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Flexible Quantum Kolmogorov Arnold Networks

Enhancing quantum KAN expressivity via Fractional order Chebyshev basis and trainable QSVT

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Bachelor's thesis, 2024-2025

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Presentation structure

1) Quantum computing
2) Kolmogorov-Arnold Networks: Classical and Quantum
3) Objectives
4) Methods
5) Results
6) Conclusion

This project has been sent to the 9th international conference on
Quantum Techniques in Machine Learning (QTML)

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Quantum computing

Qubit definition

Linear superposition of 2^n orthonormal basis states

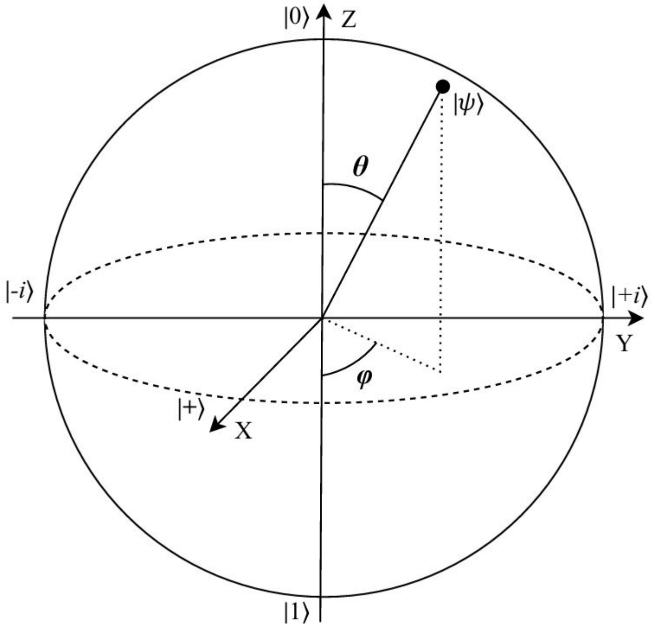
$$|\Psi\rangle = \sum_{j=0}^{2^{n-1}} a_j \, |j\rangle$$

$$a_j \in \mathbb{C}$$

Exponentially large Hilbert space

Parallelism advantage!

1- qubit system
Represented in the surface of the Bloch-Sphere

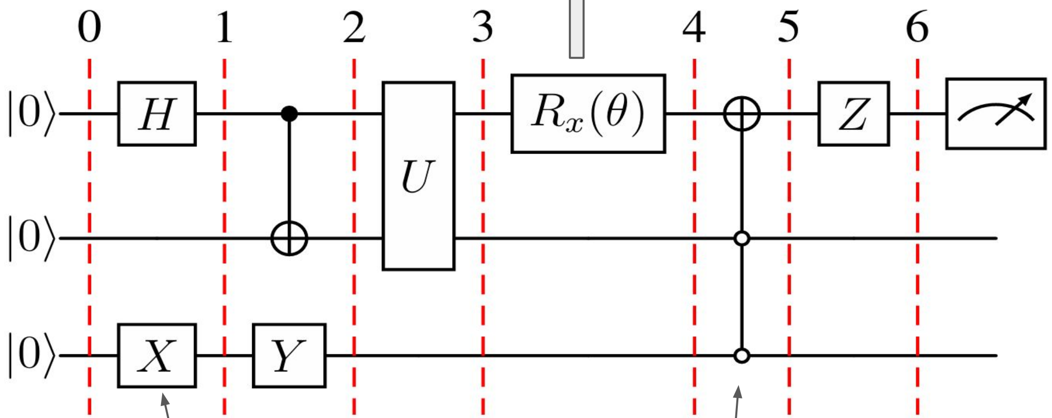


$$|\psi\rangle = \cos\frac{\theta}{2}\,|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}\,|1\rangle$$

State transformations - Quantum gates and quantum circuits

Parametrized Quantum Circuit (PQC)

PQCs open the path for Quantum ML (QML)



1-Qubit gates

Rotations around the Bloch-Sphere

n-Qubit gates

May create entanglement

Quantum circuits have a multi-qubit unitary representation

In this case, a 2^3-qubit unitary

Quantum gates are unitary matrices

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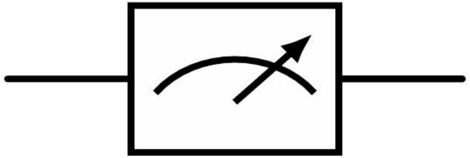
Measurements

Probabilistic result



Born rule

Probability amplitudes

$$P(|0\rangle) = |\alpha|^2$$
$$P(|1\rangle) = |\beta|^2$$

QML needs determinism!

1

An observable is defined as a single-qubit unitary matrix $\hat{O}$

2

Prepare $|\Psi\rangle$ through a quantum circuit

3

Calculate the expected measurement of $\hat{O}$ applied to $|\Psi\rangle$

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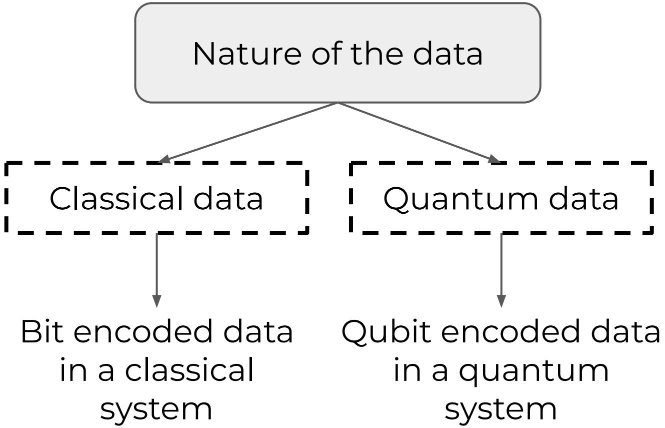
Quantum Machine Learning (QML)

Interplay between quantum computing and ML



Types of QML algorithms

	Processing and optimization	
Algorithm type	Classical	Quantum
Classical algorithms	✓	✗
Hybrid algorithms	✓	✓
Quantum algorithms	✗	✓

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Kolmogorov-Arnold Networks: Classical and Quantum

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KAN - Kolmogorov Arnold Networks (classical)

Inspired on the Kolmogorov Arnold representation theorem (KART)

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

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

φ's can be parametrized! ⇨ High expressive models!

