Mathematics of Deep Learning, Summer Term 2020 Week 4

## Kolmogorov–Arnold Representation

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# Overview of Week 4

## Hilbert's 13th Problem

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- 3 Approximate Hashing for Specific Functions
- 4 Approximate Hashing for Generic Functions
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- 6 Approximation by Networks of Bounded Size

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#### Sources for this lecture:

- Arnold (1958): On the representation of functions of several variables
- Torbjörn Hedberg: The Kolmogorov Superposition Theorem. In Shapiro (1971): Topics in Approximation Theory
- Philipp Christian Petersen (Faculty of Mathematics, University of Vienna): Course on Neural Network Theory.

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Hilbert's 13th Problem

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### Hilbert's 13th problem

Can the roots of the equation

$$x^7 + ax^3 + bx^2 + cx + 1 = 0$$

be represented as superpositions of continuous functions of two variables?

### Remark:

- This is the general form of a septic equation after some algebraic transformations. The roots are functions of (a, b, c).
- A single superposition is w(u(a, b), v(b, c)), and a double superposition is w(u(p(a, b), q(b, c)), v(r(b, c), s(c, a))).
- More generally, the question becomes: Do functions of three variables exist at all, or can they be represented as superpositions of functions of less than three variables?

Conjecture: Hilbert conjectured that such reductions to smaller numbers of variables are impossible. The strongest supporting evidence is:

### Theorem (Vitushkin 1955)

There is a polynomial such that neither the polynomial itself nor any function sufficiently close to it (in the sense of uniform convergence) can be decomposed into a simple superposition of continuous functions of two variables in any region or in any system of coordinates. Remark: Kolmogorov interpreted Hilbert's problem using dimension theory:

- Let  $N(\epsilon)$  be the smallest number of  $\epsilon\text{-balls}$  needed to cover a metric space X.
- On  $X = [0,1]^n$  one has  $\dim(X) := \liminf_{\epsilon \to 0} \frac{-\log N(\epsilon)}{\log \epsilon} = n$ .
- On  $X = C^{s}([0,1]^{n})$  one has  $\dim(X) := \liminf_{\epsilon \to 0} \frac{-\log \log N(\epsilon)}{\log \epsilon} = n/s.$
- In this sense, Hölder functions of 3 variables are strictly richer than Hölder functions of 2 variables.
- However, as we will see, this argument does not generalize to continuous functions.

### Theorem (Kolmogorov 1956)

Any continuous function f of  $n \in \mathbb{N}$  variables can be represented as a finite number of superpositions of functions of 3 variables. For instance, for n = 4 one has

$$f(x_1, x_2, x_3, x_4) = \sum_{i=1}^{4} g^i (u(x_1, x_2, x_3), v(x_1, x_2, x_3), x_4)$$

for some continuous functions  $g^i, u, v \colon \mathbb{R}^3 \to \mathbb{R}$ .

# Sketch of Proof: Reduction to three variables

### Sketch of Proof:

• The level sets (aka. contour lines) of a continuous function form a tree (Kronrod, Menger):



Figure: Figure from Arnold (1956)

Sketch of Proof: Reduction to three variables (cont.)

 Any continuous function of n variables can be written as a sum of n+1 continuous functions with standard trees, i.e., trees which do not depend on the given function (Kolmogorov):

$$f(x_1, \dots, x_n) = \sum_{i=1}^{n+1} f^i(x_1, \dots, x_n).$$

 Each of function f<sub>i</sub> can be written as a one-parameter family of functions of n - 1 variables:

$$f(x_1, \dots, x_n) = \sum_{i=1}^{n+1} f_{x_n}^i(x_1, \dots, x_{n-1})$$

# Sketch of Proof: Reduction to three variables (cont.)

• Each of the functions  $f_{x_n}^i$  factors through a function on the corresponding standard tree:

$$f(x_1, \dots, x_n) = \sum_{i=1}^{n+1} g_{x_n}^i(\ell^i(x_1, \dots, x_{n-1})).$$



Figure: Figure from Arnold (1956)

