HM

Deep Dive: Kolmogorov-Arnold Networks (KANs)

Accuracy, Interpretability, and Scaling Beyond MLPs

Team KAN (replace names)

Advanced Deep Learning Deep Dive

Roadmap

Part I: Motivation + Theory

- Why move non-linearities to edges?
- KAT vs UAT (theorem shift)

Part II: Architecture + Training

- KAN layer = matrix of 1D functions
- Splines, residual activation, grid updates

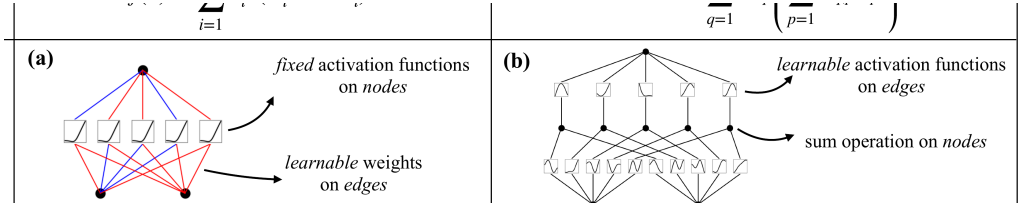
Part III: Accuracy + Scaling

- Scaling laws (alpha 4) and grid extension
- PDE + symbolic regression benchmarks

Part IV: Interpretability + Critique

- Sparsification, pruning, symbolification
- Practical limits and open questions

MLP vs KAN (shallow): where does nonlinearity live?



Shallow MLP vs shallow KAN (Fig. 0.1a,b). [Liu+25]

Key idea

- MLP: fixed activation σ on nodes; learn weights $w_{j,i}$ on edges.
- KAN: learn 1D edge functions $\varphi_{q,p}$; nodes only sum inputs.
- Intuition: learn expressive 1D building blocks, then compose across layers.

Shallow formulas

- MLP / UAT-style:

$$f(\boldsymbol{x}) \approx \sum_{j=1}^{m} a_j \sigma\left(\boldsymbol{w}_j^T \boldsymbol{x} + b_j\right)$$

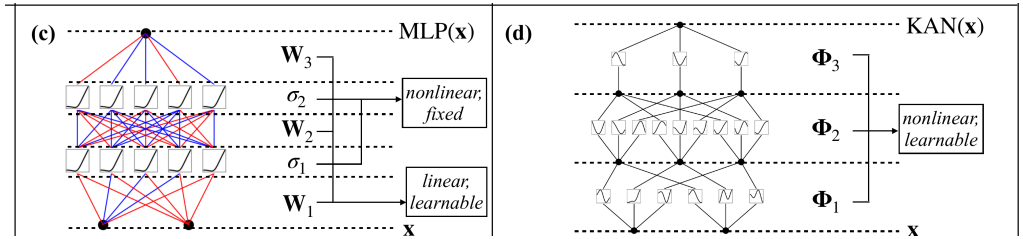
- KAN / KAT-style:

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

[Cyb89, HSW89, Kol57, Liu+25]

Connections: fixed vs learnable nonlinearity; inductive bias towards symbolic/compositional structure.

MLP vs KAN (deep): what gets learned?



Deep MLP vs deep KAN (Fig. 0.1c,d). [Liu+25]

Deep takeaway

- Deep MLPs: learn linear maps $\boldsymbol{W}_l$; nonlinearity stays fixed.
- Deep KANs: learn function matrices $\boldsymbol{\Phi}_l$ (one 1D function per edge).
- Practical upside: plot/inspect learned edge functions directly.

Deep composition

- Deep MLP:

$$\mathrm{MLP}(\boldsymbol{x}) = (\boldsymbol{W}_{L-1} \circ \sigma \circ \boldsymbol{W}_{L-2} \circ \ldots \circ \sigma \circ \boldsymbol{W}_0)(\boldsymbol{x})$$

- Deep KAN:

$$\mathrm{KAN}(\boldsymbol{x}) = (\boldsymbol{\Phi}_{L-1} \circ \ldots \circ \boldsymbol{\Phi}_0)(\boldsymbol{x})$$

[Cyb89, HSW89, Liu+25]

Interpretation

- MLP: learn linear maps $\boldsymbol{W}$; nonlinearity is fixed.
- KAN: learn edge functions $\varphi_{l,j,i}$; nodes are sums.