Empirically generalize KART

KAN layer

$$\Phi^{(l)} = \left(\sum_{p=1}^{N^{(l-1)}} \phi_{p,1}^{(l)}(x_p), \ldots, \sum_{p=1}^{N^{(l-1)}} \phi_{p,N^{(l)}}^{(l)}(x_p) \right)$$

KAN

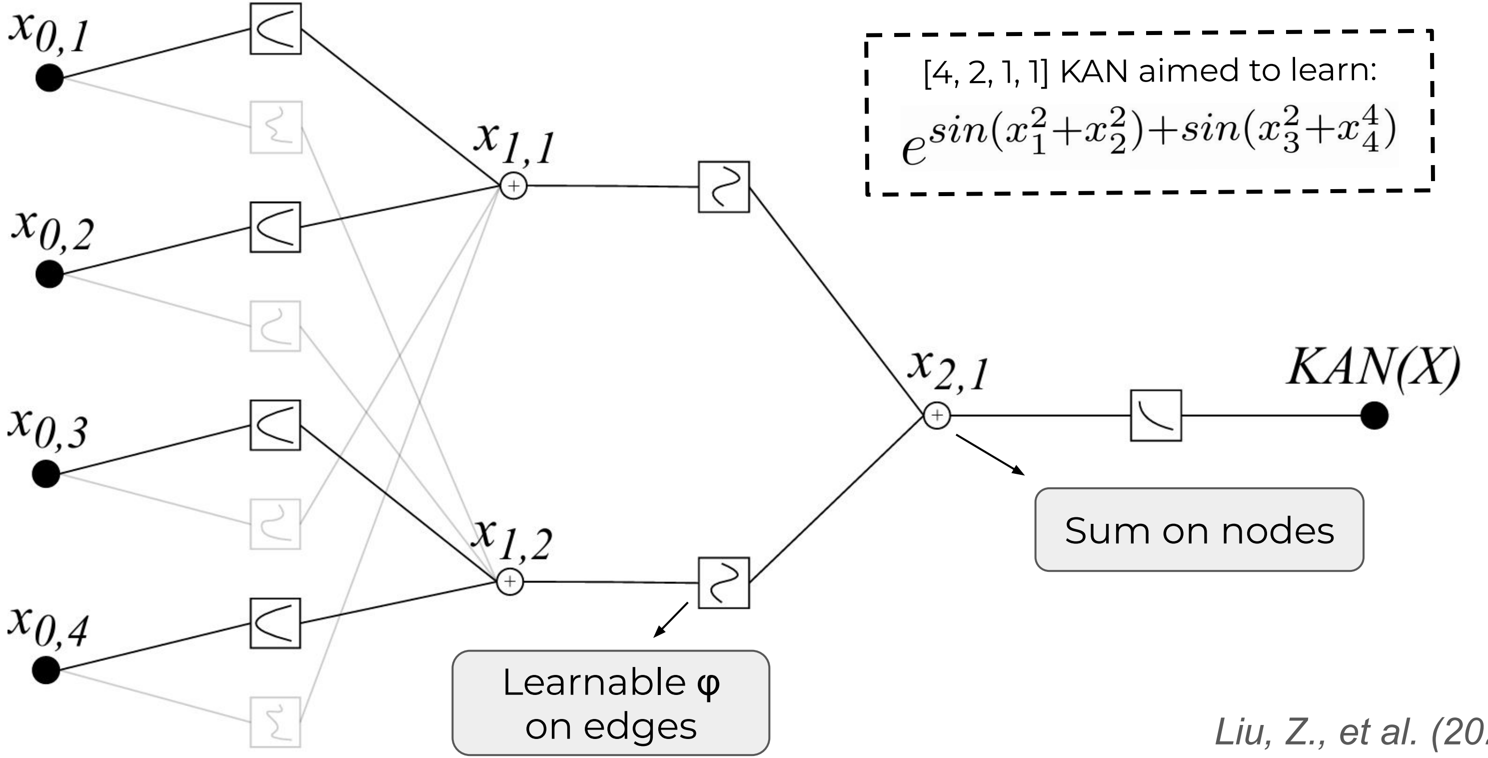
$$\mathrm{KAN}(\mathbf{x}) = \Phi^{(L)} \circ \ldots \circ \Phi^{(1)}(\mathbf{x})$$

Liu, Z., et al. (2024)

KAN - Architecture (classical)

[4, 2, 1, 1] KAN aimed to learn:

$$e^{sin(x_1^2+x_2^2)+sin(x_3^2+x_4^4)}$$



Liu, Z., et al. (2024)

Quantum KANs: State-of-the-art approaches

Name	*Abbreviation*
Quantum Kolmogorov-Arnold Networks	**QKAN**
Variational Quantum Kolmogorov-Arnold Networks	VQKAN
Adaptive Variational Quantum Kolmogorov-Arnold Networks	AVQKAN
Enhanced Variational Quantum Kolmogorov-Arnold Networks	EVQKAN
Quantum Kolmogorov-Arnold Networks by combining Quantum signal processing circuits	-

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QKAN: general idea

Based on Quantum Singular Value Transformation (QSVT) and linear algebra over Block Encodings (BEs)

QSVT forms basis functions which are Linearly combined to form activations

Unitary encoding an N-dimensional input vector

Input BE

$$U_X = \begin{bmatrix} X & * \\ * & * \end{bmatrix}$$

$$X = diag\left(x_1, x_2, \ldots, x_{N=2^n} \right)$$

QSVT + Quantum linear algebra

Output BE

$$U_{QKAN} = \begin{bmatrix} QKAN(X) & * \\ * & * \end{bmatrix}$$

$$QKAN(X) = diag\left(\mathrm{KAN}(\mathbf{x}) = \Phi^{(L)} \circ \ldots \circ \Phi^{(1)}(\mathbf{x})\right)$$

Unitary encoding a K-dimensional output vector

Ivashkov, P., et al. (2024)

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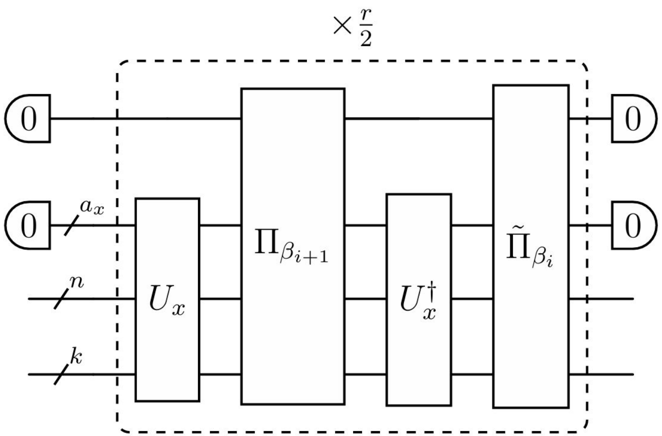
QKAN: QSVT

Applies a polynomial transformation to the singular values of a BE'd matrix

$$\begin{bmatrix} X & * \\ * & * \end{bmatrix} \xrightarrow{\text{QSVT}} \begin{bmatrix} P^{SV}(X) & * \\ * & * \end{bmatrix}$$



QKAN: CHEB-QKAN

Paper proposal

Use Chebyshev polynomials as basis functions

$$T_r(x) = \cos(r\theta)$$

where $x = \cos(\theta)$ and $x \in [-1, 1]$

Easy to implement through the QSVT routine

Chebyshev Approximation is universal

$$f(x) \approx \sum_{r=0}^{d} w_r T_r(x)$$

Ivashkov, P., et al. (2024)