# Sketch of Proof: Reduction to three variables (cont.)

• Embedding the trees in a plane with a two-dimensional coordinate system (u, v) transforms this into:

$$f(x_1,\ldots,x_n) = \sum_{i=1}^{n+1} g_{x_n}^i (u^i(x_1,\ldots,x_{n-1}), v^i(x_1,\ldots,x_{n-1})).$$

• This yields 3-variate functions  $g_i$  and (n-1)-variate functions  $u^i, v^i$ :

$$f(x_1,\ldots,x_n) = \sum_{i=1}^{n+1} g^i (u^i(x_1,\ldots,x_{n-1}), v^i(x_1,\ldots,x_{n-1}), x_n).$$

 Applying this construction iteratively to u<sup>i</sup> and v<sup>i</sup> yields the reduction to superpositions of functions of 3 variables.

- Repetition: State Hilbert's 13th problem and describe how Kolmogorov cast it in the frameworks of dimension and graph theory.
- Check: What happens to Hilbert's problem when continuous functions are replaced by measurable or arbitrary functions?
- Background: Find out about generalizations, limitations, and open problems related to Hilbert's thirteenth problem.

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Kolmogorov–Arnold Representation

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# Kolmogorov-Arnold Representation

## Theorem (Kolmogorov-Arnold 1956-1957)

For every  $n \in \mathbb{N}_{\geq 2}$ , there exist  $\varphi_{i,j} \in C([0,1])$  such that any  $f \in C([0,1]^n)$  can be represented as

$$f(x_1,\ldots,x_n) = \sum_{i=1}^{2n+1} g_i\left(\sum_{j=1}^n \varphi_{i,j}(x_j)\right),$$

for some  $g_i \in C(\mathbb{R})$ .

#### Remark:

- This disproves Hilbert's conjecture and shows that "the only" multivariate function is a sum.
- The inner functions  $\varphi_{i,j}$  are universal, i.e., they do not depend on f.
- The outer functions  $g_i$  can be learned by linear regression.

## Theorem (Sprecher 1965, Köppen 2002)

For every  $n \in \mathbb{N}_{\geq 2}$ , there exists a continuous function  $\varphi : \mathbb{R} \to \mathbb{R}$  and constants  $a, \lambda_j \in \mathbb{R}$  such that any  $f \in C([0,1]^n)$  can be represented as

$$f(x_1,\ldots,x_n) = \sum_{i=1}^{2n+1} g_i\left(\sum_{j=1}^n \lambda_j \varphi(x_j+ia)\right),\,$$

for some  $g_i \in C(\mathbb{R})$ .

#### Remark:

- The function  $\varphi$  and the constants  $\lambda_j$  and a can be constructed explicitly and are universal, i.e., independent of f.
- Sprecher's representation can be interpreted as a neural network.
- There are many further versions of the Kolmogorov–Arnold theorem with varying regularity and structural assumptions.

## Sprecher's Refinement: Universal Inner Function



Figure: Sprecher's universal inner functions  $\varphi$  (left) and  $\psi_1$  (right), where  $\psi_i(x_1, x_2) := \lambda_1 \varphi(x_1 + ia) + \lambda_2 \varphi(x_2 + ia)$  for some constants  $\lambda_1, \lambda_2, a$ . [Leni Fougerolle Truchetet 2008]

### Remark:

• The inner functions in the Kolmogorov–Arnold representation theorem can be interpreted as hash functions.

Background:

- Hash functions are widely used in computer science for array indexing operations.
- They map high-dimensional/unstructured/variable-length data to scalar hash values.
- Hash functions should be fast to compute and should be "nearly" injective, i.e., minimize duplication of output values.

# Hashing and Kolmogorov-Arnold Representation

#### Lemma

For each  $i \in \{1, \dots, 2n+1\}$ , Sprecher's inner function

$$\psi_i \colon [0,1]^n \ni (x_1,\ldots,x_n) \mapsto \sum_{j=1}^n \lambda_j \varphi(x_j+ia) \in \mathbb{R}$$

is injective on a countable dense subset  $D \subseteq [0,1]^n$ .

#### Remark:

- It is sufficient to establish injectivity of  $\psi(x) := \sum_j \lambda_j \varphi(x_j)$  on D.
- This follows from the following two facts:  $\phi$  takes rational values on D, and the coefficients  $\lambda_j$  are independent over the rational numbers.
- Of course,  $\psi$  is not injective everywhere; otherwise the Kolmogorov–Arnold theorem would be trivial.

