KAN Tutorial Slides

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Kolmogorov-Arnold Representation Theorem

Let $\Omega \subset \mathbb{R}^d$ be a bounded domain and let $f : \Omega \to \mathbb{R}$ be a continuous function; i.e. $f \in C(\Omega)$. Then there exist continuous univariate functions

$$\Phi_q : \mathbb{R} \to \mathbb{R}, \quad q = 1, \ldots, 2d + 1;$$

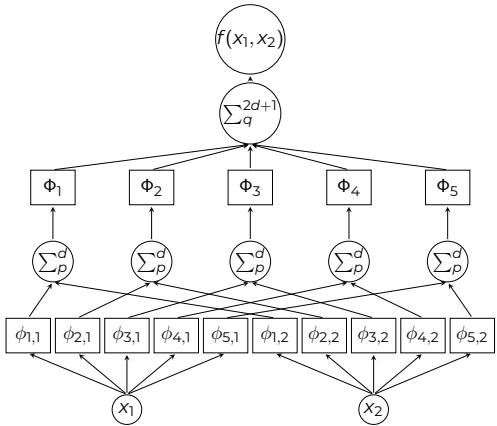
and continuous univariate functions

$$\phi_{pq} : \mathbb{R} \to \mathbb{R}, \quad p = 1, \ldots, d; \quad q = 1, \ldots, 2d + 1;$$

such that for every $\mathbf{x} = (x_1, \ldots, x_d) \in \Omega$,

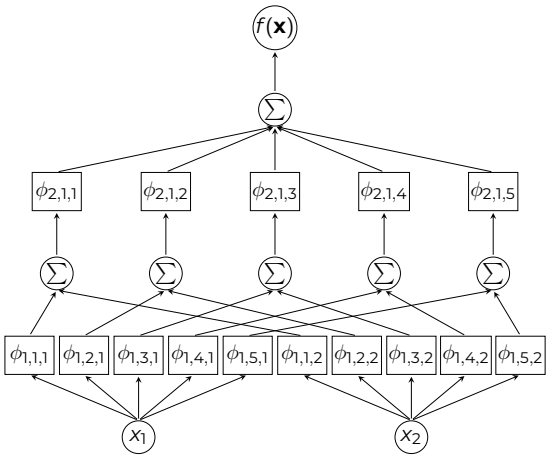
$$f(\mathbf{x}) = \sum_{q=1}^{2d+1} \Phi_q \left(\sum_{p=1}^{d} \phi_{pq}(x_p) \right).$$

Kolmogorov–Arnold Representation Theorem



The theorem states that any $f(x_1, x_2)$ can be written as a sum of univariate compositions.
The diagram shows this expression visually: each block represents a component of the decomposition.
Together, they form a **Kolmogorov–Arnold Network (KAN)**.

Kolmogorov–Arnold Networks

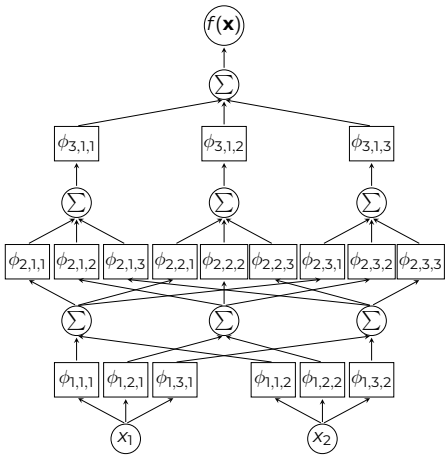


In a network setting, each univariate function is written as $\phi_{d,p,q}$, where:

- d: layer depth
- p: output node index
- q: input node index

This network is a **KAN [2,5,1]**: it has 2 inputs, one hidden layer with 5 nodes, and 1 output.

Kolmogorov–Arnold Networks



KAN [2,3,3,1]: 2 inputs, two hidden layers of 3, 1 output.

Why go deeper?

- **Theory:** Any continuous $f(\mathbf{x})$ admits a shallow KAN $[l,\ 2\,l+1,\ 1]$.
- **Practice:** Deeper KANs can model non-continuous functions. Depth improves expressivity.

B-Splines

$\phi_{d,p,q}$ can be chosen from any family of continuous univariate functions.
A common choice is the **B-spline** family.
A B-spline of k-order is defined as:

$$B_k(x) = \sum_{i=0}^{G+k-1} P_i N_{i,k}(x)$$

where G is the number of segments (grid size),
$N_{i,k}(x)$ are the basis functions of k-order (for a total of $G + k$),
and P_i are the control points coefficients (spline weights).

