KAN: Kolmogorov–Arnold Networks

Liu, Ziming, et al. "Kan: Kolmogorov-arnold networks." arXiv preprint arXiv:2404.19756 (2024).

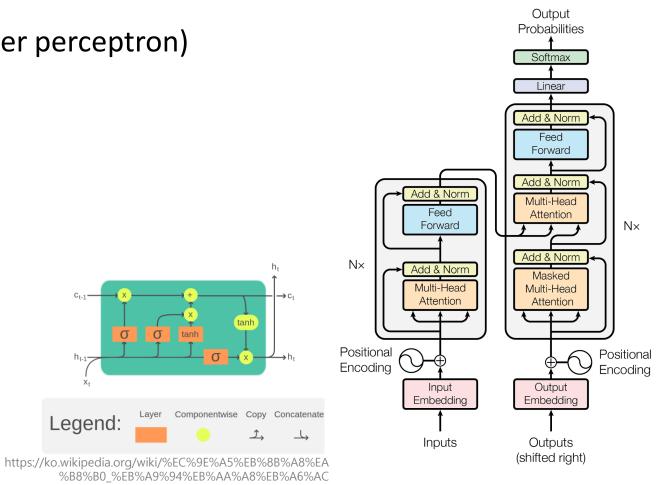
> Presenter: PhD Student @ CSE, Yonsei Univ. Jin-Duk Park

Reading Group Material 2024.05.29

Introduction

What Current AI Heavily Relies On

- Modern AI relies on MLP (multi-layer perceptron) architecture
- Transformer, RNN, LSTM, CNN...: based on MLP
- However, are MLPs the best nonlinear regressors we can build?
 - less efficient
 - less interpretable



LSTM

Transformer

Introduction

KAN: Alternatives to MLPs?

- KAN is proposed as alternatives to MLPs!
- Kolmogorov–Arnold Networks (KAN) is getting lots of attention nowadays!: LinkedIn, X (Twitter), Reddit...



Backgrounds <u>Universal Approximation Theorem (UAT)</u>

- UAT is a theoretical background of modern deep learning
- UAT says that a single MLP layer can approximate any continuous functions

Universal approximation theorem — Let $C(X, \mathbb{R}^m)$ denote the set of continuous functions from a subset X of a Euclidean \mathbb{R}^n space to a Euclidean space \mathbb{R}^m . Let $\sigma \in C(\mathbb{R}, \mathbb{R})$. Note that $(\sigma \circ x)_i = \sigma(x_i)$, so $\sigma \circ x$ denotes σ applied to each component of x.

Then σ is not polynomial if and only if for every $n \in \mathbb{N}$, $m \in \mathbb{N}$, compact $K \subseteq \mathbb{R}^n$, $f \in C(K, \mathbb{R}^m)$, $\varepsilon > 0$ there exist $k \in \mathbb{N}$, $A \in \mathbb{R}^{k \times n}$, $b \in \mathbb{R}^k$, $C \in \mathbb{R}^{m \times k}$ such that

$$\sup_{x\in K} \|f(x)-g(x)\| where $g(x)=C\cdot igl(\sigma\circ (A\cdot x+b)igr)$$$

https://en.wikipedia.org/wiki/Universal_approximation_theorem

Kolmogorov-Arnold Representation Theorem (KAT)

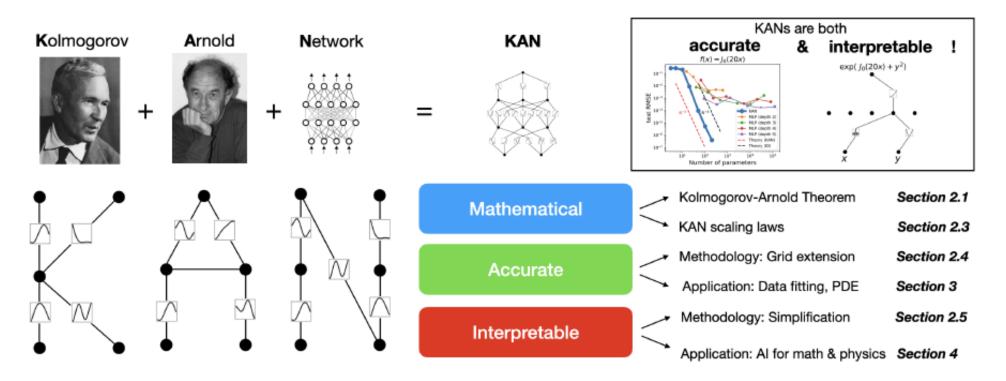
- KAT is a representation theroem
- It says that any continous f can be represented as a finite "composition" of continous functions of a single variable and addition