# Space-filling curves

- Intuitively, the inverse of a hash function  $[0,1]^n \rightarrow [0,1]$  is a space-filling curve, i.e., a surjective continuous map  $[0,1] \rightarrow [0,1]^n$ .
- For Sprecher's hash function, this is made precise as follows: By carefully examining the properties of ψ, one may construct an "inverse" map λ : [0, 1] → [0, 1]<sup>n</sup> with the following properties:

#### Lemma

• The map  $\lambda : [0,1] \rightarrow [0,1]^n$  is a space-filling curve.

2 Its image may be approximated by discrete curves  $\Lambda_k$  as  $k \to \infty$ .

#### Remark:

• By the Hahn–Mazurkiewicz theorem, a non-empty Hausdorff topological space is a continuous image of the unit interval if and only if it is compact, connected, locally connected, and second-countable.

# Space-filling curves



# Questions to Answer for Yourself / Discuss with Friends

- Repetition: Recall and compare the presented versions of the Kolmogorov–Arnold Theorem.
- Check: Why exactly does the Kolmogorov-Arnold representation theorem disprove Hilbert's conjecture?
- Check: Show that there is no continuous bijection  $[0,1]^n \rightarrow [0,1]$  for any  $n \geq 2$ .
- Discussion: How would you implement Sprecher's theorem using neural networks? Do you think this could work well for supervised learning?

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## Approximate Hashing for Specific Functions

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#### Lemma

There exists a linear map  $\ell \colon \mathbb{R}^n \to \mathbb{R}$  whose restriction to rational numbers is injective.

#### Proof:

- n = 2: Set  $\ell(x, y) = x + \lambda y$  for any irrational number  $\lambda$ .
- $n \geq 2$ : Set  $\ell(x_1, \ldots, x_n) := \lambda_1 x_1 + \cdots + \lambda_n x_n$ , where  $\lambda_i$  are independent over  $\mathbb{Q}$ , e.g.  $\lambda_i = \pi^{i-1}$  or some other powers of any transcendental number.

#### Remark:

- Thus, any  $f: \mathbb{Q}^n \to \mathbb{R}$  can be written as  $f = g \circ \ell$ , where  $\ell$  is the above linear hashing function. However, g cannot be chosen continuously, and the approximation error cannot be controlled on non-rational numbers—a more elaborate construction is needed.
- We fix an irrational number  $\lambda \in \mathbb{R} \setminus \mathbb{Q}$  throughout this section.

#### Remark:

- The key step in the proof of the Kolmogorov-Arnold theorem is the construction of approximate hashing functions.
- This is done here for a given specific function and in the next section for generic functions.
- We restrict ourselves to bivariate functions.

### Definition (Approximate hashing functions, specific f)

A function  $\varphi \in C([0,1],\mathbb{R}^5)$  is called approximate hashing function for  $f \in C([0,1]^2)$  if there exists  $g \in C(\mathbb{R})$  such that

$$\sup_{t \in \mathbb{R}} |g(t)| \le 1/7, \quad \sup_{x,y \in [0,1]} \left| f(x,y) - \sum_{i=1}^{5} g(\varphi_i(x) + \lambda \varphi_i(y)) \right| < 7/8.$$

#### Lemma

For any  $f \in C^2([0,1]^2)$  with  $||f||_{\infty} \leq 1$ , the set of approximate hashing functions for f is open and dense in  $C([0,1], \mathbb{R}^5)$ .

#### Proof:

- The set is open, since if g works for a particular  $\varphi$ , it does so for every nearby  $\varphi$ .
- It remains to show that the set is dense in  $C([0,1],\mathbb{R}^5)$ .
- Thus, given  $\epsilon > 0$  and  $\chi \in C([0,1], \mathbb{R}^5)$ , we have to find an approximate hashing function  $\varphi$  for f such that  $\|\varphi \chi\| \leq \epsilon$ .

# Proof: Approximate Hashing for a Specific Function

- Divide [0,1] into  $N \in \mathbb{N}$  intervals, cut out the *i*-th fifth of each interval, and color all remaining intervals red.
- Approximate  $\chi_i$  (gray) by functions  $\varphi_i$  (blue), which are constant on red intervals of type *i*.



