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Gary Nan Tie, August 25, 2024

Abstract

Kolmogorov-Arnold Networks (KAN) are concatenated layers of univariate function matrices. We introduce two structured DCD matrix forms to sparsify layers, and learn the univariate functions (e.g. B-splines or wavelets).

Sparse Kolmogorov-Arnold Networks

KAN architecture

The shape of a Kolmogorov-Arnold Network (KAN) is represented by an integer array:

$$[n_0, n_1, \dots, n_L]$$

where n_i is the number of nodes in the i^{th} layer of the computational graph. We denote the i^{th} neuron in the L^{th} layer by (L, i) , and the activation value of (L, i) neuron by $x_{L,i}$. Between layer L and layer $L+1$, there are $n_L n_{L+1}$ activation functions.

The activation function that connects (L, i)

and $(L+1, j)$ is denoted by $\varphi_{L,j,i}$,

$$L = 0, \dots, L-1, \quad i = 1, \dots, n_L, \quad j = 1, \dots, n_{L+1}$$

The pre-activation of $\varphi_{l,j,i}$ is $x_{l,i}$ and
 the post-activation of $\varphi_{l,j,i}$ is $\tilde{x}_{l,j,i} \triangleq \varphi_{l,j,i}(x_{l,i})$.

The activation value of the $(L+1, j)$ neuron is the
 sum of all incoming post-activations:

$$x_{L+1,j} \triangleq \sum_{i=1}^{n_L} \tilde{x}_{L,j,i} = \sum_{i=1}^{n_L} \varphi_{L,j,i}(x_{L,i}), \quad j=1, \dots, n_{L+1}$$

In matrix form, this reads

$$x_{L+1} = \Phi_L x_L \quad \text{where} \quad \Phi_L = [\varphi_{L,j,i}]$$

is the matrix of univariate functions corresponding
 to the L^{th} KAN layer. A general KAN network
 is a composition of L layers: given an input vector
 $x \in \mathbb{R}^{n_0}$, the output of KAN is

$$\text{KAN}(x) = (\Phi_{L-1} \circ \Phi_{L-2} \circ \dots \circ \Phi_1 \circ \Phi_0) x$$

Sparse structured Φ_l matrices

Let filter $h = (h_1, \dots, h_n)$ and circulant matrix

$$C(h) \triangleq \begin{bmatrix} h_1 & \cdot & \cdot & h_{n-1} & h_n \\ h_n & h_1 & & & h_{n-1} \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & & & \cdot & \cdot \\ h_2 & \cdot & \cdot & h_n & h_1 \end{bmatrix}$$

Let gate $g = (g_1, \dots, g_n)$ and diagonal matrix

$$D(g) \triangleq \begin{bmatrix} g_1 & & \bigcirc \\ & g_2 & \\ \bigcirc & & \cdot \\ & & & \cdot \\ & & & & g_n \end{bmatrix}$$

Two observations:

- (1) If matrix A has rank r , then A can be written as a sum of r rank-1 matrices. Now any rank-1 matrix is a DCD, so any matrix A of rank r is the sum of r DCD matrices.

(2) Observe that any Toeplitz matrix, often arising in signal processing, is the sum of a pair of DCDs, because any Toeplitz matrix can be decomposed into the sum of a circulant matrix C and a skew circulant matrix S ; now note both C and S are DCD matrices. Moreover, any matrix A can be written as a product of Toeplitz matrices. Hence any matrix A can be written as a concatenation of $(DCD + DCD)$ operators.

For these reasons, we are interested in DCD operators to sparsify Φ_L . We now propose two sparse structured matrix forms for the univariate function matrices Φ_L when $n_i = n \ \forall i$.

Unstructured Φ_L has n^2 functions to learn.

In the following, the filters h, r, s and gates f, g, p, q are B-splines or wavelets to be learned.

$$(1) \text{ TriAd } \Phi_L \triangleq \sum_{i=1}^N D(f^i) C(h^i) D(g^i)$$

has $N3n$ functions to learn

$$(2) \text{ Centipede } \Phi_L \triangleq T_N \dots T_2 T_1$$

$$\text{where } T_i = [D(p^i) C(r^i) D(q^i) + D(f^i) C(s^i) D(g^i)]$$

has $N6n$ functions to learn.

So if hyperparameter N is chosen so that $N \ll n$

then $N6n < n^2$ and Φ_L is relatively sparse.

□

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