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

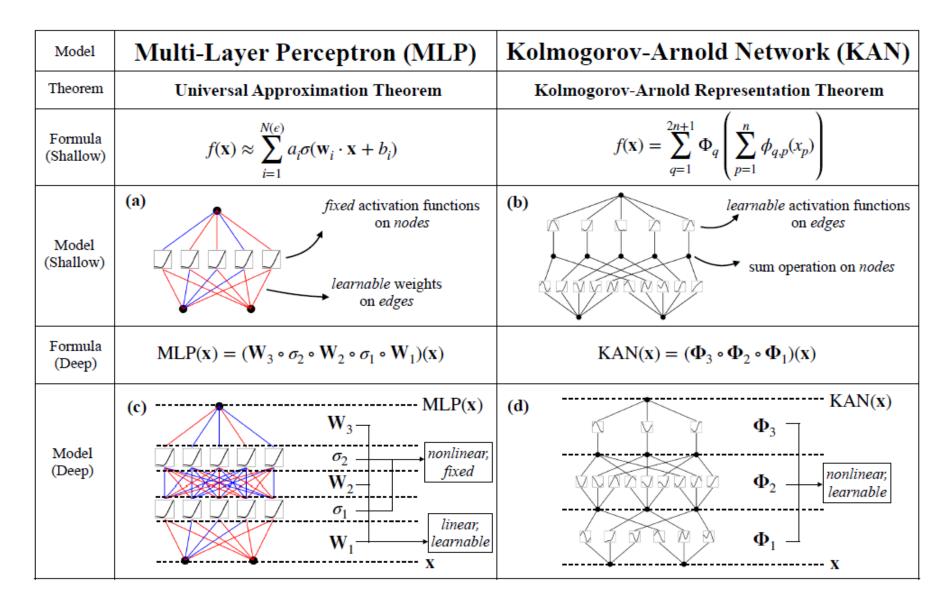
where $\phi_{q,p}\colon [0,1] o \mathbb{R}$ and $\Phi_q\colon \mathbb{R} o \mathbb{R}$.

KAN KAN: Overview

- Built upon KAT, KAN is..
 - Mathematical
 - Accurate
 - Interpretable !



KAN KAN: Overview



KAN KAN Architecture

- Revisit KAT
- Generalize KAT
 -> KAN layer

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

- 1. 2n+1 width
- 2. Only two-layer non-linearities

generalize

Arbitrary widths and depths -> KAN

$$f(\mathbf{x}) = \sum_{i_{L-1}=1}^{n_{L-1}} \phi_{L-1,i_L,i_{L-1}} \left(\sum_{i_{L-2}=1}^{n_{L-2}} \cdots \left(\sum_{i_2=1}^{n_2} \phi_{2,i_3,i_2} \left(\sum_{i_1=1}^{n_1} \phi_{1,i_2,i_1} \left(\sum_{i_0=1}^{n_0} \phi_{0,i_1,i_0}(x_{i_0}) \right) \right) \right) \right) \cdots \right)$$

KAN KAN Architecture

• KAN layer

$$\mathbf{x}_{l+1} = \underbrace{\begin{pmatrix} \phi_{l,1,1}(\cdot) & \phi_{l,1,2}(\cdot) & \cdots & \phi_{l,1,n_{l}}(\cdot) \\ \phi_{l,2,1}(\cdot) & \phi_{l,2,2}(\cdot) & \cdots & \phi_{l,2,n_{l}}(\cdot) \\ \vdots & \vdots & & \vdots \\ \phi_{l,n_{l+1},1}(\cdot) & \phi_{l,n_{l+1},2}(\cdot) & \cdots & \phi_{l,n_{l+1},n_{l}}(\cdot) \end{pmatrix}}_{\mathbf{\Phi}_{l}} \mathbf{x}_{l},$$

