KAN: Kolmogorov–Arnold Networks

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Kolmogorov-Arnold Representation Theorem

For a smooth $f: [0,1]^n \to \mathbb{R}$

$$f(\mathbf{x}) = f(x_1, \cdots, x_n) = \sum_{q=0}^{2n} \Phi_q(\sum_{p=1}^n \phi_{q,p}(x_p)).$$

where $\phi_{q,p}: [0,1] \to \mathbb{R}$ and $\Phi_q: \mathbb{R} \to \mathbb{R}$ are continuous.

• Summing and composition of univariate functions. Potentially address the curse of dimensionality (COD).

• Φ_q and $\phi_{q,p}$ not necessarily smooth. In practice we may need more than two layers (but normally it suffices with two layers).

Kolmogorov–Arnold Networks (KANs)

Model	Multi-Layer Perceptron (MLP)	Kolmogorov-Arnold Network (KAN)	
Theorem	Universal Approximation Theorem	Kolmogorov-Arnold Representation Theorem	
Formula	$f(\mathbf{x}) \sim \sum_{k=1}^{N(\epsilon)} a \sigma(\mathbf{w} \cdot \mathbf{x} + \mathbf{b})$	$f(\mathbf{x}) = \sum_{n=1}^{2n} \Phi_n \left(\sum_{n=1}^{n} \phi_{n-1}(x_n) \right)$	

Fitting Special Functions

We compare KANs and MLPs on four toy example, among which are exponential and Bessel functions.

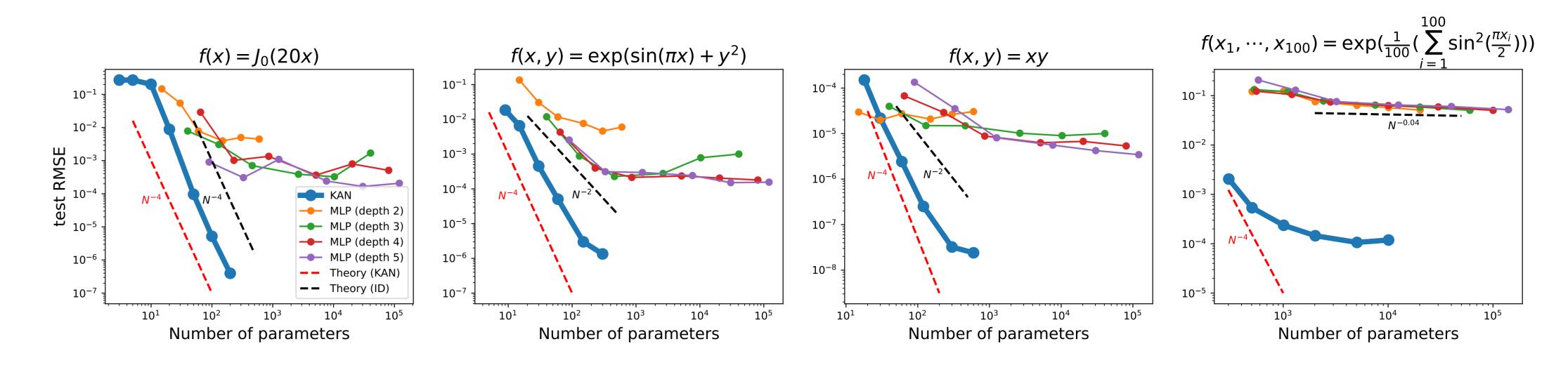
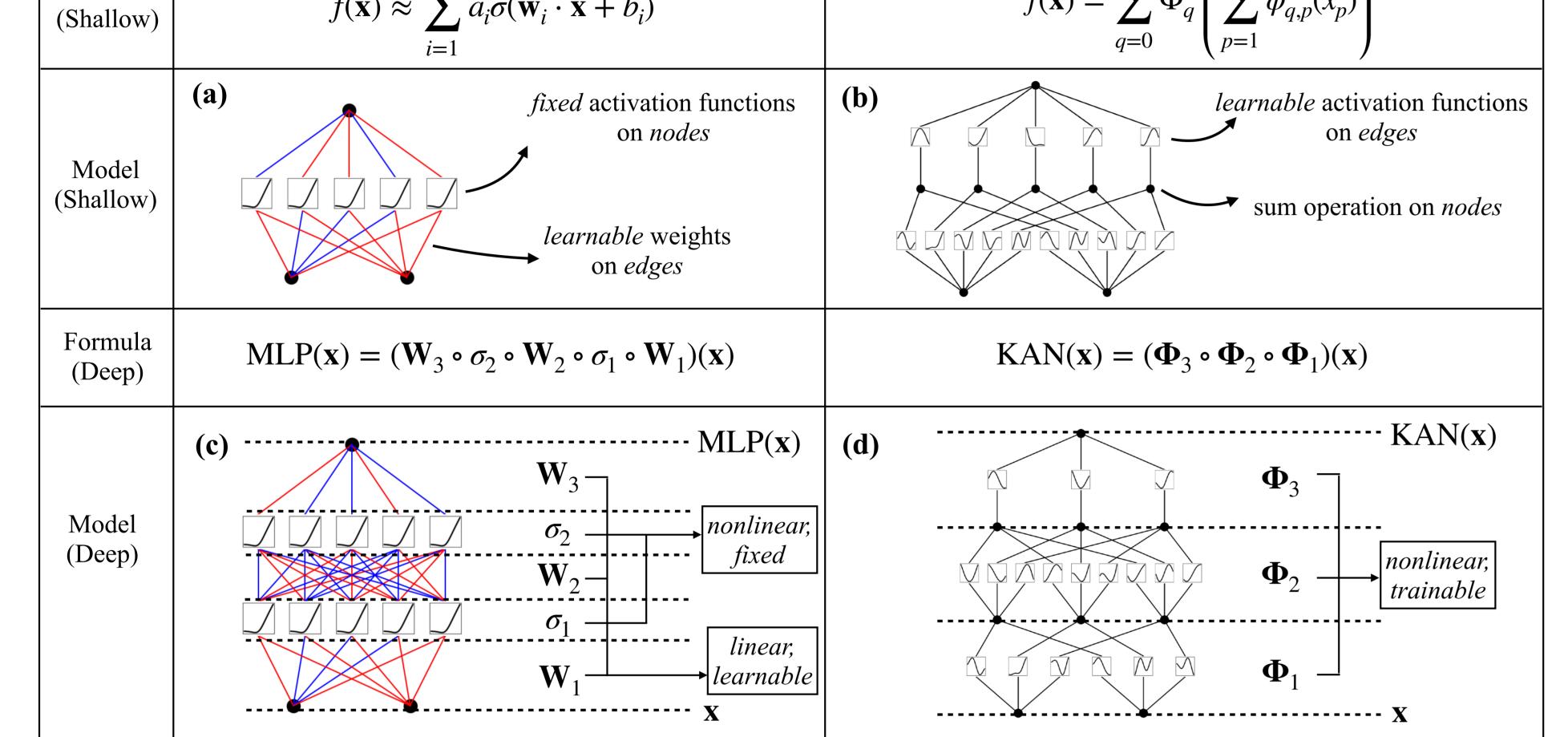