CHEB-QKAN Layer - step 1: Dilate

Objective: Accommodate space for the layer nonlinearities

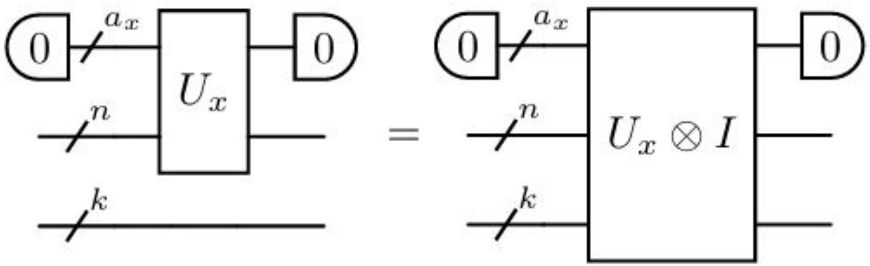
Layer output size

$$\text{DILATE:} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix}_{BE} \rightarrow \begin{matrix} K \left\{ \begin{matrix} x_1 \\ \vdots \\ x_1 \end{matrix} \right. \\ \\ \\ \\ \end{matrix} \begin{bmatrix} x_1 \\ \vdots \\ x_1 \\ \vdots \\ x_N \\ \vdots \\ x_N \end{bmatrix}_{BE}$$

$\mathbf{x} \in [-1, 1]^N$

Layer input vector

Layer input size



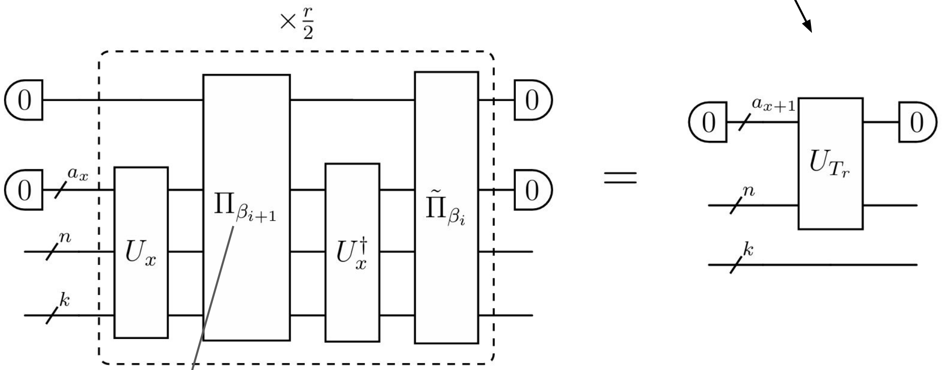
Ivashkov, P., et al. (2024)

CHEB-QKAN Layer - step 2: Cheb

QSVT

One for each degree

$$\text{CHEB:} \begin{bmatrix} x_1 \\ \vdots \\ x_1 \\ \vdots \\ x_N \\ \vdots \\ x_N \end{bmatrix}_{BE} \rightarrow \begin{bmatrix} T_r(x_1) \\ \vdots \\ T_r(x_1) \\ \vdots \\ T_r(x_N) \\ \vdots \\ T_r(x_N) \end{bmatrix}_{BE}$$



Objective: Form basis functions

$$\Pi_\beta = \begin{bmatrix} e^{-i\beta} & 0 & 0 & 0 \\ 0 & e^{i\beta} & 0 & 0 \\ 0 & 0 & e^{i\beta} & 0 \\ 0 & 0 & 0 & e^{i\beta} \end{bmatrix}$$

where $\beta_1 = (1-r)\frac{\pi}{2}$ and $\beta_{i>1} = \frac{\pi}{2}$ with $i \in [1, r]$

$$U_{T_0} = \begin{bmatrix} T_0(x_1) \\ \vdots \\ T_0(x_1) \\ \vdots \\ T_0(x_N) \\ \vdots \\ T_0(x_N) \end{bmatrix}_{BE} \quad U_{T_1} = \begin{bmatrix} T_1(x_1) \\ \vdots \\ T_1(x_1) \\ \vdots \\ T_1(x_N) \\ \vdots \\ T_1(x_N) \end{bmatrix}_{BE} \quad \dots \quad U_{T_r} = \begin{bmatrix} T_r(x_1) \\ \vdots \\ T_r(x_1) \\ \vdots \\ T_r(x_N) \\ \vdots \\ T_r(x_N) \end{bmatrix}_{BE}$$

Ivashkov, P., et al. (2024)

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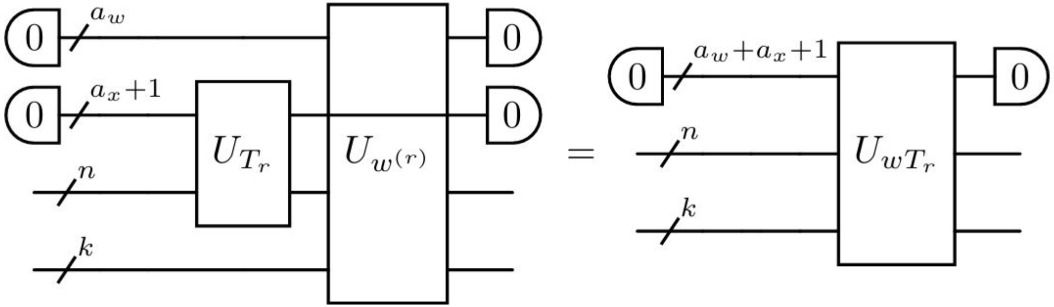
CHEB-QKAN Layer - step 3: Mul

$$\text{MUL:}\quad \begin{bmatrix} T_r(x_1) \\ \vdots \\ T_r(x_1) \\ \vdots \\ T_r(x_N) \\ \vdots \\ T_r(x_N) \end{bmatrix}_{BE} \rightarrow \begin{bmatrix} w_{11}^{(r)} T_r(x_1) \\ \vdots \\ w_{1K}^{(r)} T_r(x_1) \\ \vdots \\ w_{N1}^{(r)} T_r(x_N) \\ \vdots \\ w_{NK}^{(r)} T_r(x_N) \end{bmatrix}_{BE}$$



Objective: Form learnable Chebyshev approximation coefficients

Chebyshev approx order

d weight matrices for every NxK activation function

Encoded as BEs

Ivashkov, P., et al. (2024)