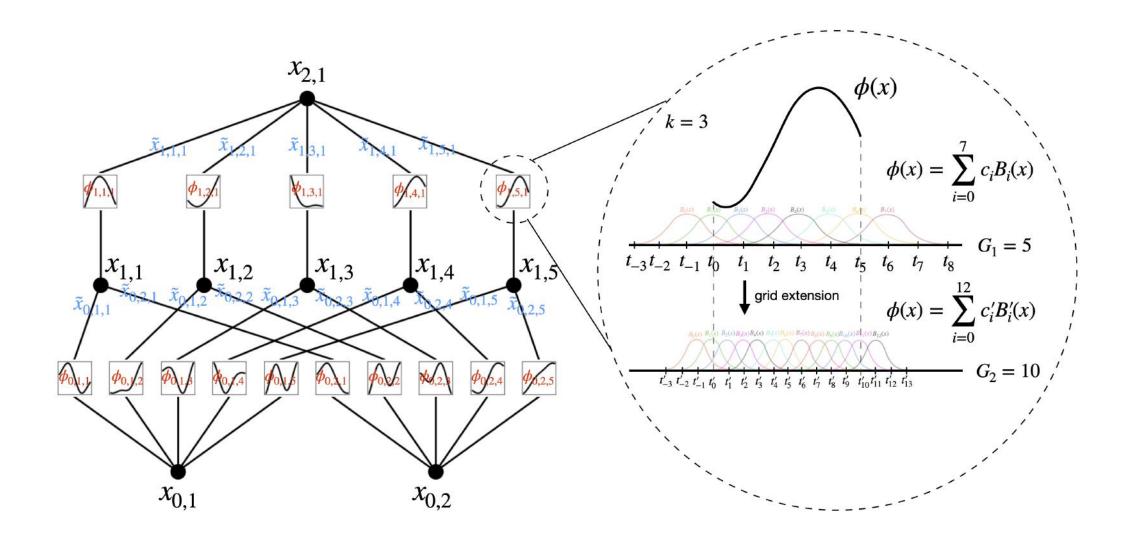
• Deep KAN

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

$$\mathbf{\mathbf{x}}$$

$$\mathbf{MLP}(\mathbf{x}) = (\mathbf{W}_{L-1} \circ \sigma \circ \mathbf{W}_{L-2} \circ \sigma \circ \cdots \circ \mathbf{W}_1 \circ \sigma \circ \mathbf{W}_0) \mathbf{x}.$$

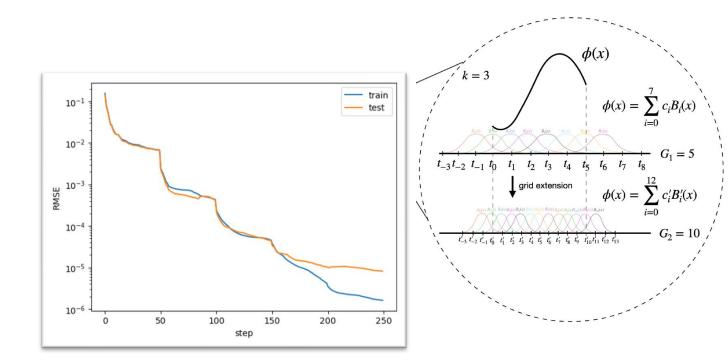
KAN KAN Architecture



KAN Grid Extention

- Neural scaling law: for improving accuracy
- Contrast to MLP, KAN: easy to fine-graining (w/o retraining larger model)
- Coarse grid to fine grid while training

$$\{c'_j\} = \underset{\{c'_j\}}{\operatorname{argmin}} \mathbb{E}_{x \sim p(x)} \left(\sum_{j=0}^{G_2+k-1} c'_j B'_j(x) - \sum_{i=0}^{G_1+k-1} c_i B_i(x) \right)^2,$$



KAN <u>Comparison: KAN(KAT) vs MLP(UAT)</u>

Model	Multi-Layer Perceptron (MLP)	Kolmogorov-Arnold Network (KAN)				
Theorem	Universal Approximation Theorem	Kolmogorov-Arnold Representation Theorem				
Formula (Shallow)	$f(\mathbf{x}) \approx \sum_{i=1}^{N(e)} a_i \sigma(\mathbf{w}_i \cdot \mathbf{x} + b_i)$	$f(\mathbf{x}) = \sum_{q=1}^{2n+1} \Phi_q \left(\sum_{p=1}^n \phi_{q,p}(x_p) \right)$				
Model (Shallow)	(a) fixed activation functions on nodes learnable weights on edges	(b) <i>learnable</i> activation functions on <i>edges</i> sum operation on <i>nodes</i>				
Formula (Deep)	$MLP(\mathbf{x}) = (\mathbf{W}_3 \circ \sigma_2 \circ \mathbf{W}_2 \circ \sigma_1 \circ \mathbf{W}_1)(\mathbf{x})$	$KAN(\mathbf{x}) = (\mathbf{\Phi}_3 \circ \mathbf{\Phi}_2 \circ \mathbf{\Phi}_1)(\mathbf{x})$				
Model (Deep)	(c) W_3 $MLP(x)$ W_3 σ_2 $nonlinear; fixed$ W_2 σ_1 $linear; learnable$ W_1 X	(d) Φ_3 KAN(x) Φ_2 <i>nonlinear;</i> <i>learnable</i> <i>k</i>				

