Kolmogorov-Arnold Networks

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10 June 2024

Welcome to the inaugural Sim-Eval literature review!

I'm trying to keep this informal – teaching is the best way of learning, and we all benefit from sharing knowledge.

My background is in math, so expect a bit more of the underlying theory here!

Agenda:

What's a KAN (and what's an MLP)?

What can a KAN represent?

Why are KANs interesting?

Some bookkeeping notes:

For simplicity, assume that the functions we care about are *scalar-valued* and *of multiple variables*, i.e.

$$f\colon \mathbb{R}^n \longrightarrow \mathbb{R}$$

Parts of this are intentionally abstract, so as to not get into the weeds of technical examples. Expect a fair bit of hand-waving.

Primer: a gentle (re)introduction to the multi-layer perceptron

Canonically, a "shallow" multi-layer perceptron is *two layers*. (This will be important for the literature!) A multi-layer perceptron in the shallow case is represented as

$$f: \ \mathbb{R}^n \longrightarrow \mathbb{R}$$

$$\hat{f}(x) = \sum_{i}^{N(\varepsilon)} a_i \sigma \left[\mathbf{W}_i \mathbf{x} + b_i \right]$$

Note the width $N(\varepsilon)$ is a function of the precision ε.

$$\hat{f}(x) = \sum_i a_i \sigma \left[\mathbf{W}_i \mathbf{x} + b_i \right]$$

where:

b_i	is the bias *(affine!)*
$\mathbf{x}$	is the i th input vector
$\mathbf{W}_i$	is the i th weight matrix *(learned!)*
σ	is the activation function *(e.g. ReLU, sigmoid,* tanh...*)*
a_i	are elements of the outermost weight matrix

In the shallow case, a_i can be denoted by a row vector.

$$\hat{f}(x) = \sum_i^d a_i \sigma \left[\mathbf{W}_i \mathbf{x} + b_i \right]$$

(a)

fixed activation functions
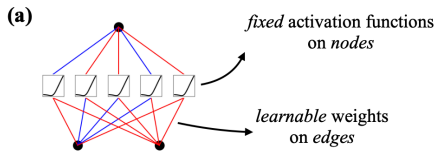on *nodes*

learnable weights
on *edges*

Figure: *A shallow 2-layer multi-layer perceptron.* $d = 2$, $n = 2$.

Interesting side note: more generally, for arbitrarily deep networks, a *multi-layer* perceptron is really just a composition of (affine!) linear transformations separated by non-linear activations.

$$MLP(\mathbf{x}) = [\mathbf{W}_d \circ \sigma_d \circ \mathbf{W}_{d-1} \circ \sigma_{d-1} \circ \ldots \mathbf{W}_1 \circ \sigma_1 \circ] (\mathbf{x})$$
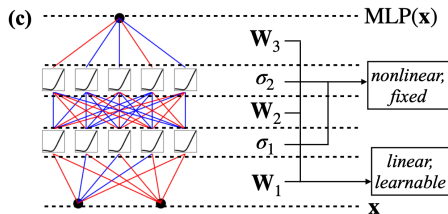

Figure: *A deep multi-layer perceptron.*

$$\hat{f}(x) = \sum_{i}^{N(\varepsilon)} a_i \sigma \left[\mathbf{W}_i \mathbf{x} + b_i \right]$$

Question: What can a multi-layer perceptron represent?
Answer Anything!*

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Answer Anything![*]

Let $D \subset \mathbb{R}^n$ be compact[1]. $f \colon D \longrightarrow \mathbb{R}$ be an *arbitrary nonlinear function*, and let $\hat{f} \colon D \longrightarrow \mathbb{R}$ denote a shallow (*n.b.* 2-layer) multi-layer perceptron, denoted by

$$\hat{f}(x) = \sum_{i}^{N(\varepsilon)} a_i \sigma \left[\mathbf{W}_i \mathbf{x} + b_i \right]$$

where $N(\varepsilon)$ is the *number of neurons.* In the shallow case this is = the width.

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[1] Compact denotes some notion of "closed and bounded" – the n-dimensional equivalent of a closed interval $[a, b] \subset \mathbb{R}$.

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Theorem
Universal approximation (2-layer network). *For arbitrary $\varepsilon \in \mathbb{R} > 0$, there exists $N(\varepsilon)$ such that*

$$|f(x) - \hat{f}(x)| \leq \varepsilon$$

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So we can model basically anything! But...

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The million-dollar question:

What is $N(\varepsilon)$?

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We don't know, in general! The universal approximation theorem guarantees no bounds on N. For deep networks, we do know that it's possibly poorly behaved ($N \propto \exp(d)$, the layer depth of the network).

Why does this make sense? Because we are fitting a "mostly linear" model to an "arbitrary non-linear" function. We need "a lot of linear pieces" to get good at modeling funky nonlinear functions.
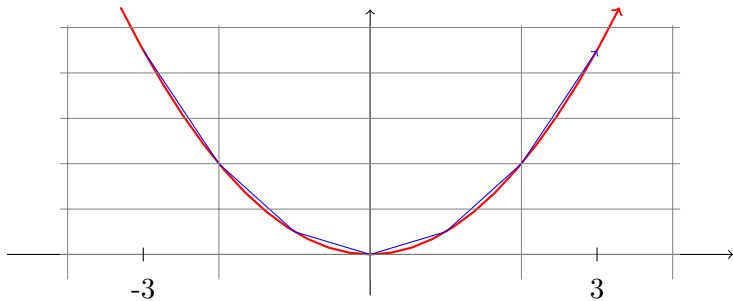

Figure: *It takes a lot of line segments to approximate this quadratic, and as soon as we leave $[-3, 3]$, the error in our approximation blows up!*

Enter the notion of *neural scaling laws*.