UAT vs KAT: what do they guarantee?

UAT (MLPs)

- Statement: 2-layer nets can approximate any continuous f on a compact domain.
- Learnable parts: $\boldsymbol{W}, \boldsymbol{b}$ (activations fixed).
- Caveat: existence result; rates can still suffer from dimensionality.

$$f(\boldsymbol{x}) \approx \sum_{j=1}^{m} a_j \sigma\left(\boldsymbol{w}_j^T \boldsymbol{x} + b_j\right)$$

[Cyb89, HSW89]

KAT (Kolmogorov–Arnold)

- Statement: represent $f : [0,1]^n \to \mathbb{R}$ via sums of 1D functions + addition.
- Promise: reduce multivariate learning to learning many 1D functions.
- Caveat: worst-case representations can be highly non-smooth/fractal.

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

[BG09, GP89, Kol57, Liu+25, Sch21]

KAN viewpoint: assume smooth/compositional structure; learn φ with splines and add depth to avoid pathological 2-layer forms. [Liu+25, PBL20]

KAN layer mechanics

Each layer is a matrix of learnable 1D functions:

$$x_{l+1,j} = \sum_{i=1}^{n_l} \varphi_{l,j,i}(x_{l,i})$$

$$\boldsymbol{x}_{l+1} = \boldsymbol{\Phi}_l \boldsymbol{x}_l$$

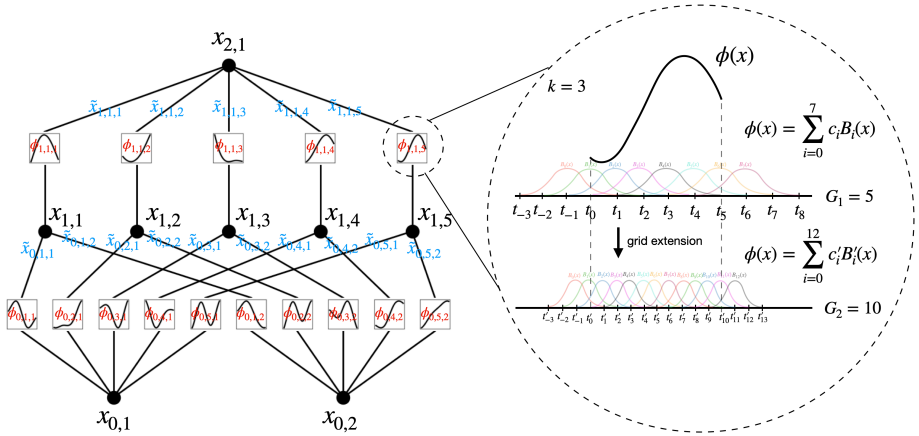
[Liu+25]

Each edge function is a residual spline:

$$\varphi(x) = w_b b(x) + w_s \sum_i c_i B_{i(x)}$$

[De 78, Liu+25]

Residual $b(x)$ defaults to SiLU; spline coefficients are trainable.



B-spline parametrization and grid refinement. [Liu+25]

Training and optimization tricks

Optimization details

- Residual activation: $\varphi(x) = w_b b(x) + w_s \ \mathrm{spline}(x)$.
- Initialize spline near zero; initialize w_b like Xavier.
- Update spline grids as activation ranges drift.

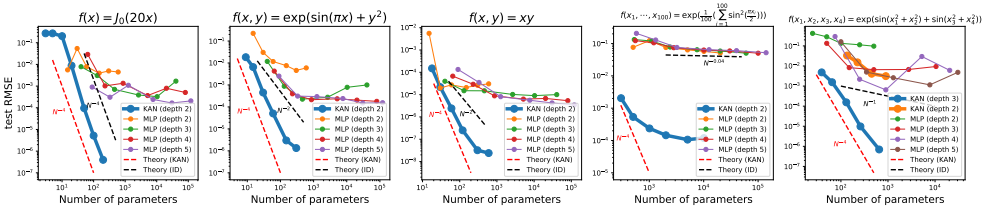
Connections

- Initialization and stability in deep networks
- Loss landscapes and optimization schedules
- Bias–variance trade-off when increasing capacity