KAN Implementation Details

• Residual activation functions Scaling factor, trainable $\phi(x) = w (b(x) + \text{spline}(x)).$

$$b(x) = silu(x) = x/(1 + e^{-x})$$

spline(x) =
$$\sum_{i} c_i B_i(x)$$

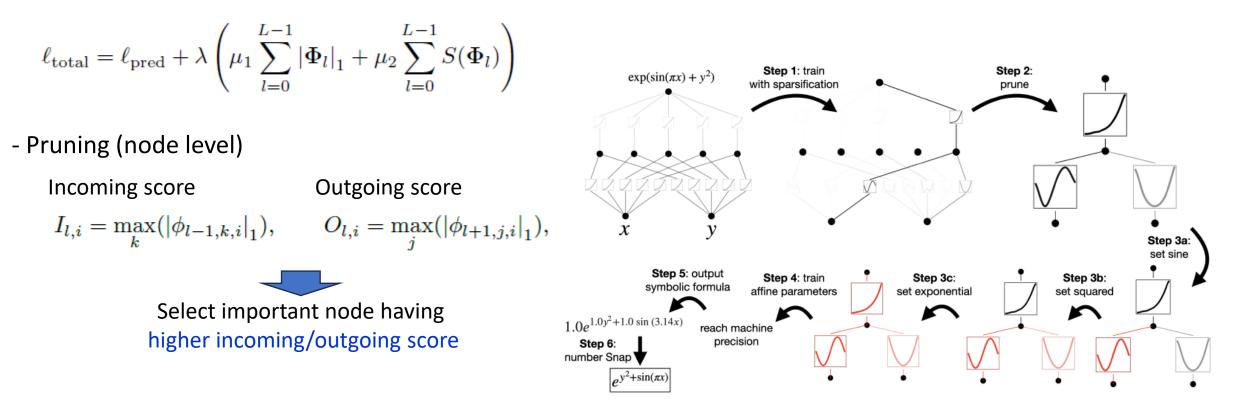
Trainable B-splines (basis)

• Initialization

-
$$c_i \sim N(0, \sigma^2)$$
 with small σ (~zero init)
- $w \sim Xavier$ [1]

Interpretability of KAN <u>Sparsification</u>

- Sparse regularization + pruning -> interpretable KAN
 - Sparse regularization

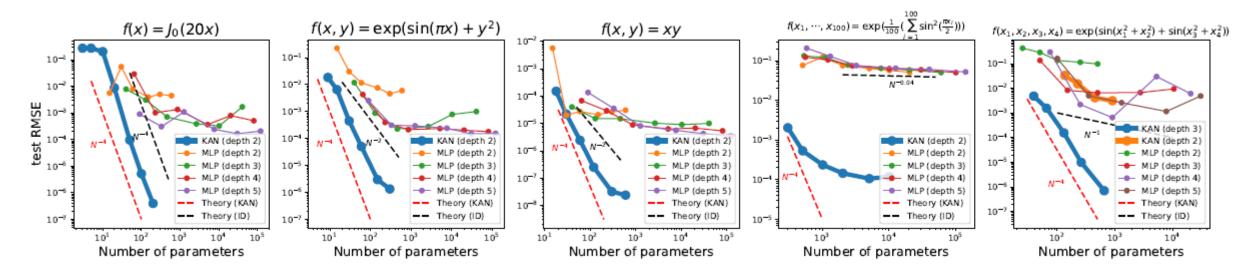


- Symbolification

Sympy to compute symbolic formula of the output node

Accuracy Test

Toy Example & Special Functions

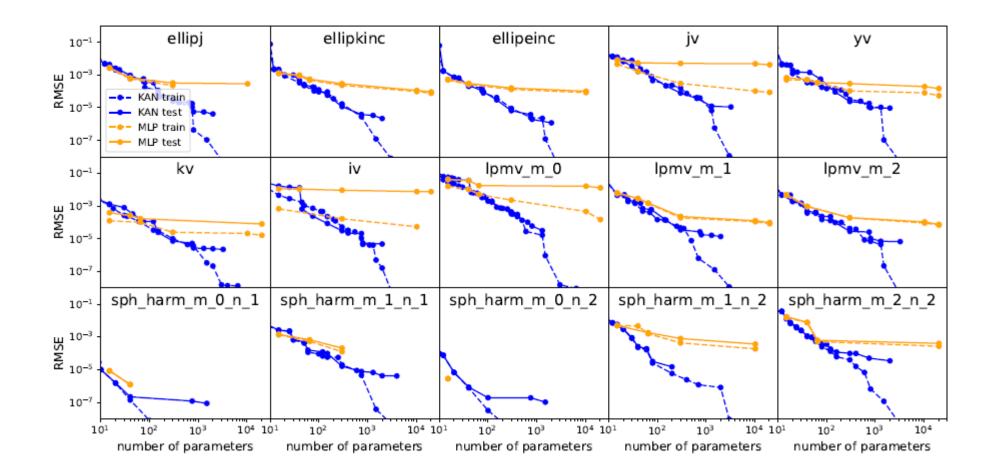


- Toy example
- KANs can almost saturate the steeper red lines
- While MLPs are not

- 1) $f(x) = J_0(20x)$, which is the Bessel function. Since it is a univariate function, it can be represented by a spline, which is a [1, 1] KAN.
- (2) $f(x,y) = \exp(\sin(\pi x) + y^2)$. We know that it can be exactly represented by a [2, 1, 1] KAN.
- (3) f(x, y) = xy. We know from Figure 4.1 that it can be exactly represented by a [2, 2, 1] KAN.
- (4) A high-dimensional example $f(x_1, \dots, x_{100}) = \exp(\frac{1}{100} \sum_{i=1}^{100} \sin^2(\frac{\pi x_i}{2}))$ which can be represented by a [100, 1, 1] KAN.
- (5) A four-dimensional example $f(x_1, x_2, x_3, x_4) = \exp(\frac{1}{2}(\sin(\pi(x_1^2 + x_2^2)) + \sin(\pi(x_3^2 + x_4^2)))))$ which can be represented by a [4, 4, 2, 1] KAN.

