Lecture 12: DNN Approximation - KST

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2022 Summer Mini Course Tianyuan Mathematical Center in Central China Topic 3: Results by Kolmogorov-Arnold Representtion Theory

Kolmogorov-Arnold representation theorem (KST):

Theorem

 $\forall f(\mathbf{x}) \in C^0([0,1]^d)$, $\exists \psi_p(x)$ and $\phi(x)$ defined on $\mathbb R$ such that

$$f(\mathbf{x}) = \sum_{q=1}^{2d+1} a_q \phi(\sum_{p=1}^d b_{pq} \psi_p(x_p)).$$

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But $\psi_p(x)$ and $\phi(x)$ are pathological.

- What if we use DNN to approximate $\psi_p(x)$ and $\phi(x)$?
- $\psi_p(x)$ and $\phi(x)$ might be exponentially bad in d.

Key ideas

- J. Braun, M. Griebel, On a constructive proof of Kolmogorov's superposition theorem, Constr. Approx. 30 (2009) 653-675.
- Montanelli, Y., Error bounds for deep ReLU networks using the Kolmogorov-Arnoldsuperposition theorem, Neural Networks, 2020.
 - · Apply ReLU in the constructive proof.
 - Check the moduli of continuity of inner and outer functions.

Observation: Hölder continuity of the inner function with constants $(\nu, \alpha) = (O(\log d), \frac{1}{O(\log d)})$.

Theorem (Approximation of the inner function)

Let $d \ge 2$ and ψ be the inner function in KST. $\forall \epsilon \in (0,1)$, there is a ReLU DNN $\widetilde{\psi}$ that has a size

$$W \leq c_1(d)\epsilon^{-[1+\log_2(d+1)]/2} \ll O(\epsilon^{-d}),$$

such that $\|\psi - \widetilde{\psi}\|_{L^{\infty}} \le \epsilon$, with a constant $c_1(d)$.

Observation:

$$\phi_j^r(x) = \frac{1}{m+1} \sum_{\ell=1}^r \sum_{\mathbf{d} \in (D_\ell)^d} e_{\ell-1}(\mathbf{d}) \mathcal{NN} \left(\mathbf{d} + jO(d^{-2}); x \right),$$

Theorem (Approximation of the outer functions)

Let $f:[0,1]^d\to\mathbb{R}$ be a continuous function, and ϕ_j^r be the (2d+1) outer functions in KST at iteration $r.\ \forall \epsilon\in(0,1)$, there are ReLU DNNs $\widetilde{\phi}_j^r$ that have a size

$$W \leq c_2(d,f)\epsilon^{-1/2},$$

such that $\|\phi_j^r - \widetilde{\phi}_j^r\|_{L^{\infty}} \le \epsilon$, with a constant $c_2(d, f)$.

Theorem (Approximation of continuous functions using KST)

Let $f: [0,1]^d \to \mathbb{R}$ be a continuous function. Then, for any scalar $0 < \epsilon < 1$, there is a ReLU DNN \widetilde{f}_r that has a size $W < (2d^2 + d) \circ (d f) e^{-1+\log_2(d+1)}/2 + (2d+1) \circ (d f) e^{-1/2}$

$$W \leq (2d^2 + d)c_3(d, f)\epsilon^{-1 + \log_2(d+1)]/2} + (2d + 1)c_4(d, f)\epsilon^{-1/2},$$

such that $\|f - \widetilde{f}_r\|_{L^{\infty}([0,1]^d)} \le \epsilon$ with $c_3(d,f)$ and $c_4(d,f)$ as constants. Remark: unspecified constants may results in the curse of dimensionality.

Elementary universal activation function (EUAF)

A continuous activation function without gradient vanishing

$$\sigma_1(x) = |x - 2\lfloor \frac{x+1}{2} \rfloor|,$$

$$\sigma_2(x) := \frac{x}{|x|+1},$$

$$\sigma(x) := \left\{ \begin{array}{ll} \sigma_1(x) & \text{for } x \in [0, \infty), \\ \sigma_2(x) & \text{for } x \in (-\infty, 0). \end{array} \right.$$

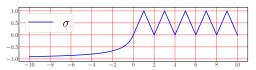


Figure: An illustration of σ on [-10, 10].

Theorem (EUAF approximation in d-dimensions)

Arbitrarily small error with a fixed number of neurons for $C([0,1]^d)$.

■ For any $\epsilon > 0$, there exists ϕ of width 36d(2d + 1) and depth 11 s.t.

$$||f(x) - \phi(x)||_{L^{\infty}([0,1]^d)} \le \epsilon$$

Shen, Y., and Zhang (arXiv:2107.02397)

Theorem (EUAF representation in *d*-dimensions)

Exact representation with a fixed number of neurons for classification functions.