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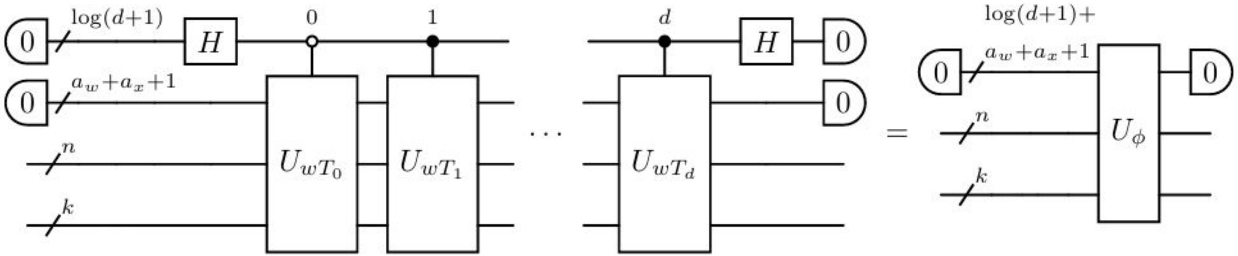
CHEB-QKAN Layer - step 4: LCU

Activation function between p-th input node and q-th output node

$$\text{LCU:}\quad \begin{bmatrix} w_{11}^{(r)}T_r(x_1) \\ \vdots \\ w_{1K}^{(r)}T_r(x_1) \\ \vdots \\ w_{N1}^{(r)}T_r(x_N) \\ \vdots \\ w_{NK}^{(r)}T_r(x_N) \end{bmatrix}_{BE} \rightarrow \begin{bmatrix} \phi_{11}(x_1) \\ \vdots \\ \phi_{1K}(x_1) \\ \vdots \\ \phi_{N1}(x_N) \\ \vdots \\ \phi_{NK}(x_N) \end{bmatrix}_{BE}$$



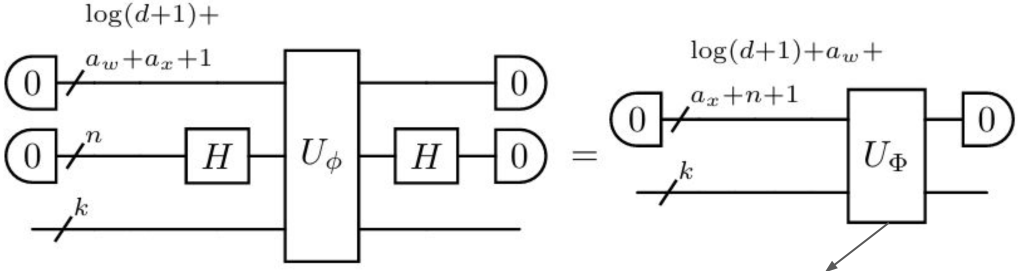
$$\phi_{pq}(x) := \frac{1}{d+1}\sum_{r=0}^{d} w_{pq}^{(r)}T_r(x_p)$$

Objective: Form the NxK activation functions

Ivashkov, P., et al. (2024)

CHEB-QKAN Layer - step 5: SUM (Final step!)

$$\text{SUM:} \begin{bmatrix} \phi_{11}(x_1) \\ \vdots \\ \phi_{1K}(x_1) \\ \vdots \\ \phi_{N1}(x_N) \\ \vdots \\ \phi_{NK}(x_N) \end{bmatrix}_{BE} \rightarrow \begin{bmatrix} \frac{1}{N}\sum_{p=1}^{N} \phi_{p1}(x_p) \\ \vdots \\ \frac{1}{N}\sum_{p=1}^{N} \phi_{pK}(x_p) \end{bmatrix}_{BE}$$



layer output BE!!

Objective: Sum all activation functions that go to the same output neuron

To form **multi-layer** QKAN models:

$$U_\Phi \longrightarrow U_x$$

Use layer output BE as input BE for the next layer

Forms

U_{CHEB} CHEB - QKAN

Ivashkov, P., et al. (2024)

Objectives

Objectives of this work

Current limitations	Objectives
CHEB-QKAN may be limited in expressive power	Increase the expressivity of QKAN-based models
Lack of empirical research on QKAN-based models	Provide empirical research on QKAN-based models for the classical-to-classical setting

Methods

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Generalized Fractional order of the Chebyshev Functions (GFCF) transformation

GFCFs

Fractional degree

$$ {}_{\eta}FT_r^{\alpha}(x) = T_r\left(1 - 2\left(\frac{x}{\eta}\right)^{\alpha}\right) $$

where $\alpha, \eta \in \mathbb{R}_+$ and $x \in [0, \eta]$

Defines a universal basis of functions well suited for representing fractional growths

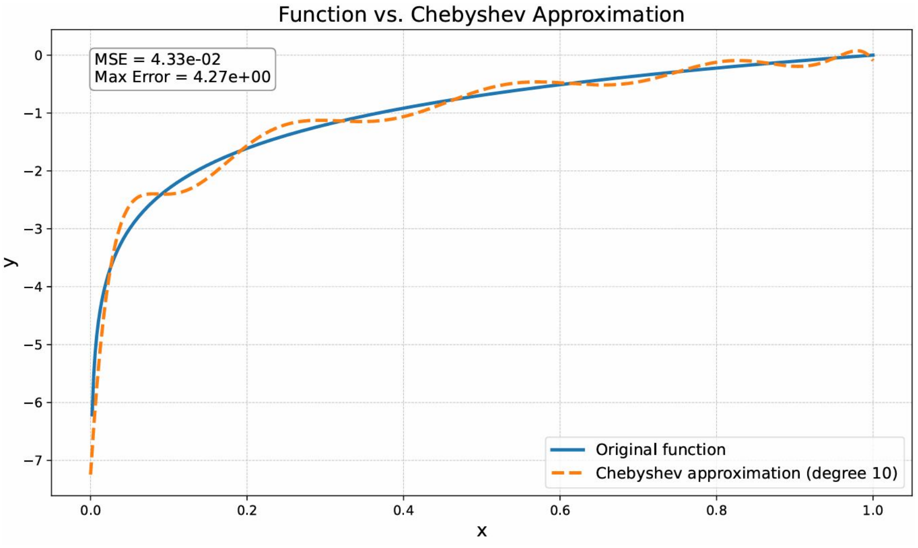
GFCF approximation

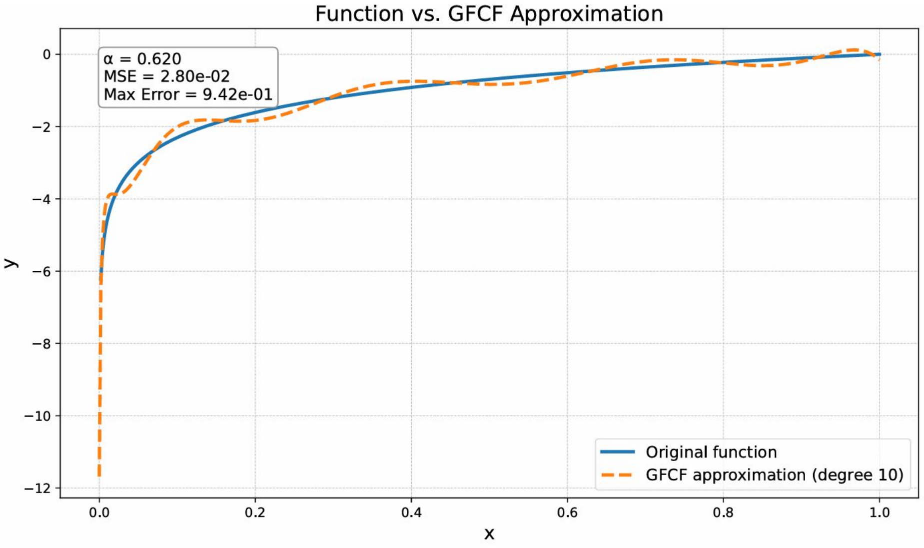
$$ f(x) \approx \sum_{r=0}^{d} {}_{\eta}FT_r^{\alpha}(x) a_r $$

Can converge faster than Chebyshev approximation for some functions

Kourosh, P. and Mehdi, D (2017)

Approximation of log(x) - Chebyshev vs GFCF





Lower MSE!