Figure 2. KANs can almost saturate the fastest scaling law predicted by our theory ($\alpha = 4$), while MLPs scales slowly and plateau quickly.

Solving Partial Differential Equations (PINNs)

We consider a Poisson equation with zero Dirichlet boundary data. For $\Omega = [-1, 1]^2$, consider the PDE



We parametrize the learnable activation functions by B-splines.

Approximation Theory

Suppose that a function $f(\mathbf{x})$ admits a smooth representation

$$f = (\mathbf{\Phi}_{L-1} \circ \mathbf{\Phi}_{L-2} \circ \cdots \circ \mathbf{\Phi}_1 \circ \mathbf{\Phi}_0)\mathbf{x}$$

 $u_{xx} + u_{yy} = f$ in Ω , u=0 on $\partial\Omega$.

 $f = -\pi^2(1+4y^2)\sin(\pi x)\sin(\pi y^2) + 2\pi\sin(\pi x)\cos(\pi y^2)$ for which $u = \sin(\pi x)\sin(\pi y^2)$ is the true solution.

We use the framework of physics-informed neural networks (PINNs) [4] with loss prescribed by

$$|\text{oss}_{\text{pde}} = \alpha |\text{oss}_i + |\text{oss}_b \coloneqq \frac{0.01}{n_i} \sum_{i=1}^{n_i} |u_{xx}(z_i) + u_{yy}(z_i) - f(z_i)|^2 + \frac{1}{n_b} \sum_{i=1}^{n_b} u^2,$$

where we use loss_i to denote the interior loss, discretized and evaluated by a uniform sampling of n_i points $z_i = (x_i, y_i)$ inside the domain, and similarly we use loss_b to denote the boundary loss, discretized and evaluated by a uniform sampling of n_b points on the boundary.