B-Splines - Basis Function

The basis functions follow the standard **Cox–de Boor recursive definition**:

$$N_{i,0}(x) = \begin{cases} 1, & t_{i-k} \leq x < t_{i-k+1}, \\ 0, & \text{otherwise} \end{cases}$$

$$N_{i,k}(x) = \frac{x - t_{i-k}}{t_i - t_{i-k}} N_{i,k-1}(x) + \frac{t_{i+1} - x}{t_{i+1} - t_{i-k+1}} N_{i,k-1}(x), \quad k > 0,$$

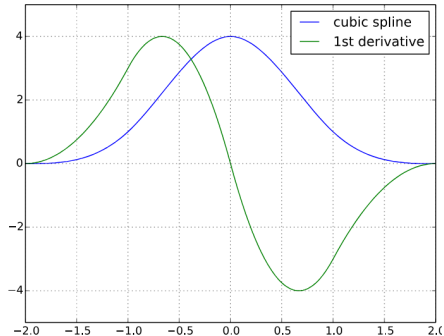
where **t** is the **knot vector**, a non-decreasing sequence of real numbers of length $(G + 2k + 1)$, being $\mathbf{t} = (t_{-k}, \ldots, t_0, \ldots, t_G, \ldots t_{G+k})$.

B-Splines - Knot Vector

Clamped knot vector $\mathbf{t}$ on $[a, b]$, with uniform knots:

$$t_{-k} = \cdots = t_0 = a,$$
$$t_G = \cdots = t_{G+k} = b,$$
$$t_j = a + \frac{j}{G}(b - a), \quad j = 0, \ldots, G$$

Ensures interpolation at the endpoints and smoothness (C^{k-1}) inside the interval.



$\mathbf{t} = (-2, -2, -2, -2, -1, 0, 1, 2, 2, 2, 2)$
$\mathbf{P} = (0, 0, 0, 6, 0, 0, 0)$

B-Splines as KAN Edges

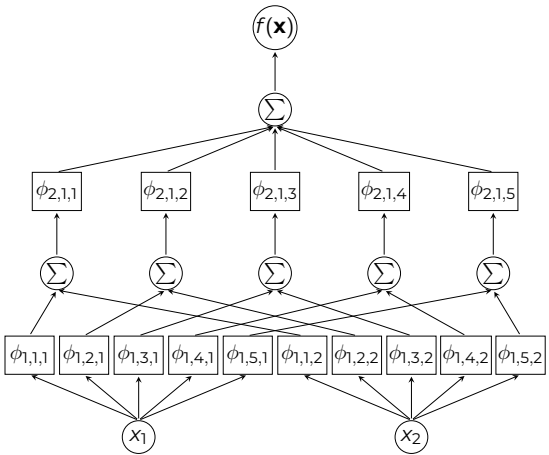
All univariate functions share the same spline degree k and number of control points n. Each $\phi_{d,p,q}$ combines a basis function (similar to residual connections) with a B-spline expansion:

$$\phi(x) = w_b\, b(x) + w_s \sum_{i=0}^{G+k-1} P_i\, N_{i,k}(x)$$

Here, w_b is the learnable weight of the basis function, w_s is the weight for the spline, and the control point coefficients P_i scale the individual B-spline functions directly. We choose the basis as:

$$b(x) = \mathrm{SiLU}(x) = \frac{x}{1 + e^{-x}}$$

KAN Parameters



Hyperparameters

- G: grid size (no. intervals).
- k: B-spline order.

Learnable parameters
(for each edge)

- P_i: control points, $i \in [0, G + k - 1]$.
- w_b: basis weight.
- w_s: spline weight.