- It can be arranged that each function  $\varphi_i$  assumes distinct rational numbers on each of the red intervals, and that these numbers are distinct for different *i*.
- Moreover, for sufficiently large  $N, \|\varphi \chi\| \leq \epsilon,$  as desired.
- $\bullet\,$  Furthermore, by the uniform continuity of f on  $[0,1]^2,$  we can make N even larger to get

$$|f(x,y) - f(x',y')| \le 1/7$$
 whenever  $\max\{|x - x'|, |y - y'|\} \le 4/N.$ 

# Proof: Approximate Hashing for a Specific Function

- The function ψ<sub>i</sub>(x, y) := φ<sub>i</sub>(x) + λφ<sub>i</sub>(y) is constant on red rectangles of type i, which are defined as products of red intervals of type i.
- The irrational numbers, which the functions ψ<sub>i</sub> assume on rectangles of type i, are all distinct for different rectangles and/or different i.
- Thus, there is  $g \in C(\mathbb{R})$  such that  $g(\psi_i(x, y)) = \pm 1/7$  if (x, y) belongs to a red rectangle of type i where  $f \ge 0$ .
- Without loss of generality,  $\|g\| \le 1/7$ .
- Intuitively, g tracks the sign of f on each rectangle.

## Proof: Approximate Hashing for a Specific Function

• For any point (x, y), consider the approximation error

$$\left| f(x,y) - \sum_{i=1}^{5} g(\psi_i(x,y)) \right|.$$
 (\*)

- If  $f(x,y) \ge 1/7$ , then  $f \ge 0$  on each red rectangle containing (x,y).
- There are at least 3 such rectangles because out of 5 types, one may fail on the *x*-axis and another one on the *y*-axis.
- Thus, the majority of the summands in (\*) tracks the sign of *f* correctly, and the approximation error is bounded by 6/7.
- If  $|f(x,y)| \le 1/7$ , the approximation error is again bounded by 6/7, regardless of correct or incorrect tracking.
- As 6/7 < 7/8, we have shown that  $\varphi$  is an approximate hashing function, which is  $\epsilon$ -close to  $\chi$ .

- Repetition: Recall the definition of and main result on approximate hashing.
- Background: Refresh your memory of algebraic closures and the definition of algebraic and transcendental numbers, if necessary.
- Check: Draw the red rectangles of types 1 to 5 and verify that each point is contained in at least three rectangles.
- Check: What is the role of the numbers 5 and 1/7 in the lemma? Can they be altered?

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## Approximate Hashing for Generic Functions

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# Approximate Hashing for Generic Functions

### Remark:

• As before, we fix an irrational number  $\lambda \in \mathbb{R} \setminus \mathbb{Q}$ .

### Definition (Approximate hashing functions)

A function  $\varphi \in C([0,1],\mathbb{R}^5)$  is called approximate hashing function if for any  $f \in C([0,1]^2)$ , there exists  $g \in C(\mathbb{R})$  such that

$$\|g\|_{\infty} \leq \frac{1}{7} \|f\|_{\infty}, \qquad \left\|f - \sum_{i=1}^{5} g \circ \psi_{i}\right\|_{\infty} \leq \frac{8}{9} \|f\|_{\infty},$$

where  $\psi_i(x, y) = \varphi_i(x) + \lambda \varphi_i(y)$ .

#### Remark:

• Compared to hashing for specific functions *f*, this definition imposes the hashing property simultaneously for all *f* and with a slightly worse error bound.

# Approximate Hashing for Generic Functions

#### Lemma

The set of approximate hashing functions is dense in  $C([0,1], \mathbb{R}^5)$ .