[Liu+25]

Accuracy & Scaling

How KANs generalize and grow



Fast scaling trends on structured function classes. [Liu+25]

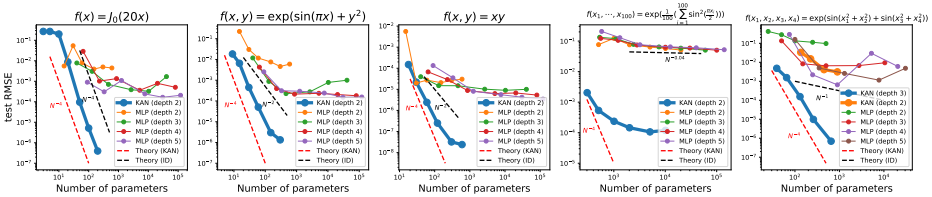
Scaling laws

Theory + observation

- Smooth-KAT bound: $|f - \mathrm{KAN}_G| \leq CG^{-(k+1)}$ (cubic: $k = 3 \to \alpha \approx 4$).
- Comparison: manifold view ($\alpha \approx \frac{k+1}{d}$) vs arity view ($\alpha \approx \frac{k+1}{2}$).
- Empirically: KANs reach steeper scaling than MLPs on compositional data.

[De 78, Liu+25, MLT23, SK20]

Connections: scaling laws; approximation theory; bias–variance trade-off.



Scaling vs MLP baselines. [Liu+25]

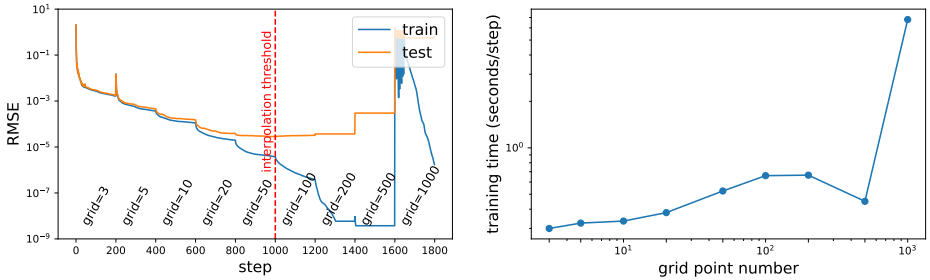
Grid extension: fine-grain without retraining

Key idea

- Start with coarse grids, then refine spline knots.
- Initialize finer grids by least-squares fit to the coarse spline.
- Produces staircase-like drops in loss after each extension.

[Liu+25]

Connections: model scaling vs training schedules; KAN adds explicit fine-graining.



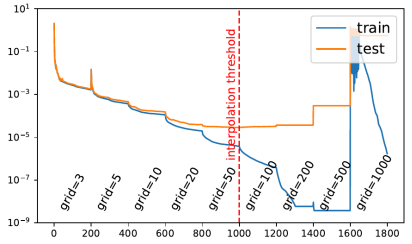
Grid extension illustration. [Liu+25]

Grid extension: why it works

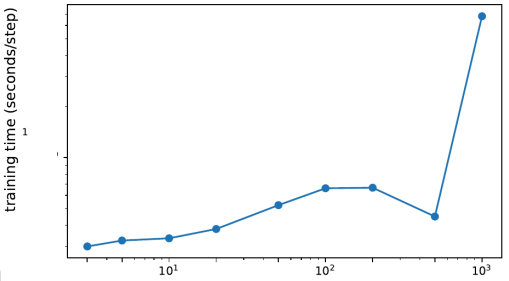
Why grid extension works

- External dofs: graph structure (width/depth) learns compositional structure.
- Internal dofs: spline grid points learn 1D functions precisely.
- Grid extension: increase internal dofs without re-initializing.
- Warm-start: least-squares fit a finer spline to the coarse spline (per edge).
- Effect: staircase-like loss drops after each refinement; cost grows with grid size.