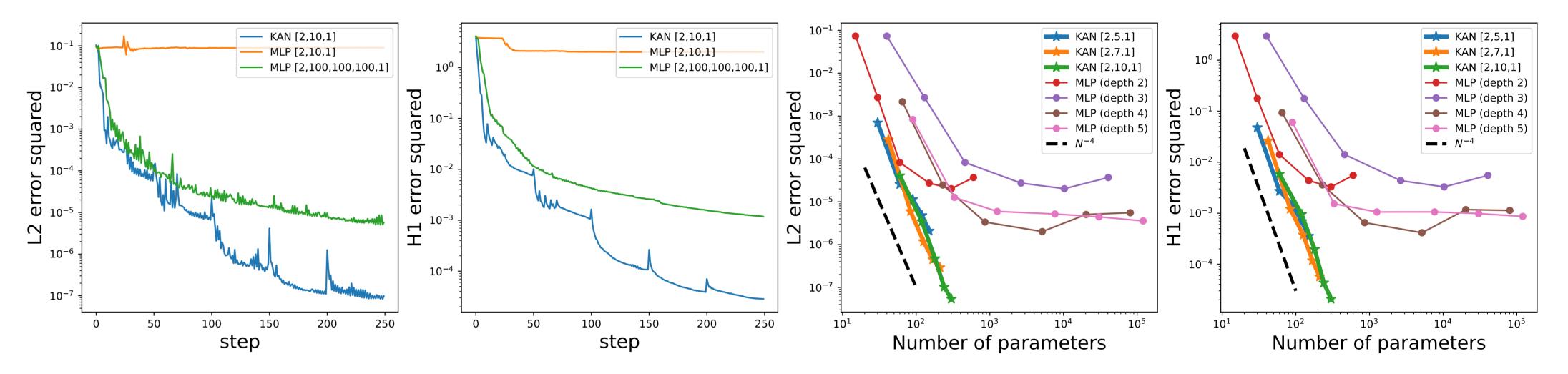


Figure 3. The PDE example. We plot L2 squared and H1 squared losses between the predicted solution and ground truth solution. First and second: training dynamics of losses. Third and fourth: scaling laws of losses against the number of parameters. KANs converge faster, achieve lower losses, and have steeper scaling laws than MLPs.



where $\Phi_{l,i,j}$ are smooth with derivatives uniformly bounded up to k + 1-th order. Then using k-th order B-splines with G + 1 grid points as activation functions, there exist $\Phi_{l,i,j}^G$ such that for any $0 \le m \le k$, we have the bound

 $\|f - (\mathbf{\Phi}_{L-1}^G \circ \mathbf{\Phi}_{L-2}^G \circ \cdots \circ \mathbf{\Phi}_1^G \circ \mathbf{\Phi}_0^G) \mathbf{x}\|_{C^m} \leq C G^{-k-1+m}.$

