that a good but imperfect model G will produce an orbit, denoted as $\text{Orbit}_{\mathbf{G}}(\mathbf{x}_0) = {\mathbf{x}_0, \mathbf{G}(\mathbf{x}_0), \mathbf{G}^2(\mathbf{x}_0)...} \equiv {\mathbf{x}_0, \tilde{\mathbf{x}}_1, \tilde{\mathbf{x}}_2,...}$ that stays close to Orbit $_F(\mathbf{x}_0)$. If the model is good in the sense that a pointwise error $e(x) = |\mathbf{G}(x) - \mathbf{F}(x)|$ on the domain $\mathbf{x} \in \mathcal{D}$ satisfies in terms of the sup-norm, $||e||_{\infty} := \sup_{\mathbf{x} \in \mathcal{D}} |e(\mathbf{x})| < \epsilon$ for some small $\epsilon > 0$, then at each step of the model the error is small: $\tilde{\mathbf{x}}_{i+1} = \mathbf{G}(\tilde{\mathbf{x}}_i)$ $F(\tilde{x}_i)+\epsilon_i$ and with each step error, $0 \leq |\epsilon_i| < \epsilon$. Nonetheless a small normed error of the function difference be-

FIG. 4. KAN applied to a chaotic ecosystem. (a) KAN structure with 3 input and 3 output nodes. (b) Training and testing loss curves. (c) KAN generated attractor during the training phase (orange), which agrees completely with the ground truth (blue). (d-f) KAN generated time series (orange) in agreement with the true time series (blue). (g-j) Similar to (c-f) but for the testing phase. Due to chaos, the KAN generated time series diverges from the true ones from the same initial condition, but the KAN attractor agrees with the true one. The true Lyapunov exponents are [0.0053, 0, −0.2288]. The exponents of the KAN-generated attractor are consistent: $[0.0095, -5.8 \times 10^{-6}, -0.3932]$. The errors arise from the implicit numerical evaluation of the Jacobian matrix.

tween the system and model alone does not prevent the model from producing an unrealistic orbit $Orbit_G(i\mathbf{x}_0)$ that behaves quite differently from any orbit of \bf{F} , e.g., a model orbit that diverges to infinity even if the true orbit produces bounded attractor. Furthermore, it is even more difficult to consider a model orbit that has statistical properties such as the invariant measure of a chaotic attractor analogous to the attractor of the true system.

The KAN was represented as an efficient way to replace a standard multi-layer perceptron (MLP) [\[53\]](#page-5-10) and, in so doing, the weights of edges are in principle eliminated, but in practice they are absorbed into representing the various activation functions at the vertices of the network. That is, in stating the basic form of a KAN as $G(x) = \sum_{q=1}^{2n+1} \Phi_q \circ \sum_{p=1}^{n} \phi_{q,p}(x_p)$, in practice each ac-

tivation function $\phi_{q,p}$ was represented as a cubic spline numerically [\[53\]](#page-5-10), and therefore each has many internal fitted parameters of the scalar piecewise cubics. Collecting all these as the set of parameters $\Theta_{q,p}$ for each $\phi_{q,p}$, and Θ_q for each Φ_q , we can state the complete collection of parameters $\Theta = \bigcup_q(\Theta_q) \cup (\bigcup_{q,p} \Theta_{q,p})$ and rewrite the function to emphasize the internal parameters: $G_{\Theta}(x) = \sum_{q=1}^{2n+1} \Phi_{q,\Theta_q} \circ \sum_{p=1}^n \phi_{q,p,\Theta+q,p}(x_p)$, and for a multivariate argument $x = (x_1, x_2, ..., x_d) \in \mathbb{R}^d$. It is shown [\[53\]](#page-5-10) that a regularized fit to the data by a loss function $\mathcal{L}(\mathcal{D};\Theta)$ (over a data set $\mathcal D$ with respect to the fitting parameters Θ), with an objective of data fidelity as least squares fit across the data set balanced against L_2 norm on the parameters to prevent overfitting.

While excellent fit when optimizing $\mathcal{L}(\mathcal{D};\Theta)$ was observed, it is possible to emphasize sparsification. That is, one or some of the activation functions may be set to zero, a procedure that was called "pruning" [\[53\]](#page-5-10). This procedure is possible when the representation of the activation functions by splines is sufficiently fine so that there are more parameters than data points. In such case, $\mathcal{L}(\mathcal{D};\Theta)$ will generally have nontrivial level sets. The sparsification concept speaks to one of the many reasons to exploit these level sets, generally in terms of machine-learning interpretability, where the fitted KAN model is pushed toward just a few physics recognizable activation functions and the residual in a few terms is collected. The mathematical reason this kind of procedure is possible hinges on the implicit function theorem [\[59\]](#page-5-15). In brief, the KAN model function $G_{\Theta}(x)$ can be varied smoothly with respect to the fitting parameters so that $\mathcal{L}(\mathcal{D}; \Theta) = c$ is constant for a given parameter c. Therefore even following numerical optimization to a small value c, there will generally be smooth level sets with respect to the Θ parameters to emphasize other goals of explainability. A smooth implicit function $\Theta = h(s)$ exists under the conditions of a nonsingular Jacobian derivative $D_{\Theta} \mathcal{L}$ that continues a c-level set, and in principle this level of constancy $\mathcal{L}(\mathcal{D}; h(s)) = c$ set may intersect the other useful or desirable interpretabile states, including sparsification.

To summarize, we exploited KANs to solve the problem of data-driven model discovery for any dynamical systems including those for which the popular sparsityoptimization approach to finding the governing equations fails. Our result may be understood as realizing shadowing in the functional space where KANs find certain functions that produce the same dynamics. These functions may or may not have the same mathematical forms as the governing equations of the system and may even be implicit with a numerical representation. In the space of all functions, an infinite number of such "shadowing" functions may exist. We demonstrated that KAN-based machine learning can indeed find many of them, depending on the neural-network architecture.

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