Approximation power of deep networks

Matus Telgarsky <mjt@illinois.edu> (with help from many friends!)

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$$\int \ell(f(x), y) \, \mathrm{d}P(x, y)$$
 vs. $\int \ell(g(x), y) \, \mathrm{d}P(x, y)$.

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▶ **Upper bounds:** If $\ell(\cdot, y)$ is 1-Lipschitz,

$$\int \left[\ell(g(x), y) - \ell(f(x), y)\right] \mathrm{d}P(x, y) \leq \left|g(x) - f(x)\right| \mathrm{d}P(x, y);$$

we make this small everywhere (universal/uniform/ $L_{\infty}(P)$ apx), or in $L_1(P)$.

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▶ Lower bounds: we want large error on a large set; as a surrogate, |g - f| large in $L_1(P)$ or $L_1(Unif)$. By deep networks we mostly mean

$$x \mapsto A_L \sigma_{L-1} \left(\cdots \sigma_1 (A_1 x + b_1) \cdots \right) + b_L,$$

where nonlinearity/activation/transfer σ_i is applied coordinate-wise.

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We'll mostly stick to the ReLU $z \mapsto \max\{0, z\}$ (Fukushima '80); it's easy to convert.







 $x\mapsto 2\cdot 1\!\!1[x\!-\!3\geq 0]\!+\!1[x\!-\!5\geq 0]\!+\!2\cdot 1\!\!1[x\!-\!7\geq 0]\!-\!1\!\!1[x\!-\!13\geq 0]\cdots$



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Remark. By contrast, polynomials struggle with flat regions.





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$$f(x) = f(0) + \int_0^x f'(b) \, \mathrm{d}b = f(0) + \int_0^\infty \mathbb{1}[x - b \ge 0] f'(b) \, \mathrm{d}b.$$

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Remarks.

- ► Infinite width network!
- ▶ Refined average-case estimate! (Captures flat regions.)





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(In some sense optimal (Savarese-Evron-Soudry-Srebro '19).)







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Caveats:

- ▶ Representation size may have blown up.
- ▶ Not our original goal.





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Supporting hyperplanes! ... oops.

Fix #1: product halfspaces together! (we'll return to this...)Fix #2: add a layer, thresholding at 3.5!...how about one ReLU/hidden layer?



Fix #3: add all the hyperplanes!



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Bad news: good apx seems to require 2^d nodes... (We'll come back to this.)

Combinations of radial bumps.



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$$\left| f(x) - \int f(z)p(x-z) \, \mathrm{d}z \right| = \left| f(x) - \int f(x-z)p(z) \, \mathrm{d}z \right|$$
$$= \left| \int f(x)p(z) \, \mathrm{d}z - \int f(x-z)p(z) \, \mathrm{d}z \right| \le \int \left| f(x) - f(x-z) \right| p(z) \, \mathrm{d}z,$$

which is small if $p(z) \approx 0$ for large ||z||.

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which is small if $p(z) \approx 0$ for large ||z||. Size estimate: $(d \cdot \text{Lip}/\epsilon)^{\mathcal{O}(d)}$. (Mhaskar-Michelli '92, BJTX '19.)

So far:

- ► Easy univariate constructions.
- ▶ 3-layer box constructions over \mathbb{R}^d : size $(\text{Lip}/\epsilon)^{\mathcal{O}(d)}$.
- ▶ 2-layer RBF convolutions over \mathbb{R}^d : size $\left(\frac{d \cdot \operatorname{Lip}}{\ell}\right)^{\mathcal{O}(d)}$.

Remarks.

- ▶ Impractical constructions! Bad Lipschitz constants.
- ▶ Contrast with polynomials: flat pieces.
- ▶ Usefuleness of infinite width! Note also:

$$\mathbb{E}\sigma_{\mathbf{r}}(a^{\mathsf{T}}x) = \frac{1}{2}\mathbb{E}|a^{\mathsf{T}}x| = \frac{\|x\|}{\sqrt{2\pi}}.$$

Poor complexity measures outside univariate!

Interlude: three questions

- 1. Are fixed DN architectures closed under addition?
- 2. Can RNNs model Turing Machines?



3. Given continuous $g : \mathbb{R}^d \to \mathbb{R}$, can we construct custom univariate activations so that

$$g(x) \stackrel{!}{=} \sum_{i=0}^{2d} f_i\left(\sum_{j=1}^d h_{i,j}(x_j)\right)?$$







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$$\mathbb{1}\left[\|x\|_{\infty} \le 1\right] = \prod_{i=1}^{d} \mathbb{1}\left[|x_i| \le 1\right] \quad \text{and} \quad \prod_{i=1}^{d} \cos(x_i)^p.$$



Univariate bump: $\cos(x)^p$ for large p. Multivariate bump:

$$\mathbb{1}[\|x\|_{\infty} \le 1] = \prod_{i=1}^{d} \mathbb{1}[|x_i| \le 1]$$
 and $\prod_{i=1}^{d} \cos(x_i)^p$.