[Liu+25]



Staircase loss drops after each refinement. [Liu+25]



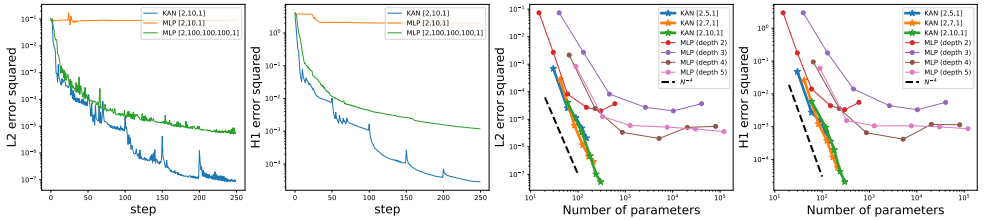
Training time vs grid size. [Liu+25]

Accuracy results: PDEs and scientific fitting

Results

- PDE solving: Poisson equation solved with smaller KANs at higher accuracy.
- Special functions + Feynman datasets show strong sample efficiency.
- Suggests KANs as compact, high-precision function approximators.

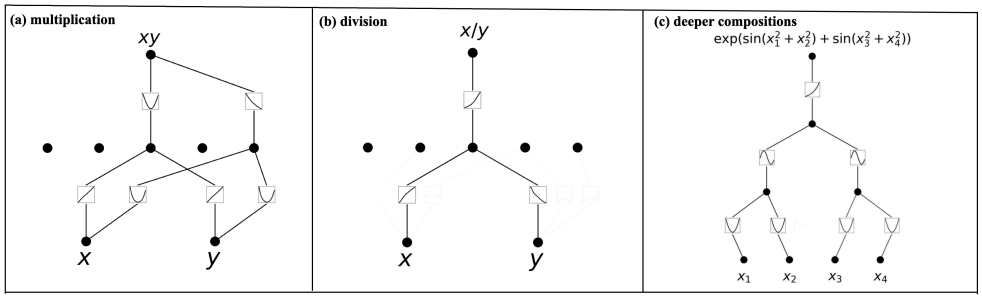
[Liu+25]



PDE benchmark results. [Liu+25]

Interpretability & Science

From pruning to symbolic laws



Symbolic recovery examples from pruned/simplified KANs. [Liu+25]

Interpretability toolkit: sparsify, prune, symbolify

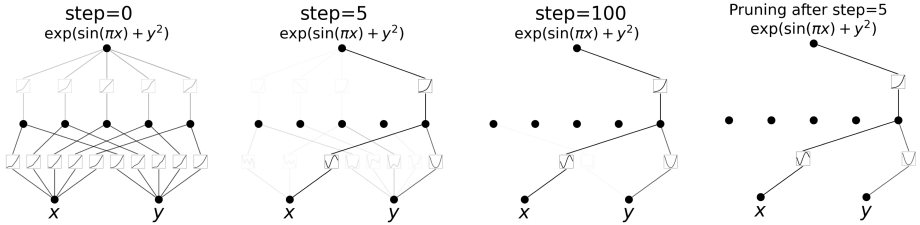
Four steps to a formula

- Sparsify: encourage few active edges (L1 + entropy).
- Visualize: inspect learned 1D edge functions $\varphi_{l,j,i}$.
- Prune: drop inactive nodes to a minimal shape $[n_0, ..., n_L]$.
- Symbolify: snap splines to analytic forms with an affine wrapper

$$y \approx cf(ax + b) + d$$

(grid search for a, b; linear regression for c, d).

[Liu+25]



Sparsification + pruning yields simpler, more interpretable KANs.
[Liu+25]