Accuracy Test

Toy Example & Special Functions (Cont'd)



• Performs well than MLPs, on special functions

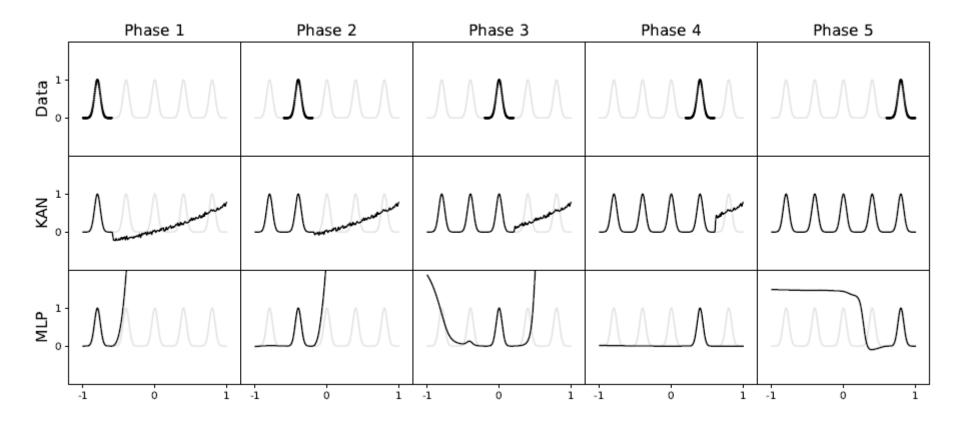
Accuracy Test

Feynman Datasets

• Many physics equations collected by Feynman

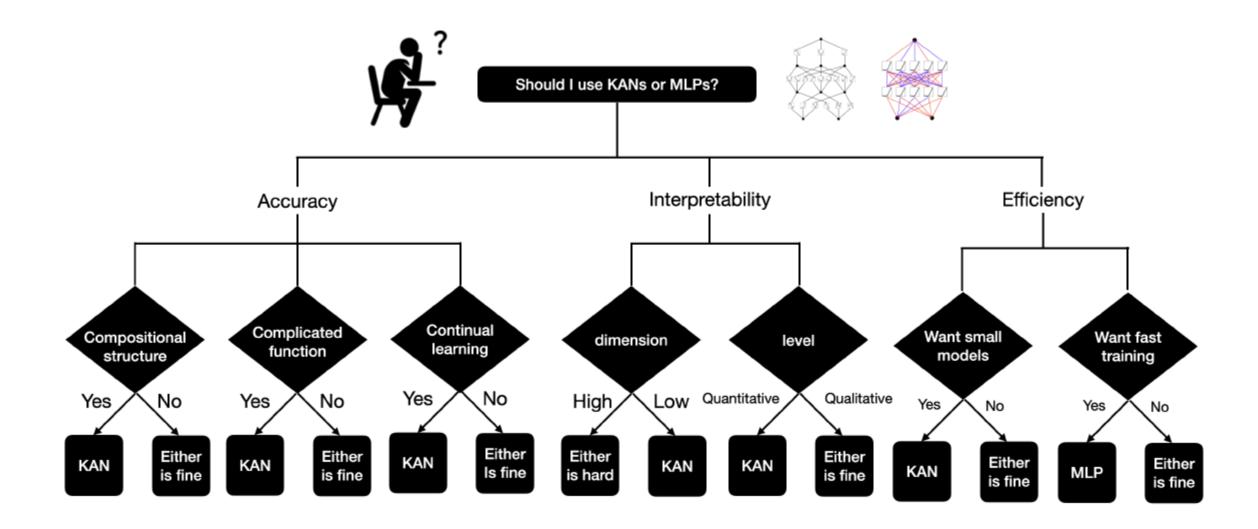
			Descent							
Feynman Eq.	Original Formula	Dimensionless formula	Variables	Human-constructed KAN shape	Pruned KAN shape (smallest shape that achieves RMSE < 10 ⁻²)	Pruned KAN shape (lowest loss)	Human-constructed KAN loss (lowest test RMSE)	Pruned KAN loss (lowest test RMSE)	Unpruned KAN loss (lowest test RMSE)	MLP Ioss (Iowest test RMSE)
I.6.2	$\exp(-\frac{\theta^2}{2\sigma^2})/\sqrt{2\pi\sigma^2}$	$\exp(-\frac{\theta^2}{2\sigma^2})/\sqrt{2\pi\sigma^2}$	θ, σ	[2,2,1,1]	[2,2,1]	[2,2,1,1]	$7.66 imes 10^{-8}$	$2.86\times\mathbf{10^{-6}}$	4.60×10^{-8}	1.45×10^{-4}
I.6.2b	$\exp\left(-\frac{(\theta-\theta_1)^2}{2\sigma^2}\right)/\sqrt{2\pi\sigma^2}$	$\exp\left(-\frac{(\theta-\theta_1)^2}{2\sigma^2}\right)/\sqrt{2\pi\sigma^2}$	θ, θ_1, σ	[3,2,2,1,1]	[3,4,1]	[3,2,2,1,1]	1.22×10^{-3}	$4.45 imes 10^{-4}$	1.25×10^{-3}	7.40×10^{-4}
L9.18	$\frac{Gm_1m_2}{(x_2-x_1)^2+(y_2-y_1)^2+(z_2-z_1)^2}$	$\frac{a}{(b-1)^2+(c-d)^2+(c-f)^2}$	a,b,c,d,e,f	[6,4,2,1,1]	[6,4,1,1]	[6,4,1,1]	1.48×10^{-3}	$8.62 imes 10^{-3}$	$6.56 imes 10^{-3}$	1.59×10^{-3}
L12.11	$q(E_f + Bv\sin\theta)$	$1 + a \sin \theta$	a, θ	[2,2,2,1]	[2,2,1]	[2,2,1]	2.07×10^{-3}	1.39×10^{-3}	$9.13 imes 10^{-4}$	$6.71 imes 10^{-4}$
L13.12	$Gm_1m_2(\frac{1}{r_2}-\frac{1}{r_1})$	$a(\frac{1}{b}-1)$	a, b	[2,2,1]	[2,2,1]	[2,2,1]	7.22×10^{-3}	4.81×10^{-3}	$2.72 imes 10^{-3}$	1.42×10^{-3}
L15.3x	$\frac{x-ut}{\sqrt{1-(\frac{u}{a})^2}}$	$\frac{1-a}{\sqrt{1-b^2}}$	a, b	[2,2,1,1]	[2,1,1]	[2,2,1,1,1]	$7.35 imes10^{-3}$	$1.58 imes 10^{-3}$	1.14×10^{-3}	$8.54\times\mathbf{10^{-4}}$