GFCFs for QKAN - classical processing step

Assuming a normalized classical input in [0, η]

Apply GFCF transformation prior to QKAN ingestion

$$\mathbf{x}_{\text{norm}} \in [0, \eta]^N \quad \Longrightarrow \quad \mathbf{x}_{gfcf} = 1 - 2\left(\frac{\mathbf{x}_{\text{norm}}}{\eta}\right)^{\alpha}$$

where $\alpha, \eta \in \mathbb{R}_{>0}$

α

Can be made trainable to increase expressivity → Basis functions adapt themselves to fractional growths

Flexible QKAN (Flex-QKAN)

Idea

Parametrize QSVT angles

$$\cancel{\text{where } \beta_1 = (1-r)\frac{\pi}{2} \text{ and } \beta_{i>1} = \frac{\pi}{2} \text{ with } i \in [1, r]}$$

$$\beta_1, \ldots, \beta_r \longrightarrow \boxed{\text{Trainable!}}$$

Why?

Learnable polynomial basis functions

$$F_1^{\beta_1}(x) \ldots F_d^{\beta_1 \ldots \beta_d}(x)$$

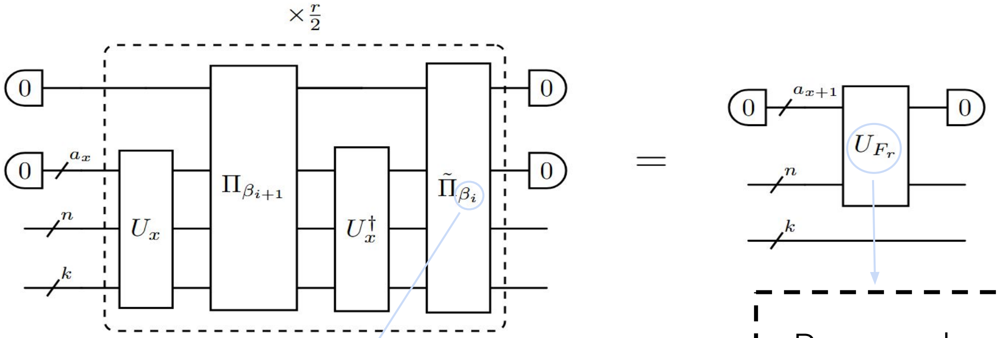
Implications

Augmented expressivity

Choose the best polynomial basis for each specific problem

Flex-Step and U_{FLEX}

Flex-Step



Trainable

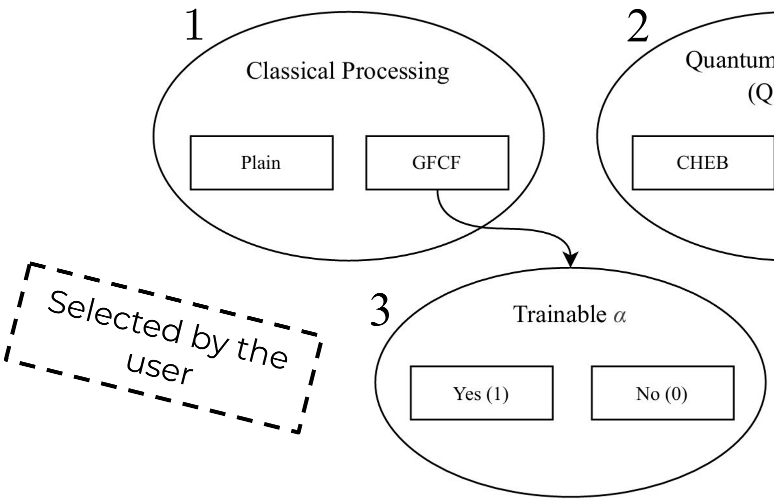
Renamed as U_{Fr}

Multi-layer Flex-QKAN

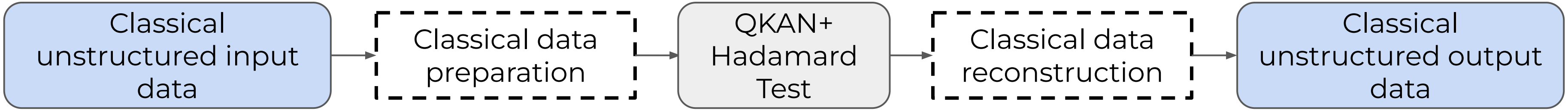
U_{FLEX}

GFCF + U_{FLEX} to increase even more the expressivity!

Classical-to-Classical QKAN framework: CCQKAN



Model Name
Plain-CHEB
Plain-Flex
GFCF-CHEB-0
GFCF-CHEB-1
GFCF-Flex-0
GFCF-Flex-1



$\mathbf{x}_{in} \in \mathbb{R}^N$

Models pipeline

$\mathbf{x}_{out} \in \mathbb{R}^K$

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CCQKAN models initialization

Implemented as a Python class:

1) Initialization parameters
Network structure
Degree of approximation
GFCF flag
α and η
Trainable α flag
Flex flag
Input + Output domains

2) Trainable Parameters initialization:

Parameter	**Initialization**
Weights	Random or fixed 0.5
α	User's choice
QSVT angles	Chebyshev
Output domain	User's choice

CCQKAN models end-to-end pipeline I

0

Classical unstructured input data ingestion

$\mathbf{x}_{in} \in \mathbb{R}^N$

1

Classical data preparation

Plain models

$$\underbrace{\mathbf{x}_{in} \longrightarrow \mathbf{x}_{plain} \in [-1,1]^N}_{\text{min-max norm}} \longrightarrow \mathbf{X}_{plain} = \begin{bmatrix} x_{\text{plain}_1} & 0 & \cdots & 0 \\ 0 & x_{\text{plain}_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & x_{\text{plain}_N} \end{bmatrix}$$