Proof:

- Let U<sub>k</sub> be the sets of approximate hashing functions of f<sub>k</sub>, for some dense sequence (f<sub>k</sub>)<sub>k∈ℕ</sub> in the unit sphere of C([0, 1]<sup>2</sup>).
- The sets  $U_k$  are open and dense. By Baire's category theorem, its intersection U is dense.
- Any function  $\varphi \in U$  is an approximate hashing function: for any f with  $\|f\|_{\infty} \leq 1$ , there exists  $f_k$  and g such that

$$\left\| f - \sum_{i} g \circ \psi_{i} \right\|_{\infty} \leq \| f - f_{k} \|_{\infty} + \left\| f_{k} - \sum_{i} g \circ \psi_{i} \right\|_{\infty}$$
$$\leq \left( \frac{8}{9} - \frac{7}{8} \right) + \frac{7}{8} = \frac{8}{9}.$$

• Extend to general f by scaling.

- Repetition: What is the difference between hashing for specific versus generic functions, and how does the former imply the latter?
- Background: Refresh your memory of the Baire category theorem if necessary.
- Discussion: Can you strengthen the proof to get monotonically increasing approximate hashing functions?

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## Proof of the Kolmogorov-Arnold Theorem

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# Kolmogorov-Arnold Representation, Refined Version

Remark: The approximate hashing results imply the following refined version of the Kolmogorov–Arnold representation theorem:

#### Theorem (Kolmogorov–Arnold representation, refined version)

For any  $n \in \mathbb{N}_{\geq 2}$ , there exist  $\lambda_1, \ldots, \lambda_n \in \mathbb{R}$  and  $\varphi_1, \ldots, \varphi_{2n+1} \in C([0,1])$  such that any  $f \in C([0,1]^n)$  admits a representation

$$f(x_1,\ldots,x_n) = \sum_{i=1}^{2n+1} g(\lambda_1\varphi_i(x_1) + \cdots + \lambda_n\varphi_i(x_n))$$

for some continuous function g.

**Remark**: The difference to Kolmogorov's original result is that g does not depend on i.

Proof: Iterative improvement of the approximate hashing representation

- Let  $\varphi \in C([0,1], \mathbb{R}^5)$  be an approximate hashing function, define  $\psi_i(x,y) = \lambda_1 \varphi_i(x) + \lambda_2 \varphi_i(y)$  for  $\lambda_1 := 1$  and  $\lambda_2$  irrational, and define  $Tg := \sum_{i=1}^5 g \circ \psi_i$ .
- Set  $f_1 := f$  and find  $g_1$  with  $||g_1||_{\infty} \le \frac{1}{7} ||f_1||_{\infty}$  and  $||f_1 Tg_1||_{\infty} \le \frac{7}{8} ||f_1||_{\infty}$ .
- Set  $f_2 := f_1 Tg_1$  and find  $g_2$  with  $||g_2||_{\infty} \le \frac{1}{7} ||f_2||_{\infty}$  and  $||f_2 Tg_2||_{\infty} \le \frac{7}{8} ||f_2||_{\infty}$ .
- Continue to eternity. When done, set  $g = \sum_k g_k$  and note that f = Tg as required.

- Repetition: Recall the proof of the Kolmogorov-Arnold theorem via the construction of approximate hashing functions.
- Discussion: How does the proof work in higher dimensions?

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## Approximation by Networks of Bounded Size

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#### Theorem

There exists a continuous, piece-wise polynomial activation function  $\rho \colon \mathbb{R} \to \mathbb{R}$  which allows one to approximate continuous multivariate functions by realizations of neural networks with bounded size, that is, for all  $n \in \mathbb{N}$  there exists a constant C = C(n) such that

## $\forall \epsilon > 0 \ \forall f \in C([0,1]^n) \ \exists \Phi: \ \mathbf{L}(\Phi) = 3, \, \mathbf{M}(\Phi) \leq C(n), \, \|f - \mathbf{R}(\Phi)\|_\infty \leq \epsilon$

#### Remark:

- This theorem is in a sense "too good" because it provides an approximate representation of continuous functions by finitely many real numbers.
- It highlights the influence of the choice of activation function on the resulting approximation theory.
- It also points to the importance of asking for bounded weights.

### Lemma (Univariate case)

The theorem holds in the univariate case n = 1: there exists a continuous, piecewise polynomial activation function  $\rho \colon \mathbb{R} \to \mathbb{R}$  such that

$$\forall \epsilon > 0 \ \forall f \in C([0,1]) \ \exists \Phi: \ \mathbf{L}(\Phi) = 2, \quad \mathbf{M}(\Phi) \leq 3, \quad \|f - \mathbf{R}(\Phi)\|_{\infty} \leq \epsilon \,.$$

**Remark**: By translation and scaling, this extends to continuous functions f on every closed interval  $[a, b] \subseteq \mathbb{R}$ .