To remove the product:

$$\cos(x)\cos(x) = \frac{1}{2}\left(\cos(2x) + 1\right),$$

$$2\cos(x_1)\cos(x_2) = \cos(x_1 + x_2) + \cos(x_1 - x_2).$$

Weierstrass approximation theorem



Theorem (Weierstrass, 1885). Polynomials can uniformly approximate continuous functions over compact sets.

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Remarks.

- Not a consequence of interpolation: must control behavior between interpolants.
- ▶ Proofs are interesting; e.g., Bernstein (Bernstein polynomials and tail bounds), Weierstrass (Gaussian smoothing gives analytic functions). ...
- ▶ Stone-Weierstrass theorem: Polynomial-like function families (e.g., closed under multiplication) also approximate continuous function.

$$\lim_{z \to -\infty} \sigma(z) = 0, \qquad \lim_{z \to +\infty} \sigma(z) = 1,$$

and define $\mathcal{H}_{\sigma} := \left\{ x \mapsto \sigma(a^{\mathsf{T}}x - b) : (a, b) \in \mathbb{R}^{d+1} \right\}$. Then span (\mathcal{H}_{σ}) uniformly approximates continuous functions on compact sets.

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Proof #1. \mathcal{H}_{cos} is closed under products since

$$2\cos(a)\cos(b) = \cos(a+b) + \cos(a-b).$$

Now uniformly approximate fixed \mathcal{H}_{cos} with span (\mathcal{H}_{σ}) . (Univariate fitting.)

Proof #2. \mathcal{H}_{exp} is closed under products since $e^a e^b = e^{a+b}$. Now uniformly approximate fixed \mathcal{H}_{exp} with $\operatorname{span}(\mathcal{H}_{\sigma})$. (Univariate fitting.)

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Remarks.

- ► ReLU is fine: use $\sigma(z) := \sigma_{r}(z) \sigma_{r}(z-1)$.
- Size estimate: expanding terms, seem to get $(Lip/\epsilon)^{\Omega(d)}$.
- ▶ Best conditions on σ (Leshno-Lin-Pinkus-Schocken '93): theorem holds iff σ not a polynomial.
- Inner hint about DN: no need for explicit multiplication?

Other proofs.

▶ (Cybenko '89.) Assume contradictorily you miss some functions. By duality, $0 = \int \sigma(a^{\mathsf{T}}x - b) \,\mathrm{d}\mu(x)$ for some signed measure μ , all (a, b). Using Fourier, can show this implies $\mu = 0...$ ▶ (Leshno-Lin-Pinkus-Schocken '93.) If σ a polynomial, ...; else can (roughly) get derivatives of all orders, polynomials of all orders. ▶ (Barron '93.) Consider activation $x \mapsto \exp(ia^{\mathsf{T}}x)$, infinite width form $\int \exp(ia^{\mathsf{T}}x)\widetilde{f}(a) \,\mathrm{d}a.$ Take real part and sample (Maurey) to get $g \in \text{span}(\mathcal{H}_{\cos})$; convert to span(\mathcal{H}_{σ}) as before. (Funahashi '89.) Also Fourier, measure-theoretic.

"Universal approximation"

(Uniform approximation of cont. functions on compact sets).

- ▶ Elementary proof: RBF (Mhaskar-Michelli '92; BJTX '19).
- ▶ Slick proof: Stone-Weierstrass and \mathcal{H}_{cos} or \mathcal{H}_{exp} (Hornik-Stinchcombe-White, '89).
- ▶ Proof with size estimates beating (Lip/ε)^d, indeed norm of Fourier transform of gradient, related to "sampling measure": (Barron '93).

Remarks.

- Exhibits nothing special about DN; indeed, same proofs work for boosting, RBF SVM, ...
- ► Size estimates huge (soon we'll see $d^{\Omega(d)}$).
- Proofs use nice representation "tricks"; (e.g., Leshno et al "iff not polynomial").



Radial functions are easy with two ReLU layers

Consider $f(||x||^2)$ with Lipschitz constant Lip. \blacktriangleright Pick $h(x) \approx_{\epsilon} ||x||_2^2 = \sum_i x_i^2$ with $d \cdot \text{Lip}/\epsilon$ ReLU.

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- ▶ Pick $g \approx_{\epsilon} f$ with Lip/ ϵ ReLU; then

$$\begin{aligned} \left| f(\|x\|^2) - g(h(x)) \right| &\leq \left| f(\|x\|^2) - f(h(x)) \right| + \left| f(h(x)) - g(h(x)) \right| \\ &\leq \operatorname{Lip} \left| \|x\|^2 - h(x) \right| + \epsilon \leq 2\epsilon. \end{aligned}$$

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Remarks.