■ For any classification function f(x) with K classes, there exists ϕ of width 36d(2d + 1) and depth 12 s.t.

$$f(x) = \phi(x)$$

on the supports of each class.

■ Shen, Y., and Zhang (arXiv:2107.02397)





Two main ideas

■ Theorem (Kolmogorov-Arnold Superposition Theorem) $\forall f(\mathbf{x}) \in C([0,1]^d)$, there exist $\psi_p(x)$ and $\phi(x)$ in $C(\mathbb{R})$ and $b_{pq} \in \mathbb{R}$ s.t.

$$f(\mathbf{x}) = \sum_{q=1}^{2d+1} a_q \phi(\sum_{p=1}^d b_{pq} \psi_p(x_p)).$$

■ Lemma (EUAF approximation in 1D (Shen, Y., and Zhang (arXiv:2107.02397))

NNs with width 36 and depth 5 constructed with EUAF is dense in C([0,1]).

EUAF is more powerful than bit extraction.

Lemma (Curve filling in K-dimensions (Shen, Y., and Zhang (arXiv:2107.02397))

For any $K \in \mathbb{N}^+$, the following point set

$$\left\{\left[\sigma_1(\tfrac{w}{\pi+1}),\ \sigma_1(\tfrac{w}{\pi+2}),\ \cdots,\ \sigma_1(\tfrac{w}{\pi+K})\right]^T\ :\ \textbf{\textit{w}}\in\mathbb{R}\right\}\subseteq[0,1]^K$$

is dense in $[0,1]^K$, where π is the ratio of the circumference of a circle to its diameter.

Proof.

Ideas:

- \blacksquare Transcendental number + distinct rational numbers \rightarrow rationally independent numbers
- \blacksquare Rationally independent numbers + periodic functions \rightarrow dense set in $[0,1]^{\it K}$

For arbitrary K, NN with width 1 and depth 2 constructed with EAUF can fit K points up to arbitrary accuracy.

Other EUAF

- C^s EUAF
- Sigmod EUAF

Topic 4: Low-Dimensional Structure

Low-Dimensional Structure

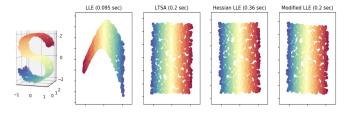


Figure: "Nearly" isometric maps.

Low-Dimensional Structure

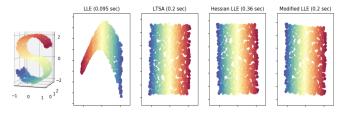


Figure: "Nearly" isometric maps.

Theorem (Theorem 3.1 of Baraniuk et al 2009)

Let \mathcal{M} be a compact $d_{\mathcal{M}}$ -dimensional Riemannian submanifold of \mathbb{R}^d . Fix $\delta \in (0,1)$ and $\gamma \in (0,1)$. Let $\mathbf{A} = \sqrt{\frac{d}{d_\delta}} \Phi$, where $\Phi \in \mathbb{R}^{d_\delta \times d}$ is a random orthoprojector with

$$extbf{ extit{d}}_\delta = \mathcal{O}\left(rac{d_\mathcal{M} \ln(d\delta^{-1}) \ln(1/\gamma)}{\delta^2}
ight).$$

If $d_{\delta} \leq d$, then with probability at least $1 - \gamma$, the following statement holds: For every $\mathbf{x}_1, \mathbf{x}_2 \in \mathcal{M}$,

$$(1-\delta)|x_1-x_2| \leq |Ax_1-Ax_2| \leq (1+\delta)|x_1-x_2|.$$



Continuous functions

Idea: data in $\mathbb{R}^d \xrightarrow{\text{random} \\ \text{projection}}$ data in $\mathbb{R}^{d_\delta} \xrightarrow{\text{neural} \\ \text{network}}$ function values

Theorem (Shen, Y., Zhang, CiCP, 2020)

 \mathcal{M} is a $d_{\mathcal{M}}$ -manifold in $[0,1]^d$. For any $L,N\in\mathbb{N}^+$, let $f:\mathcal{M}_\epsilon\to\mathbb{R}$ be a Lip. cont. function with constant 1, $p\in[1,\infty)$, then there exists $\phi\in\mathcal{NN}$ (#input = 1; maxwidth \leq max $\{8d_\delta\lfloor N^{1/d_\delta}\rfloor+4d_\delta,\ 12N+14\}$; #layer $\leq 9L+12$) such that $\|f-\phi\|_{L^p([0,1]^d,\mu_\varrho)}\leq 3\frac{4\epsilon}{1-\delta}\sqrt{\frac{d}{d_\delta}}+5\frac{16d}{(1-\delta)\sqrt{d_\delta}}N^{-2/d_\delta}L^{-2/d_\delta}.$