Rec-KAN: Recursive KAN of KANs

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Recursive KAN: KAN of KANs

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Abstract
Schematically, the architecture of a Kolmogorov-Arnold neural network (KAN) has sum operations on nodes and learnable activation functions on edges. We introduce Rec-KAN, recursive KANs, by having learnable sparse KANs on edges. Rec-KANs are interpretable, parallelizable, enjoy compositional sparsity, and have sub-quadratic runtime.

Let KAN have shape $[n_0, n_1, \ldots, n_L]$

$$x_{l+1,j} \triangleq \sum_{i=1}^{n_l} \varphi_{l,j,i}(x_{l,i}), \quad \varphi_{l,j,i} : \mathbb{R} \to \mathbb{R} \quad \text{and}$$

$$l = 0, \ldots, L-1 \qquad i = 1, \ldots, n_l \qquad j = 1, \ldots, n_{l+1}$$

in matrix form:

$$x_{l+1} = \Phi_l \, x_l, \quad (n_{l+1} \times n_l) \; \Phi_l = [\varphi_{l,j,i}]$$

Schematically, the KAN architecture has sum operations on the nodes and learnable activation functions φ on the edges. We propose Rec-KAN, recursive KANs, by having learnable sparse KANs on edges.

$$\text{Rec-KAN}(x) = (\Phi_{L-1} \circ \ldots \circ \Phi_0)\, x$$

where $\Phi_l \triangleq \Psi_1^l + \ldots + \Psi_M^l$

with KAN layer $\Psi_k^l = [\psi_{k,j,i}^l]$, $\psi_{k,j,i}^l : \mathbb{R} \to \mathbb{R}$

$$i = 1, \ldots, n_l \qquad j = 1, \ldots, n_{l+1} \qquad k = 1, \ldots, M$$

Without loss of generality, let Rec-KAN have shape

$[n_0, N, \ldots, N, n_L]$ (otherwise let $N = \max\{n_1, \ldots, n_{L-1}\}$).

Note that the intermediate layers $l = 1, \ldots, L-2$

$\Phi_l = \Psi_1^l + \ldots + \Psi_M^l$ have MN^2 activation functions

to learn! To make Rec-KAN tractable we sparsify

the Φ_l by defining $\Psi_k^l = D(f_k^l)\, C(h_k^l)\, D(g_k^l)$

where $D(f)$ is a $N \times N$ diagonal matrix with diagonal

$f = (f_1, \ldots, f_N)$ and $C(h)$ is a $N \times N$ circulant matrix

with generator $h = (h_1, \ldots, h_N)$.

In terms of number of activation functions to learn:

- sparse Rec-KAN Φ_l has $M\,3N$
- Rec-KAN Φ_l has MN^2
- unstructured KAN Φ_l has N^2

If $N > 3$ and $N > 3M$ then sparse Rec-KAN Φ_L

have the fewest activation functions to learn.

Note that $\Phi_L = \Psi_1^L + \ldots + \Psi_M^L$ can be computed

in parallel and that $\Psi_K^L(x) = \left(D(f_K^L)\, C(h_K^L)\, D(g_K^L)\right) x$

can be computed using a Fast Fourier Transform.

Case by case, there is a tradeoff between accuracy

and runtime (sparsity) to be determined.

Sparse recursive KAN, $(\Phi_{L-1} \circ \ldots \circ \Phi_0)\, x$

with $\Phi_L = \sum_{K=1}^{M} D(f_K^L)\, C(h_K^L)\, D(g_K^L)$ are:

1) interpretable

2) parallelizable

3) compositionally sparse with sub-quadratic runtime.

Layers L, nodes N, and number of DCDs M

are hyperparameters to be chosen.

Random sparse KANs

A KAN layer, matrix Φ_l, can be made sparse by using structured matrices, like sums of DCD matrices.

We can prune further with random masking.

In a sparse recursive KAN, $\Phi = \Psi_1 + \ldots + \Psi_M$,

where Ψ has form $D(f)\,C(h)\,D(g)$

$$= \begin{bmatrix} f_1 & & 0 \\ & \ddots & \\ 0 & & f_N \end{bmatrix} \begin{bmatrix} h_1 & \cdots & h_{N-1} & h_N \\ h_N & h_1 & & h_{N-1} \\ \vdots & & \ddots & \vdots \\ h_2 & \cdots & h_N & h_1 \end{bmatrix} \begin{bmatrix} g_1 & & 0 \\ & \ddots & \\ 0 & & g_N \end{bmatrix}$$

$$= \begin{bmatrix} f_1 h_1 g_1 & f_1 h_2 g_2 & \cdots & f_1 h_{N-1} g_{N-1} & f_1 h_N g_N \\ f_2 h_N g_1 & f_2 h_1 g_2 & \cdots & f_2 h_{N-2} g_{N-1} & f_2 h_{N-1} g_N \\ \vdots & \vdots & & \vdots & \vdots \\ f_N h_2 g_1 & f_N h_3 g_2 & \cdots & f_N h_N g_{N-1} & f_N h_1 g_N \end{bmatrix}$$

with $f_i, h_i, g_i : \mathbb{R} \to \mathbb{R}$

Let $g_i = \sigma_i$, Rademacher variables,

ie $\Pr(\sigma_i = \mathbb{1}) = \frac{1}{2} = \Pr(\sigma_i = \mathbb{0})$

where $\mathbb{1} : \mathbb{R} \to \mathbb{R}$ and $\mathbb{0} : \mathbb{R} \to \mathbb{R}$

$x \mapsto 1$ $\qquad$ $x \mapsto 0$

and draw M independent samples of $g = (g_1, \ldots, g_N)$

Notice Φ_L, being a random sum of DCs, has

M2N activation functions to learn and is a

form of neural architecture search.

References

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