L16.6	$\frac{u+v}{1+\frac{u+v}{n^2}}$	<u>a+b</u> 1+ab	a, b	[2,2,2,2,2,1]	[2,2,1]	[2,2,1]	1.06×10^{-3}	1.19×10^{-3}	1.53×10^{-3}	$6.20\times \mathbf{10^{-4}}$
L18.4	$\frac{m_1r_1+m_2r_2}{m_1+m_2}$	$\frac{1+ab}{1+a}$	a, b	[2,2,2,1,1]	[2,2,1]	[2,2,1]	$3.92 imes 10^{-4}$	$1.50 imes 10^{-4}$	1.32×10^{-3}	$3.68 imes 10^{-4}$
1.26.2	$\arcsin(n\sin\theta_2)$	$\arcsin(n\sin\theta_2)$	n, θ_2	[2,2,2,1,1]	[2,2,1]	[2,2,2,1,1]	1.22×10^{-1}	7.90×10^{-4}	$8.63 imes 10^{-4}$	$1.24 imes 10^{-3}$
1.27.6	$\frac{1}{\frac{1}{d_1} + \frac{1}{d_2}}$	1 1+ab	a, b	[2,2,1,1]	[2,1,1]	[2,1,1]	2.22×10^{-4}	$1.94\times\mathbf{10^{-4}}$	2.14×10^{-4}	2.46×10^{-4}
L29.16	$\sqrt{x_1^2+x_2^2-2x_1x_2\mathrm{cos}(\theta_1-\theta_2)}$	$\sqrt{1+a^2-2a\mathrm{cos}(\theta_1-\theta_2)}$	a, θ_1, θ_2	[3,2,2,3,2,1,1]	[3,2,2,1]	[3,2,3,1]	$2.36 imes10^{-1}$	$3.99 imes 10^{-3}$	$3.20 imes 10^{-3}$	$4.64 imes 10^{-3}$
L30.3	$I_{*,0} \frac{\sin^2(\frac{n\theta}{2})}{\sin^2(\frac{\theta}{2})}$	$\frac{\sin^2\left(\frac{n\theta}{2}\right)}{\sin^2\left(\frac{\theta}{2}\right)}$	n, θ	[2,3,2,2,1,1]	[2,4,3,1]	[2,3,2,3,1,1]	$3.85 imes 10^{-1}$	$1.03 imes 10^{-3}$	$1.11 imes 10^{-2}$	$1.50 imes 10^{-2}$
1.30.5	$\arcsin(\frac{\lambda}{nd})$	$\arcsin(\frac{a}{n})$	a, n	[2,1,1]	[2,1,1]	[2,1,1,1,1,1]	2.23×10^{-4}	3.49×10^{-6}	6.92×10^{-5}	$9.45 imes 10^{-8}$
1.37.4	$I_{\star}=I_1+I_2+2\sqrt{I_1I_2}{\rm cos}\delta$	$1 + a + 2\sqrt{a}\cos\delta$	a, δ	[2,3,2,1]	[2,2,1]	[2,2,1]	7.57×10^{-5}	4.91×10^{-6}	$3.41 imes 10^{-4}$	$5.67 imes 10^{-4}$
L40.1	$n_0 \exp(-\frac{m_{gx}}{k_b T})$	$n_0 e^{-a}$	n_0, a	[2,1,1]	[2,2,1]	[2,2,1,1,1,2,1]	$3.45 imes 10^{-3}$	$5.01 imes 10^{-4}$	$3.12 imes 10^{-4}$	3.99×10^{-4}
L44.4	$nk_bT\ln(\frac{V_2}{V_1})$	nlna	n, a	[2,2,1]	[2,2,1]	[2,2,1]	2.30×10^{-8}	$2.43 imes 10^{-5}$	$1.10 imes 10^{-4}$	3.99×10^{-4}
1.50.26	$x_1(\cos(\omega t) + \alpha \cos^2(wt))$	$\cos a + \alpha \cos^2 a$	a, α	[2,2,3,1]	[2,3,1]	[2,3,2,1]	1.52×10^{-4}	5.82×10^{-4}	4.90×10^{-4}	1.53×10^{-3}