GFCF models

$$\underbrace{\mathbf{x}_{in} \longrightarrow \mathbf{x}_{\text{norm}}}_{\text{min-max norm}} \in [0,\eta]^N \longrightarrow \mathbf{x}_{gfcf} = 1 - 2\left(\frac{\mathbf{x}_{\text{norm}}}{\eta}\right)^{\alpha} \longrightarrow \mathbf{X}_{gfcf} = \begin{bmatrix} x_{\text{gfcf}_1} & 0 & \cdots & 0 \\ 0 & x_{\text{gfcf}_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & x_{\text{gfcf}_N} \end{bmatrix}$$

where $\alpha, \eta \in \mathbb{R}_{>0}$

CCQKAN models end-to-end pipeline II

2

Quantum processing

if

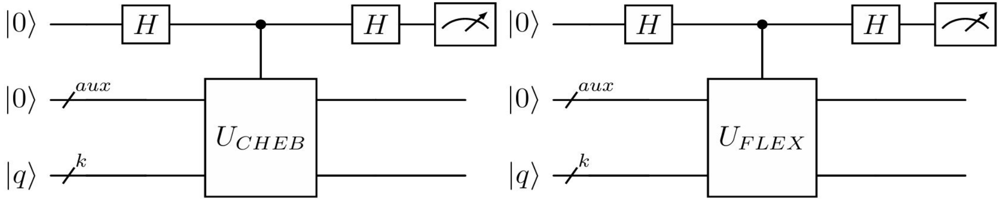
|q> = |5> = |101>

then

X_{h5}

For q in 1...K

PennyLane qnode receiving diagonal input matrix



Extract

X_{hq}

$$\mathbf{x}_h \in [-1, 1]^{K_{out}}$$

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CCQKAN models end-to-end pipeline III

3

Classical data reconstruction

$\mathbf{x}_h \in [-1, 1]^{K_{out}} \rightarrow$ Inverse step 1 normalization $\rightarrow \mathbf{x}_{out} \in \mathbb{R}^K$

Learnable output bounds

Model classical unstructured output

Results

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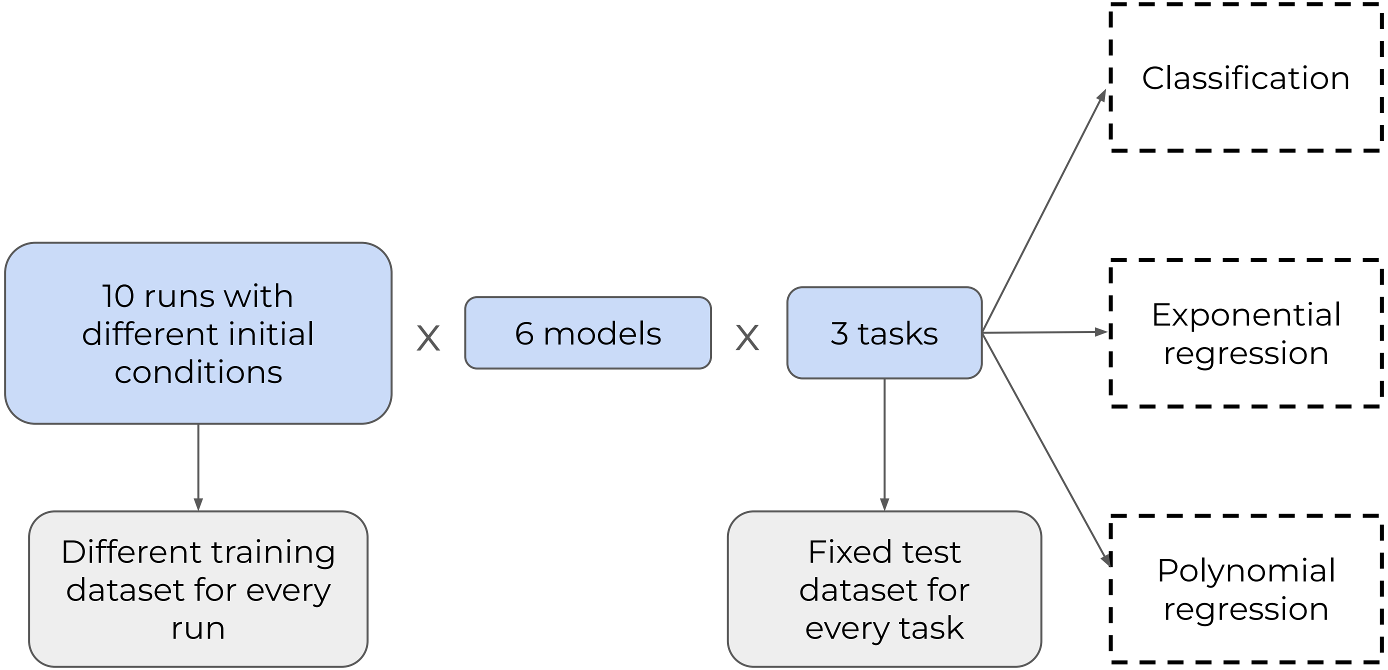
Experimental setup