KAN Backpropagation

Loss function is L2 (RMSE):

$$L = \|y - \hat{y}\|_2 = \left\| f(\mathbf{x}) - \hat{f}_d(\mathbf{x}) \right\|_2 = \left\| f(\mathbf{x}) - \sum_q \phi_{d,q}(\mathbf{x}) \right\|_2$$

Where d is the last layer, and $p = 1$ because we have a single output. The coefficients of that layer are $P_{d,q,i}$.

$$\frac{\partial L}{\partial P_{d,q,i}} = \frac{\partial L}{\partial \hat{f}_d(\mathbf{x})} \cdot \frac{\partial \hat{f}_d(\mathbf{x})}{\partial P_{d,q,i}}$$

And for the previous layer $d - 1$:

$$\frac{\partial L}{\partial P_{d-1,p,q,i}} = \frac{\partial L}{\partial \hat{f}_d(\mathbf{x})} \cdot \frac{\partial \hat{f}_d(\mathbf{x})}{\partial \hat{f}_{d-1,p}(\mathbf{x})} \cdot \frac{\partial \hat{f}_{d-1,p}(\mathbf{x})}{\partial P_{d-1,p,q,i}}$$

Capabilities of KANs with B-Splines

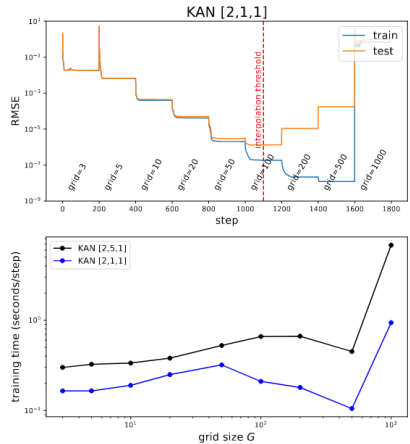
- **Grid extension**: progressively increase model capacity by refining the spline grid without retraining from scratch.
- **Continual learning**: local support ensures new information affects only nearby regions, reducing catastrophic forgetting.
- **Sparsity**: regularization and pruning remove redundant components, simplifying the model without major accuracy loss.
- **Symbolic regression**: univariate structure enables conversion of learned functions into interpretable closed-form expressions.

Capabilities - Grid Extension

Grid extension refines a trained KAN by adding more spline knots without restarting training.

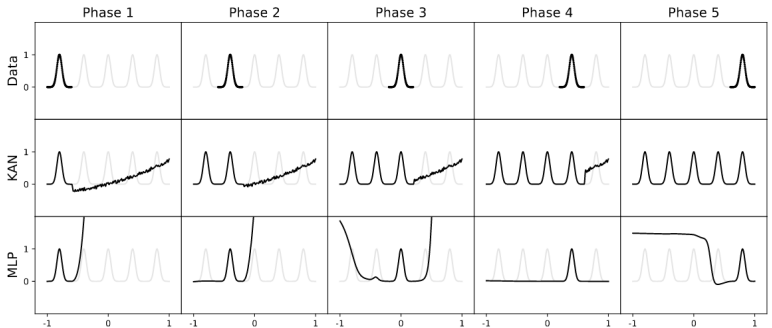
- Train on a coarse grid first.
- Add intervals to increase resolution and capacity (increase G)
- Initialize new coefficients (P_i) by least-squares fitting.
- Continue training to improve accuracy.

Test loss often improves until the parameter count roughly matches the number of data points.



Capabilities - Continual Learning

Because B-splines have **local support**, updates to $\phi(x)$ in one region of the input space affect only nearby points. This locality mitigates **catastrophic forgetting**, a common issue in MLPs where learning new data can overwrite previously acquired knowledge.

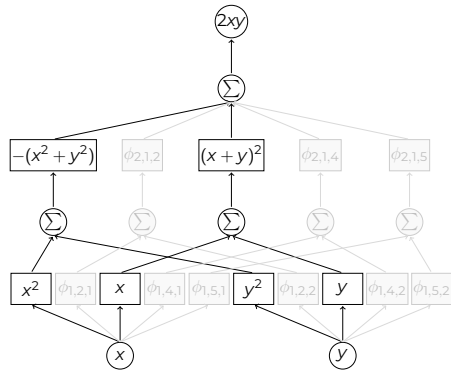


Capabilities - Sparsity

Sparsity removes unnecessary components, revealing the essential structure of our target function.

- **Regularization** drives many spline weights toward zero.
- Irrelevant edges can be pruned after training.
- The result is a compact, interpretable network.

Sparsity helps towards **interpretability**.