IL2.42	$\frac{k(T_2-T_1)A}{d}$	(a-1)b	a, b	[2,2,1]	[2,2,1]	[2,2,2,1]	8.54×10^{-4}	7.22×10^{-4}	1.22×10^{-3}	1.81×10^{-4}
IL6.15a	$\frac{3}{4\pi\epsilon} \frac{p_{dz}}{r^5} \sqrt{x^2 + y^2}$	$\frac{1}{4\pi}c\sqrt{a^2+b^2}$	a, b, c	[3,2,2,2,1]	[3,2,1,1]	[3,2,1,1]	2.61×10^{-3}	$3.28 imes 10^{-3}$	1.35×10^{-3}	$5.92 imes 10^{-4}$
IL11.7	$n_0(1 + \frac{p_d E_f \cos \theta}{k_k T})$	$n_0(1 + a\cos\theta)$	n_0, a, θ	[3,3,3,2,2,1]	[3,3,1,1]	[3,3,1,1]	$7.10 imes 10^{-3}$	8.52×10^{-3}	$5.03 imes 10^{-3}$	$5.92 imes 10^{-4}$
IL11.27	$\frac{n\alpha}{1-\frac{n\alpha}{2}}eE_f$	$\frac{n\alpha}{1-\frac{n\alpha}{2}}$	n, α	[2,2,1,2,1]	[2,1,1]	[2,2,1]	2.67×10^{-8}	4.40×10^{-8}	1.43×10^{-8}	7.18×10^{-8}
II.35.18	$\frac{no}{\exp(\frac{n-H}{k_{L}T})+\exp(-\frac{n-H}{k_{L}T})}$	$\frac{no}{exp(a)+exp(-a)}$	n_0, a	[2,1,1]	[2,1,1]	[2,1,1,1]	4.13×10^{-4}	1.58×10^{-4}	$7.71 imes 10^{-6}$	7.92×10^{-5}
IL36.38	$\frac{\mu_m B}{k_b T} + \frac{\mu_m \alpha M}{ec^2 k_b T}$	$a + \alpha b$	a, α, b	[3,3,1]	[3,2,1]	[3,2,1]	2.85×10^{-3}	1.15×10^{-3}	$3.03 imes 10^{-3}$	2.15×10^{-3}
IL38.3	$\frac{YAx}{d}$	4 6	a, b	[2,1,1]	[2,1,1]	[2,2,1,1,1]	1.47×10^{-4}	$8.78\times\mathbf{10^{-6}}$	$6.43 imes 10^{-4}$	5.26×10^{-4}
III.9.52	$\frac{p_4 E_f}{h} \frac{\sin^2((\omega - \omega_0)t/2)}{((\omega - \omega_0)t/2)^2}$	$a \frac{\sin^2(\frac{b-a}{2})}{(\frac{b-a}{2})^2}$	a, b, c	[3,2,3,1,1]	[3,3,2,1]	[3,3,2,1,1,1]	$4.43 imes 10^{-2}$	$3.90 imes 10^{-3}$	2.11×10^{-2}	$9.07 imes 10^{-4}$
III.10.19	$\mu_m \sqrt{B_x^2 + B_y^2 + B_z^2}$	$\sqrt{1 + a^2 + b^2}$	a, b	[2,1,1]	[2,1,1]	[2,1,2,1]	2.54×10^{-3}	1.18×10^{-3}	$8.16 imes 10^{-4}$	$1.67\times\mathbf{10^{-4}}$
III.17.37	$\beta(1 + \alpha \cos\theta)$	$\beta(1 + \alpha \cos\theta)$	α, β, θ	[3,3,3,2,2,1]	[3,3,1]	[3,3,1]	1.10×10^{-3}	$5.03 imes 10^{-4}$	$4.12 imes 10^{-4}$	$6.80 imes 10^{-4}$