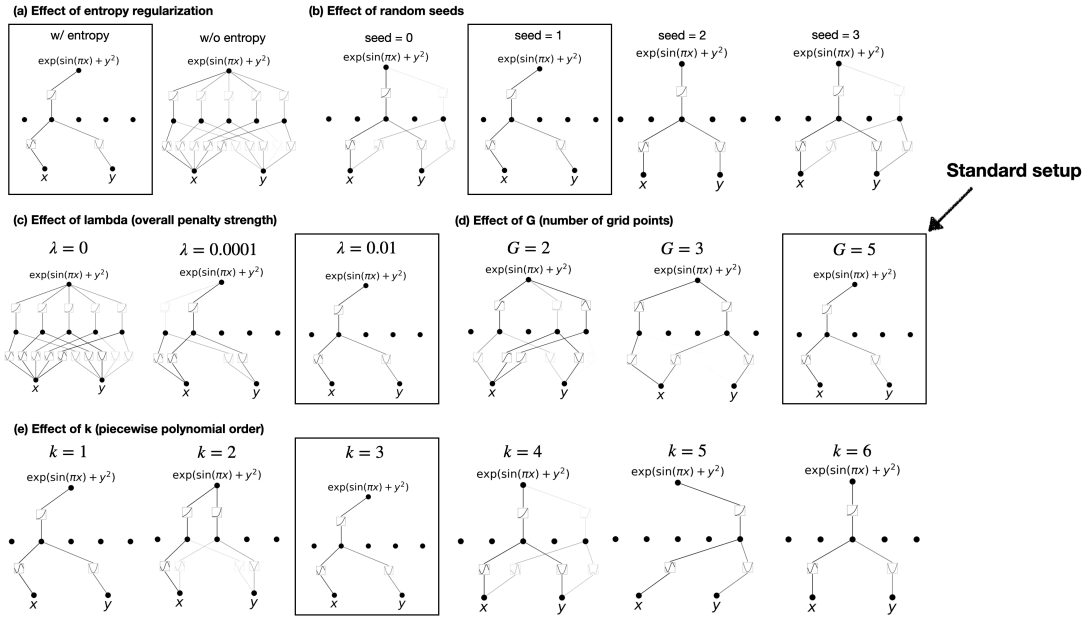
Interpretability: hyperparameters matter

What changes (and why)

- Entropy regularization: encourages sparse, readable graphs.
- λ: sparsity–accuracy trade-off; too small $\rightarrow$ dense, too large $\rightarrow$ underfit.
- Grid size G + spline order k: resolution vs compute (larger G is slower).
- Random seeds can reveal different relations in unsupervised discovery.

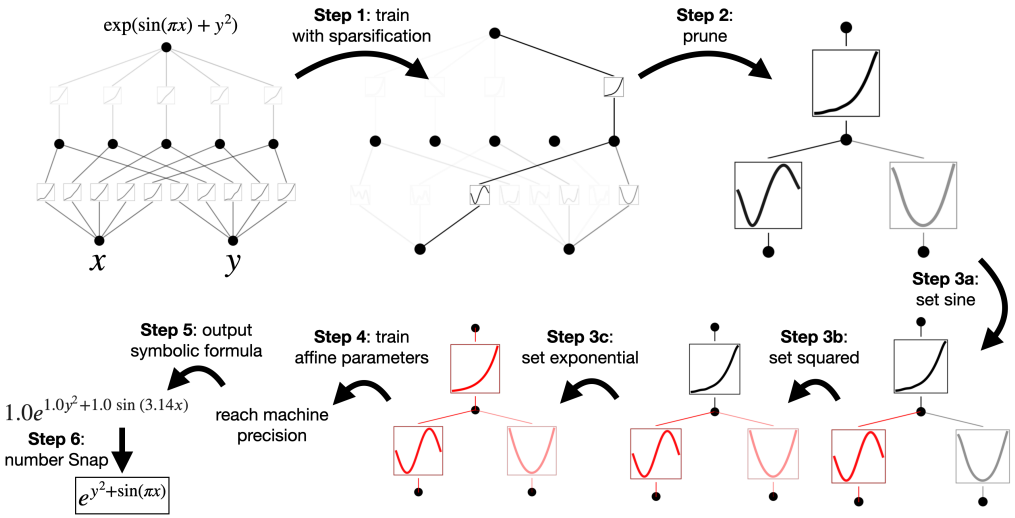
[Liu+25]

Takeaway: interpretability is an objective + design choice, not a byproduct.



Dependence on regularization, seeds, and spline resolution. [Liu+25]

Interactive symbolification (toy example)



Interactive workflow for symbolic regression with KANs. [Liu+25]

What the user does

- Train with sparsification.
- Prune to a minimal graph.
- Set/suggest symbolic forms (manual or assisted).
- Retrain only affine parameters and export the symbolic formula.