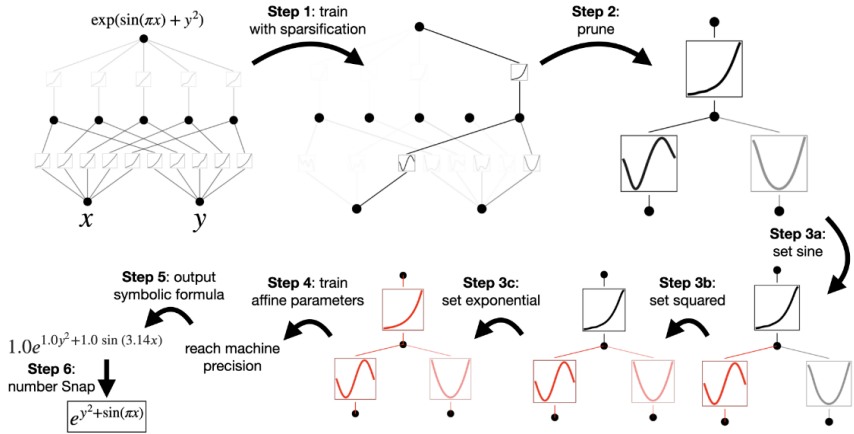
Capabilities - Symbolic Regression

KANs provide an interpretable path from neural models to closed-form expressions:

- Each learned $\phi(x)$ is a univariate function, which can often be approximated by simple analytic forms (e.g., $\sin$, $\exp$, $\log$).
- After training, these functions are “snapped” to symbolic templates via affine fitting, producing human-readable equations.
- The resulting network can be viewed as a composition graph of symbolic functions approximating $f(\mathbf{x})$.

This makes KANs suitable not only for prediction but also for **discovering interpretable laws** from data.

KAN Train Steps



Limitations of KANs

- **Parameter & memory blow-up.** For comparable width, KAN layers require substantially more parameters and activations than FC layers; memory scales poorly with I, O, B and grid/spline settings (G, k).
- **Convergence to sharp minima.** Hessian spectrum analyses show KANs tend to sharper minima $\Rightarrow$ weaker generalization (vision benchmarks).
- **Underperformance at scale.** On SciML (Neural ODEs), vision (Mixer/DeiT), and operator learning (FNO), KANs typically underperform MLPs despite higher cost.
- **Runtime/feasibility.** Longer training times and frequent OOM at moderate batch sizes on 16nB nPUs when scaling depth/width.

Limitations - Parameter Complexity

Fully Connected (FC) layer with O outputs and I inputs:

$$O \times (I + 1)$$

KAN layer (B-spline) with two shortcut weights, grid size G, k-order:

$$I \times O \times (2 + G + k)$$

Even “width-matched” KANs are often an order of magnitude larger than FC/MLP layers.

Limitations - Memory Footprint (Training)

Fully Connected (FC) layer accounting for both forward and reverse pass (one matrix each), and the coefficients (parameters):

$$O \times B + O \times B + O \times (I + 1)$$

KAN layer (B-spline)

$$I \times (1+G+k) \times B \; + \; I \times (G+k-1) \times B \; + \; I \times O \times (2+G+k)$$

KANs allocate extra tensors for B-spline evaluation and De Boor recursion.

Limitations - Convergence & Generalization

- Large-batch training tends to *sharp* minima (many large positive eigenvalues); *flat* minima correlate with better generalization.
- Empirically, KAN variants show Hessian spectra with **more positive eigenvalues** than MLP counterparts, *even at small batches*.
- **Effect:** test-time accuracy lags behind MLPs on vision tasks; e.g., DeiT on CIFAR-100 shows ∼8–12% lower Top-1 for B-spline KANs with **more** parameters.

Empirical Evidence Across Domains

Neural ODEs (SciML).

- On Lotka–Volterra, Pleiades, Spiral ODE, KAN-ODEs reach **higher final loss**; MLP-ODEs fit dynamics better.

Computer Vision.

- MLP-Mixer/Conv-Mixer/DeiT: KAN variants converge to **sharper minima** and **lower accuracy**; parameter counts are 2–3$\times$ higher for KANs at similar or worse accuracy.

Operator Learning (FNO).

- Replacing lift/projection MLPs with KANs yields **slightly worse** test loss without residuals; with residuals, small gains appear but at **prohibitive memory cost**.

References

- Liu, Ziming et al. (Feb. 2025). *KAN: Kolmogorov-Arnold Networks*. en. arXiv:2404.19756 [cs]. DOI: 10.48550/arXiv.2404.19756. URL: http://arxiv.org/abs/2404.19756 (visited on 09/19/2025).
- Pal, Avik and Dipankar Das (n.d.). "Understanding the Limitations of B-Spline KANs: Convergence Dynamics and Computational Efficiency". en. In: ().