Accuracy Test <u>Continual Learning</u>



- Toy example dataset
- KAN is more immune to catastropic forgetting
- Structure re-organization only occurs locally on KAN, while MLP is not

Summary Should I use KANs or MLPs?



Takeaway Messages

- KAN can be a potential alternatives to MLP
- However, KAN is only applied to limited dataset & settings

- Still, a lot of research projects are now going on though... (refer to: https://github.com/mintisan/awesome-kan)

Library

- pykan : Offical implementation for Kolmogorov Arnold Networks | O Stars 12k
- efficient-kan : An efficient pure-PyTorch implementation of Kolmogorov-Arnold Network (KAN).
- FastKAN : Very Fast Calculation of Kolmogorov-Arnold Networks (KAN) | Stars 194
- FasterKAN : FasterKAN = FastKAN + RSWAF bases functions and benchmarking with other KANs. Fastest KAN variation as of 5/13/2024, 2 times slower than MLP in backward speed.
- <u>TorchKAN</u>: Simplified KAN Model Using Legendre approximations and Monomial basis functions for Image Classification for MNIST. Achieves 99.5% on MNIST using Conv+LegendreKAN.
- FourierKAN: Pytorch Layer for FourierKAN. It is a layer intended to be a substitution for Linear + non-linear activation | O Stars 659
- ChebyKAN : Kolmogorov-Arnold Networks (KAN) using Chebyshev polynomials instead of B-splines.
- GraphKAN : Implementation of Graph Neural Network version of Kolmogorov Arnold Networks (GraphKAN)
- <u>FCN-KAN</u> : Kolmogorov–Arnold Networks with modified activation (using fully connected network to represent the activation) | Ostars 84
- <u>X-KANeRF</u>: KAN based NeRF with various basis functions like B-Splines, Fourier, Radial Basis Functions, Polynomials, etc | O Stars 84
- Large Kolmogorov-Arnold Networks : Variations of Kolmogorov-Arnold Networks (including CUDA-supported KAN convolutions) | O Stars 96
- FastKAN : Very Fast Calculation of Kolmogorov-Arnold Networks (KAN) | O Stars 194
- <u>xKAN</u> : Kolmogorov-Arnold Networks with various basis functions like B-Splines, Fourier, Chebyshev, Wavelets etc

Project

- <u>KAN-GPT</u> : The PyTorch implementation of Generative Pre-trained Transformers (GPTs) using Kolmogorov-Arnold Networks (KANs) for language modeling
- KAN-GPT-2: Training small GPT-2 style models using Kolmogorov-Arnold networks.(despite the KAN model having 25% fewer parameters!).
- KANeRF : Kolmogorov-Arnold Network (KAN) based NeRF | O Stars 118
- Vision-KAN : KAN for Vision Transformer | Stars 54
- Simple-KAN-4-Time-Series : A simple feature-based time series classifier using Kolmogorov-Arnold Networks |
 O Stars 66
- KANU_Net : U-Net architecture with Kolmogorov-Arnold Convolutions (KA convolutions) | O Stars 9
- kanrl : Kolmogorov-Arnold Network for Reinforcement Leaning, initial experiments | 🖸 Stars 199
- <u>kan-diffusion</u>: Applying KANs to Denoising Diffusion Models with two-layer KAN able to restore images almost
- as good as 4-layer MLP (and 30% less parameters).
- S MANARec Implementation of Kolmogorov-Arnold Network (KAN) for Recommendations | Stars 25
- <u>CF-KAN</u> : Kolmogorov-Arnold Network (KAN) implementation for collaborative filtering (CF) | O Stars 8
- X-KANeRF : X-KANeRF: KAN-based NeRF with Various Basis Functions to explain the the NeRF formula
- KAN4Graph : Implementation of Kolmogorov-Arnold Network (KAN) for Graph Neural Networks (GNNs) and
 Tasks on Graphs | Ostars 33

"Success is not final, failure is not fatal: it is the courage to continue that counts." - Winston Churchill

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