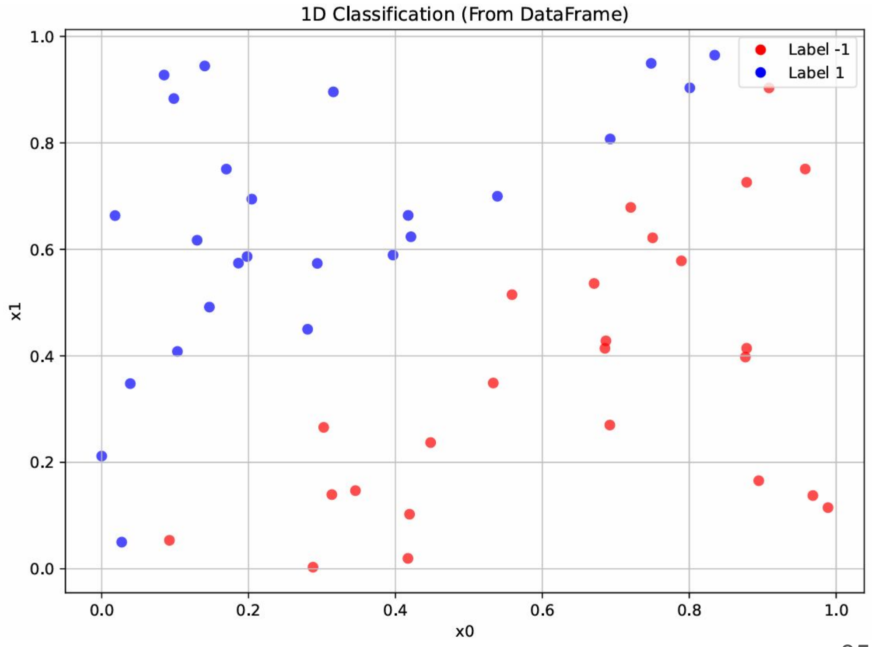


Classification task - description

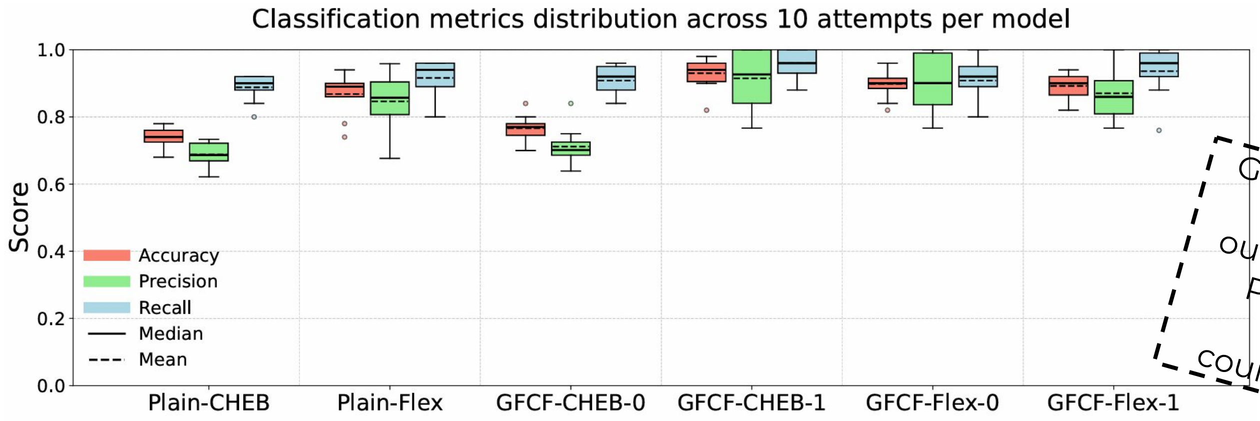
Trained as 1-d regression

Training datasets size	45
Test dataset size	50
QKAN	[1,2,1] d=2
Optimizer	Adam, 0.3
Epochs	20
Training loss	MSE
Evaluation	Accuracy, Precision, Recall

Test dataset

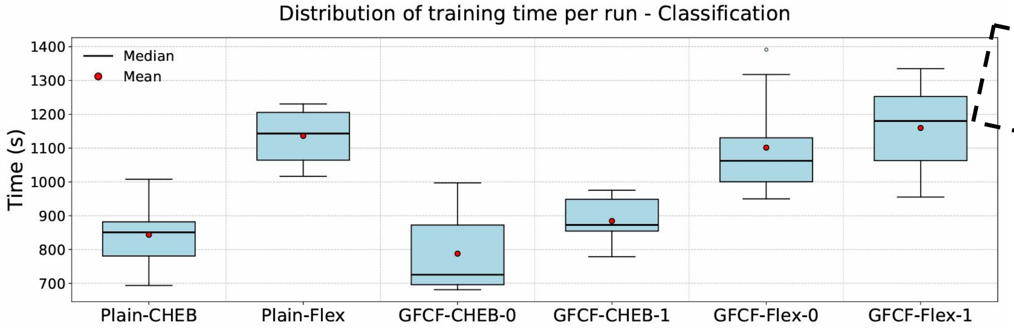


Classification task - results



GFCF and Flex methods outperformed Plain and CHEB counterparts

GFCF fixed α has the same training time as Plain!



+ expressivity
- trainability

Exponential regression task - description

Training datasets size	100
Test dataset size	50
QKAN	[4,1] d=2
Optimizer	Adam, 0.3
Epochs	55
Training loss	MSE
Evaluation	Sum Abs. Distances

$$SAD = \sum_{i=1}^{i=50} |f^{aim}(\mathbf{x})_i - \hat{f}^{aim}(\mathbf{x})_i|$$

Datasets generator

$$f_{exp}^{aim}(\mathbf{x}) = \exp\left(\sin(x_0^2 + x_1^2) + \sin(x_2^2 + x_3^2)\right)$$

Input domain: $[-1,1]^4$

Test dataset: 5 samples

x_0	x_1	x_2	x_3	$target$
0.10	0.14	0.36	-0.70	1.84
0.43	-0.12	-0.46	0.74	2.42
0.21	0.98	0.47	-0.68	4.33
0.09	-0.80	0.92	0.23	4.00
-0.15	-0.58	-0.50	-0.75	2.96

Target domain: [1.08, ,7.18]

Contextualize distance based eval.

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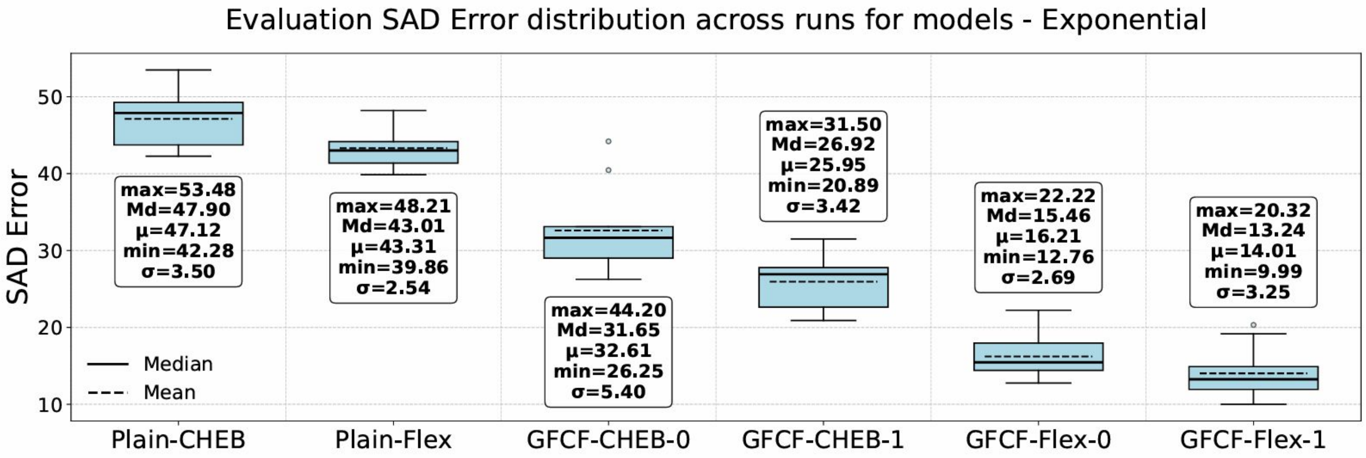
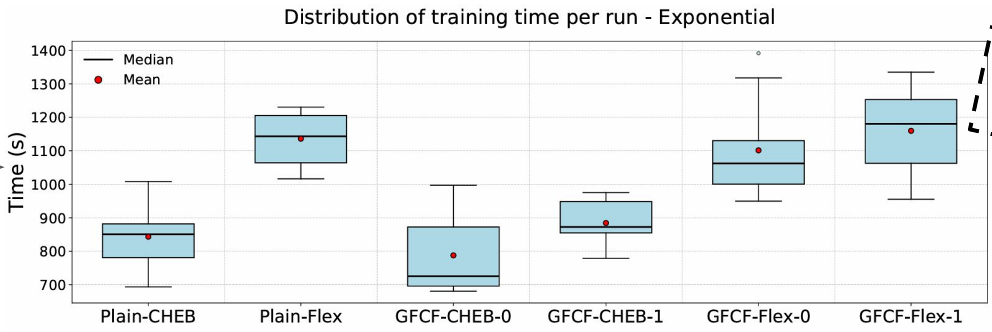
Exponential regression task - results



GFCF fixed α clearly outperformed Plain models

With no trainability cost!!