[Liu+25]

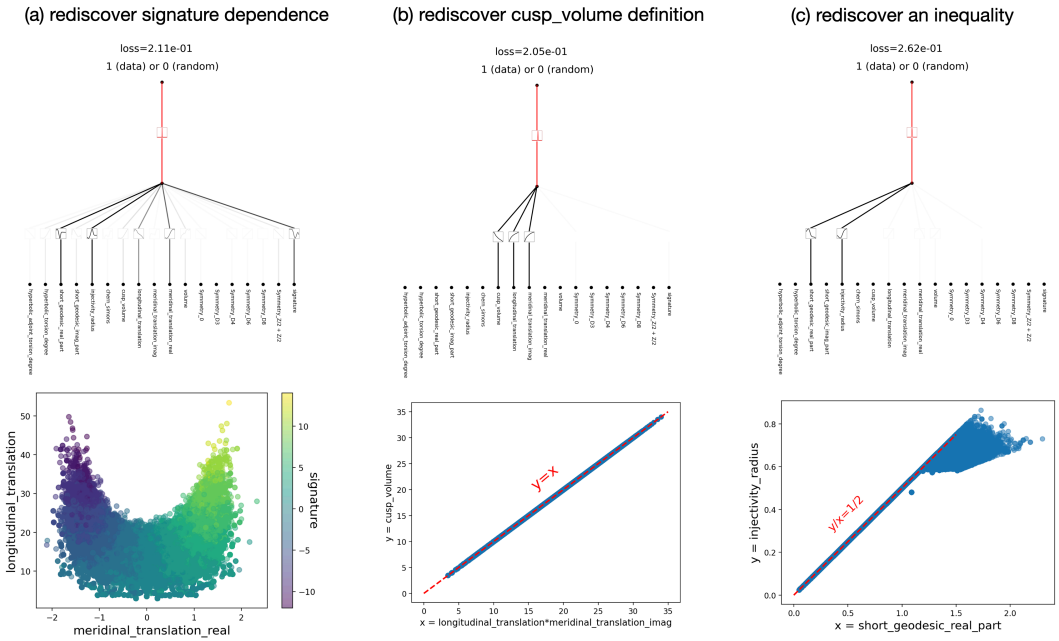
Case study (math): knot invariants (unsupervised)

Unsupervised discovery idea

- Goal: discover sparse relations among many invariants (not just predict one target).
- Train a sparse classifier KAN (shape $[18, 1, 1]$).
- Fix the last activation to a Gaussian peak at 0 $\Longrightarrow$ positives satisfy

$$\sum_{i=1}^{18} g_{i(x_i)} \approx 0$$

(read g_i off learned edges).
- Sweep seeds + λ and cluster multiple discovered relations.



Knot dataset (unsupervised): rediscovered relations. [Dav+21, Guk+23, Liu+25]

Case study (physics): mobility edges via KANs

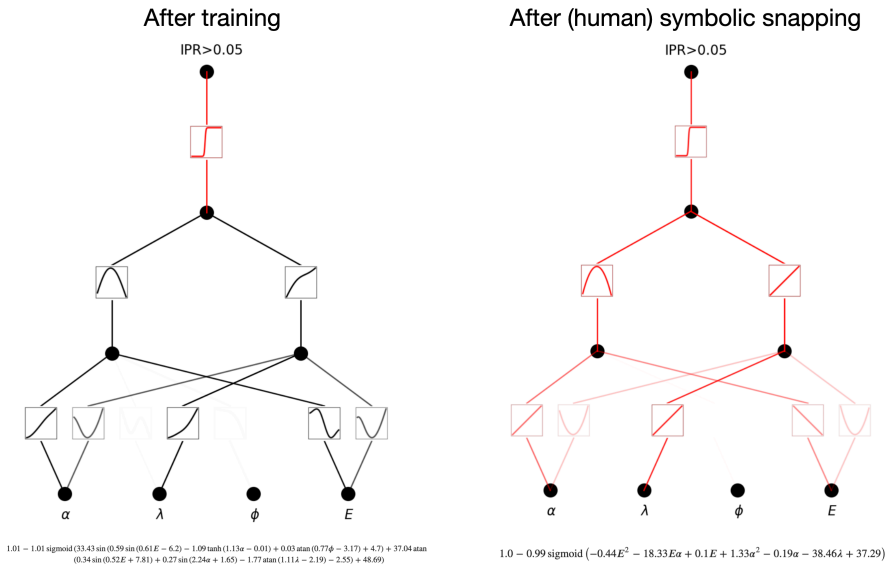
From data to an order parameter

- Goal: learn the mobility edge separating localized vs extended phases.
- Localization metric (eigenstate ψ^k):