### Proof of the lemma:

- Recall that the set  $\Pi$  of polynomials with rational coefficients is dense in the Polish space C([0, 1]), and let  $(\pi_i)_{i \in \mathbb{Z}}$  be an enumeration of  $\Pi$ .
- Define the activation function  $\rho$  by

$$\rho(x) := \begin{cases} \pi_i(x-2i), & x \in [2i, 2i+1] \\ \pi_i(1)(2i+2-x) + \pi_{i+1}(0)(x-2i-1), & x \in (2i+1, 2i+2) \end{cases}$$

- Note that, by the very definition of  $\rho,$  one has  $\rho(x+2i)=\pi_i(x)$  for  $x\in[0,1].$
- Hence, the neural network  $\Phi:=((1,2i),(1,0))$  has the desired properties.

### Proof of the theorem:

• By the Kolmogorov-Arnold theorem (refined version),

$$f = \sum_{i=1}^{2n+1} g \circ \psi_i, \quad \psi_i(x_1, \dots, x_n) = \lambda_1 \varphi_i(x_1) + \dots + \lambda_n \varphi_i(x_n).$$

for some  $g \in C(\mathbb{R})$ ,  $\lambda_1, \ldots, \lambda_n \in \mathbb{R}$  and  $\varphi_1, \ldots, \varphi_{2n+1} \in C([0, 1])$ .

- By the previous lemma,  $\varphi_i \approx \mathbb{R}(\Phi_i) \in C([0, 1])$  for some networks  $\Phi_i$  and a piece-wise polynomial activation function  $\rho$ , where  $\approx$  denotes approximation up to arbitrary accuracy.
- Then  $\psi_i \approx \mathbf{R}(\Psi_i) \in C([0,1]^n)$  for each  $i \in \{1,\ldots,2n+1\}$ , where

$$\Psi_i = (((\lambda_1, \dots, \lambda_n), 0)) \bullet \operatorname{FP}(\Phi_i, \dots, \Phi_i).$$

# Proof: Approximation of Multivariate Functions (cont.)

- By the previous lemma,  $g \approx \mathbf{R}(\Xi) \in C([-K, K])$ , where K is sufficiently large such that  $\psi_i([0, 1]^n) \subseteq [-K, K]$ .
- Then the network

$$\Phi := (((1,\ldots,1),0)) \bullet \operatorname{FP}(\Xi,\ldots,\Xi) \bullet \operatorname{P}(\Psi_1,\ldots,\Psi_{2n+1}).$$

has the desired number of layers and weights.

• Moreover,  $f \approx \mathbf{R}(\Phi)$  thanks to the estimate

$$\begin{split} \|f - \mathbf{R}(\Phi)\| &\leq \sum_{i} \|\mathbf{R}(\Xi) \circ \mathbf{R}(\Psi_{i}) - g \circ \psi_{i}\| \\ &\leq \sum_{i} \|\mathbf{R}(\Xi) \circ \mathbf{R}(\Psi_{i}) - \mathbf{R}(\Xi) \circ \psi_{i}\| + \|\mathbf{R}(\Xi) \circ \psi_{i} - g \circ \psi_{i}\|, \end{split}$$

and thanks to the uniform continuity of  $R(\Xi)$  on [-K, K].

- Repetition: Recall the approximation of univariate and multivariate functions by networks of bounded size.
- Check: Verify that the activation function  $\rho$  constructed in the univariate case is continuous.
- Discussion: What are theoretical implications to approximation theory and practical implications to supervised learning?

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Wrapup

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#### • Reading:

- Arnold (1958): On the representation of functions of several variables
- Bar-Natan (2009): Hilberts 13th problem, in full color
- Hecht-Nielsen (1987): Kolmogorov's mapping neural network existence theorem

Having heard this lecture, ...

- You can describe the Kolmogorov–Arnold representation theorem and its proof.
- You can appreciate the fundamental distinction between inner and outer network layers.
- You are aware that different choices of activation functions may lead to very different approximation theories.