+ expressivity
- trainability

Polynomial regression task - description

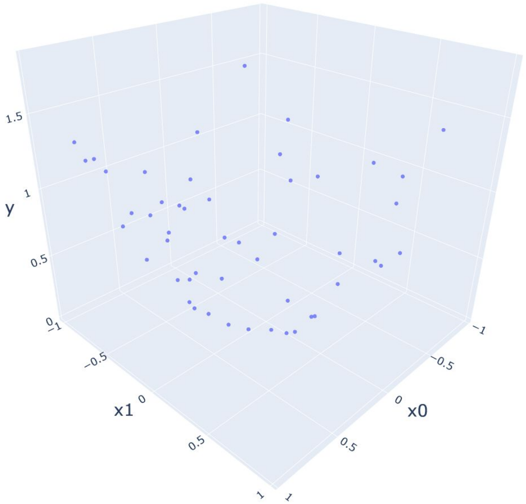
Training datasets size	100
Test dataset size	50
QKAN	[2,1] d=2
Optimizer	Adam, 0.3
Epochs	55
Training loss	MSE
Evaluation	Sum Abs. Distances

$$SAD = \sum_{i=1}^{i=50} |f^{aim}(\mathbf{x})_i - \hat{f}^{aim}(\mathbf{x})_i|$$

Datasets generator

$$f^{aim}(\mathbf{x}) = x_0^2 + x_1^2$$

Test dataset



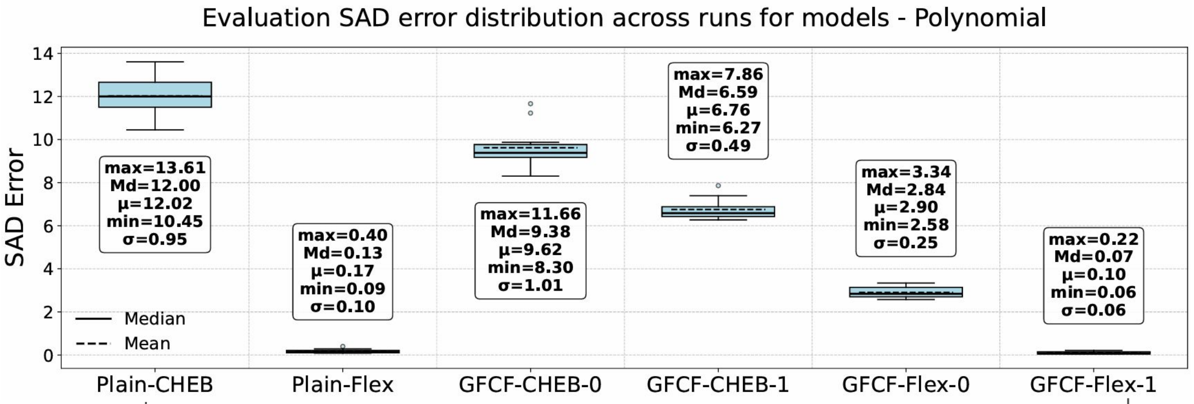
Input domain: $[-1,1]^2$

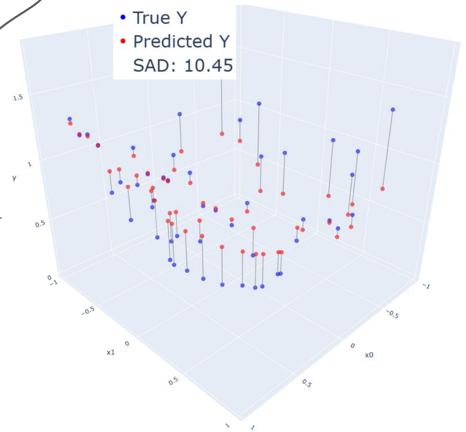
Target domain: [0.29, 1.82]

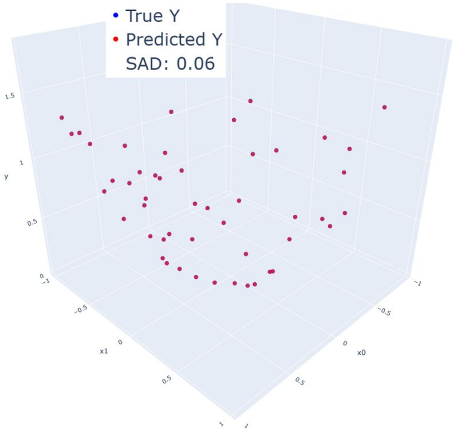
Contextualize distance based eval.

Polynomial regression task - results

Flex models performed surprisingly good here







Discussion

Expressivity is augmented

GFCF with fixed α has no trainability cost

GFCF and Flex outperformed Plain and CHEB

GFCF learnable α + Flex QKAN

Only 1 extra parameter

$\mathcal{O}(d^2)$ extra parameters

Use it if fractional growth is suspected

Once trained, forward pass is equally fast as other models. Use them!!

Conclusion

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Contributions

Augmented expressivity for QKAN-based methods

GFCF transformation

$$\mathbf{x}_{gfcf} = 1 - 2\left(\frac{\mathbf{x}_{\text{norm}}}{\eta}\right)^{\alpha}$$

Prior to BE

α learnable -> + expressivity - trainability

Improved Plain results

Flex-QKAN

Learnable polynomial basis functions

$$F_1^{\beta_1}(x) \ldots F_d^{\beta_1 \ldots \beta_d}(x)$$

+ expressivity - trainability

Improved CHEB results

Empirical research on QKAN-based models

CCQKAN framework

6 models
Plain-CHEB
Plain-Flex
GFCF-CHEB-0
GFCF-CHEB-1
GFCF-Flex-0
GFCF-Flex-1

Open source classical-to-classical QKAN based framework

Baseline established for future research

Future work

Polynomial basis functions

B-Splines

+ Locally adaptive

Implementable through QSVT

Options:

Make CCQKAN hardware compatible

1) Use FABLE to BE

2) Encode classical input as state amplitudes

Transform to BEs

Apply GFCFs on every layer

Solve the following problem:

Given a BE Ux that encodes a diagonal matrix X of a vector x ∊ RN, find a BE Uz of the diagonal matrix Z such that the diagonal values of Z are the diagonal elements of X transformed by $z = 1-2(x/\eta)^{\alpha}$

Arbitrary power to *Ux*

LCU step

- Increase expressivity on every layer

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Thank you

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