$$\mathrm{IPR}_k = \frac{\sum_n |\psi_n^k|^4}{\left(\sum_n |\psi_n^k|^2\right)^2}$$

$$D_k = -\frac{\log(\mathrm{IPR}_k)}{\log(N)}$$

- Train → sparsify/prune → symbolify to recover a compact boundary $g(\cdot) = 0$ (human-in-the-loop: constrain the symbol library).



Mobility-edge discovery before/after symbolic snapping. [And58, Liu+25]

Symbolic regression: KANs vs classic SR

Why KANs help

- Continuous search in function space (gradients) before snapping to symbols.
- Debuggable intermediate artifacts: plots of $\varphi_{l,j,i}$.
- Works even when the target is not exactly symbolic (splines as fallback).

[Liu+25]

Related SR methods

- Genetic / heuristic: Eureqa [Dub11]
- Physics-inspired: AI Feynman [Udr+20, UT20]
- NN-based: EQL [ML16], OccamNet [Dug+20]
- Program search: PySR [Cra23]

[Liu+25]

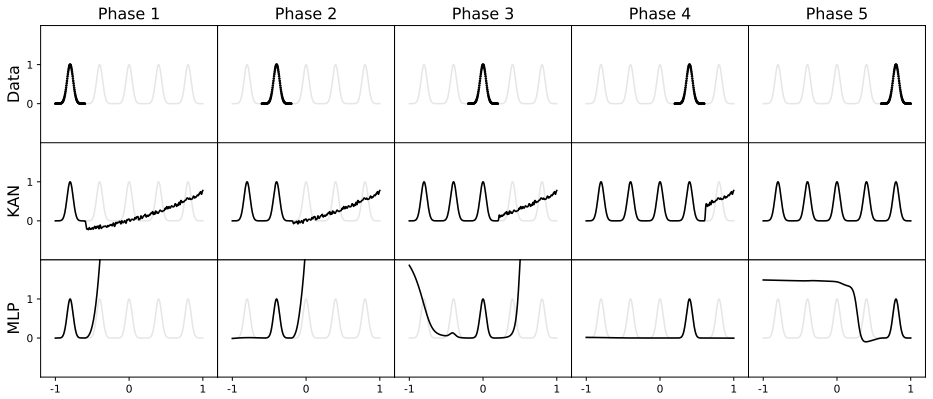
Continual learning and locality

Local plasticity

- B-spline activations are local in input space.
- Updates can be localized, reducing catastrophic forgetting.
- Promising for continual or lifelong learning regimes.

[Liu+25]

Connections: catastrophic forgetting; local adaptation; compute reuse in continual settings.



Continual learning experiments. [Liu+25]

Limitations and open questions

Practical limits

- Training is slower (poor batching; no optimized spline kernels). [Liu+25]
- Scaling claims are strongest on structured, low-data scientific tasks.
- Choosing minimal KAN shapes is still an open design problem.
- Can KANs replace MLP blocks in CNNs/Transformers without hardware regressions?

Connections: throughput vs parameter count; hardware efficiency vs expressivity.

Summary + discussion prompts

Takeaways

- KANs move nonlinearity to edges, learning 1D functions directly.
- Grid extension + spline parametrization yield strong accuracy/scaling.
- Sparsification enables symbolic interpretability (white-box ML).
- Trade-off: better accuracy/interpretability vs slower training.

Questions for the track

- Where would KANs beat MLPs (e.g., scientific regression, PDEs, transformer MLP blocks)?
- What hardware/software advances would make KANs practical?
- How should we evaluate interpretability vs performance for science?

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