In particular for L^2 or RMSE, we have the scaling table

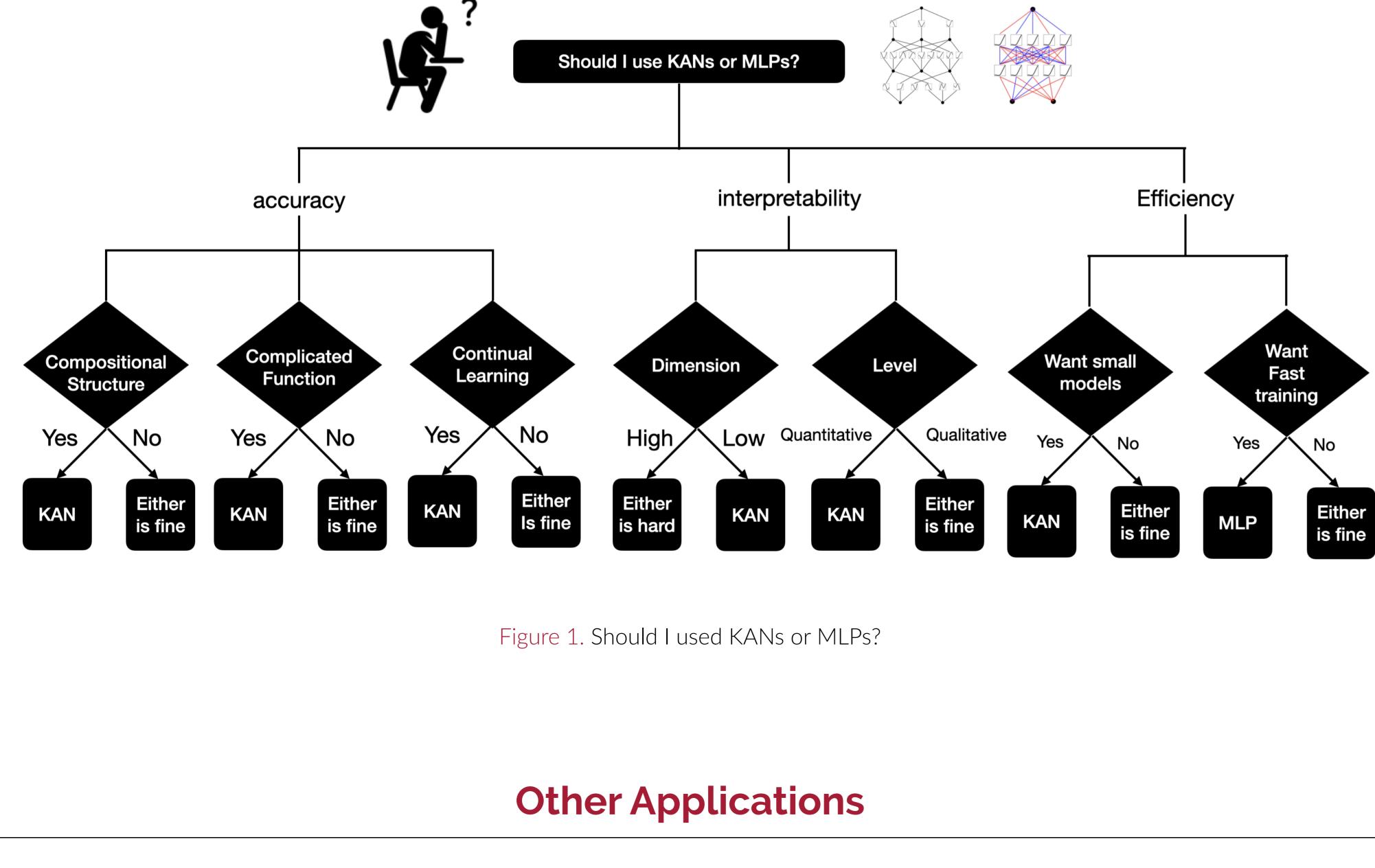
Paper	Idea	Scaling exponent α	
Sharma & Kaplan [5]	Intrinsic dimensionality	(k+1)/d	
Michaud et al. [2]	maximum arity	1	
Poggio et al. [3]	compositional sparsity	m/2	
Ours	K-A representation	k+1	

Table 1. Scaling exponents from different theories $\ell \propto N^{-\alpha}$. ℓ : test RMSE loss, N: number of model parameters, d: input intrinsic dimension, k: order of piecewise polynomial, m: derivative order as in function class W_m .

Leveraging the 1D structure to get better scaling laws

Advantages of KAN Architecture

. Interpretability: KANs with much smaller network size and fewer trainable parameters is normally comparable in performance to MLPs. This makes them ideal for model reduction or symbolic regression. 2. Accuracy: KANs can achieve much smaller error due to mesh refinement of splines, with better scaling laws.



Al for Math: Knot Theory

Method	Architecture	Parameter Count	Accuracy
Deepmind's MLP	4 layer, width-300	$\sim 3 \times 10^5$	78%
KANs	2 layer, $[17, 1, 14]$ ($G = 3, k = 3$)	~ 200	81.6%

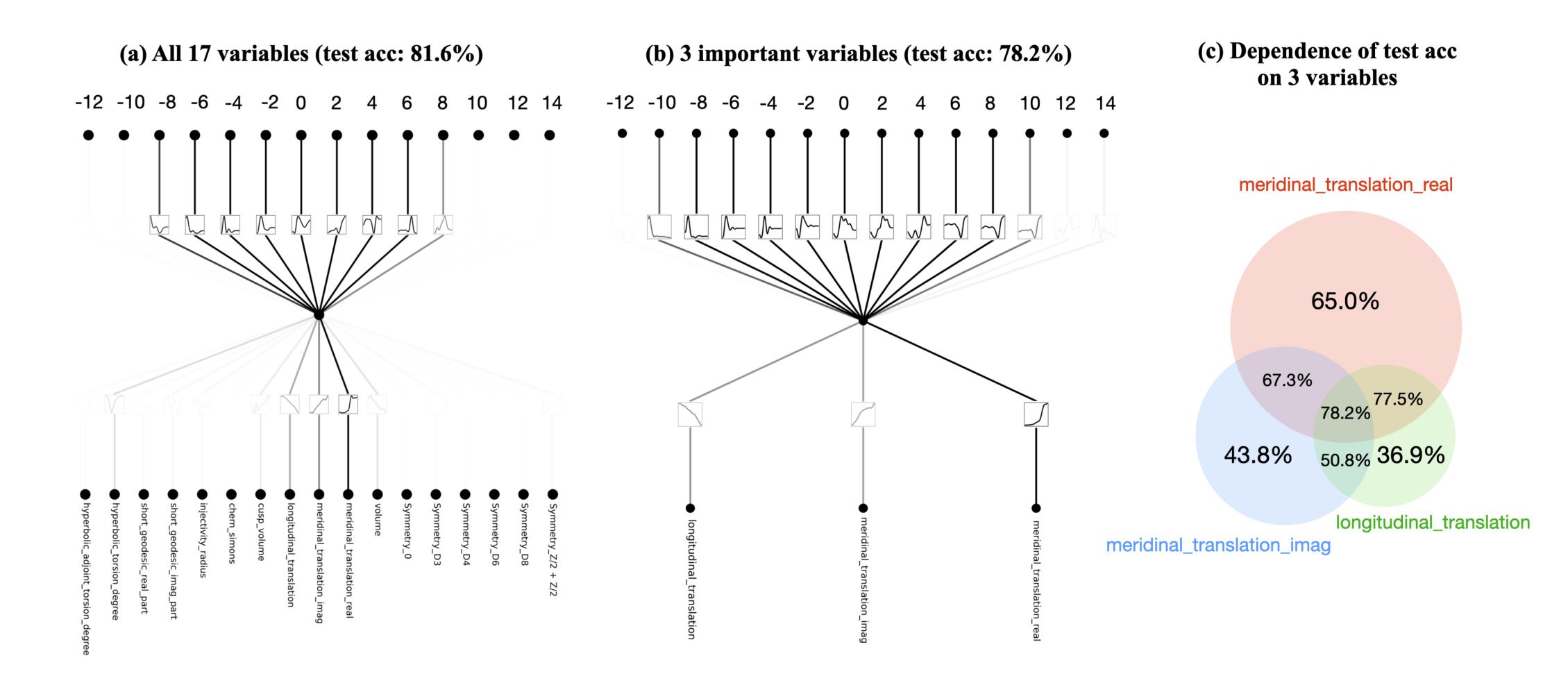


Figure 4. Knot dataset, supervised mode. With KANs, we rediscover Deepmind's results that signature is mainly dependent on meridinal translation.

In [1], supervised learning and human domain experts were combined to arrive at a new theorem relating algebraic and geometric topological invariants. Deepmind's main results for the knot theory dataset are: (1) They use network attribution methods to find the signature σ is mostly dependent on meridinal distance μ (real μ_r , imag μ_i) and longitudinal distance λ . (2) Human scientists identified that σ has high correlation with the slope $\equiv \operatorname{Re}(\frac{\lambda}{\mu}) = \frac{\lambda \mu_r}{\mu^2 + \mu^2}$ and derived a bound for $|2\sigma - \operatorname{slope}|$. KANs not only rediscover these results with much smaller networks and much more automation, but also present new results and insights.

• (What we have done:) Data regression; Anderson localization; Imaging. • (Future works:) Large Language Models.

References

- [1] Alex Davies, Petar Veličković, Lars Buesing, Sam Blackwell, Daniel Zheng, Nenad Tomašev, Richard Tanburn, Peter Battaglia, Charles Blundell, András Juhász, et al.
- Advancing mathematics by guiding human intuition with ai. Nature, 600(7887):70–74, 2021.
- [2] Eric J Michaud, Ziming Liu, and Max Tegmark. Precision machine learning. Entropy, 25(1):175, 2023.
- [3] Tomaso Poggio, Andrzej Banburski, and Qianli Liao. Theoretical issues in deep networks. Proceedings of the National Academy of Sciences, 117(48):30039–30045, 2020.
- [4] Maziar Raissi, Paris Perdikaris, and George E Karniadakis. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. Journal of Computational physics, 378:686–707, 2019.
- ^[5] Utkarsh Sharma and Jared Kaplan. A neural scaling law from the dimension of the data manifold. *arXiv preprint arXiv:2004.10802, 2020.*

https://roywangyx.github.io/

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