- ► Final size of $g \circ h$ is poly(Lip, $d, 1/\epsilon$).
- Proof style is "typical"/lazy; (problematically) pays with Lipschitz constant.
- ▶ That was easy/intuitive; how about the 2 layer case?...

Radial functions are *not* easy with only one ReLU layer (I)

Theorem (Eldan-Shamir, 2015).

There exists a radial function f,

expressible with two ReLU layers of width poly(d),

and a probability measure ${\cal P}$

so that every g with a single ReLU layer of width $2^{\mathcal{O}(d)}$ satisfies

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Proof hints.

Apply Fourier isometry and consider the transforms. Transform of g is supported on a small set of tubes; transform of f has large mass they can't reach.

Theorem (Daniely, 2017).

Let $(x, x') \sim P$ be uniform on two sphere surfaces, define $h(x, x') = \sin(\pi d^3 x^{\mathsf{T}} x')$. For any g with a single ReLU layer of width $d^{\mathcal{O}(d)}$ and weight magnitude $\mathcal{O}(2^d)$,

$$\int \left(h(x,x') - g(x,x')\right)^2 \mathrm{d}P(x,x') \ge \Omega(1),$$

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Proof hints.

Spherical harmonics reduce this to a univariate problem; apply region counting.

Approximation of high-dimensional radial functions



(A radial function contour plot.)

If we can approximate each shell, we can approximate the overall function.

Approximation of high-dimensional radial shell



Let's approximate a single shell; consider

$$x\mapsto \mathbb{1}\left[\|x\|\in [1-{}^{1}\!/\!d\ ,\ 1]\right],$$

which has a constant fraction of sphere volume.

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... but then we need to cover exponentially many caps.

Let's go back to the drawing board; what do shallow representations do exceptionally badly? Let's go back to the drawing board; what do shallow representations do exceptionally badly?

One weakness: their complexity scales with #bumps.

Consider the tent map \mathbf{t}

$$\Delta(x) := \sigma_{\mathbf{r}}(2x) - \sigma_{\mathbf{r}}(4x - 2) = \begin{cases} 2x & x \in [0, 1/2), \\ 2(1-x) & x \in [1/2, 1]. \end{cases}$$



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What is the effect of composition?

 $f(\Delta(x)) = \begin{cases} x \in [0, \frac{1}{2}) \implies f(2x) = f \text{ squeezed into } [0, \frac{1}{2}], \\ x \in [\frac{1}{2}, 1] \implies f\left(2(1-x)\right) = f \text{ reversed, squeezed.} \end{cases}$
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 Δ^k uses $\mathcal{O}(k)$ layers & nodes, but has $\mathcal{O}(2^k)$ bumps.

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Proof.

- 1. g with few oscillations can't apx oscillatory regular f.
- 2. There exists a regular, oscillatory f. $(f = \Delta^{k^2+3})$.
- 3. Width m depth $L \implies$ few $(\mathcal{O}(m^L))$ oscillations. Rediscovered many times; (T '15) gives elementary univariate argument;

multivariate arguments in (Warren '68), (Arnold ?), (Montufar, Pascanu, Cho, Bengio, '14), (BT '18), ...









g with few oscillations; f highly oscillatory, regular

$$\implies \qquad \int_{[0,1]} |\boldsymbol{g} - \boldsymbol{f}| \text{ large }.$$





$$\Rightarrow \qquad \int_{[0,1]} |g-f| \, ext{large} \; .$$





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Story from *benefits of depth*:

- Certain radial functions have polynomial width 2 ReLU layer representation, exponential width 1 ReLU layer representation.
- Δ^{k^2+3} can be written with $\mathcal{O}(k^2)$ depth and $\mathcal{O}(1)$ width, requires width $\Omega(2^k)$ if depth $\mathcal{O}(k)$.

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- Δ^{k^2+3} can be written with $\mathcal{O}(k^2)$ depth and $\mathcal{O}(1)$ width, requires width $\Omega(2^k)$ if depth $\mathcal{O}(k)$.

- Δ^k is 2^k -Lipschitz; possibly nonsensical, unrealistic.
- These results have stood a few years now; many "technical" questions, also "realistic" questions.



 $h_k :=$ piecewise-affine interpolation of x^2 at $\{0, \frac{1}{2^k}, \frac{2}{2^k}, \dots, \frac{2^k}{2^k}\}$.







$$h_1 - h_2$$
.









Thus
$$h_k(x) = x - \sum_{i \le k} \Delta^i(x)/4^i$$
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- ▶ h_k needs $k = \mathcal{O}(\ln(1/\epsilon))$ to ϵ -apx $x \mapsto x^2$ (Yarotsky, '16), with matching lower bounds.
- Squaring implies **multiplication** via polarization: $x^{\mathsf{T}}y = \frac{1}{2} \left(\|x + y\|^2 - \|x\|^2 - \|y\|^2 \right).$



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- Squaring implies **multiplication** via polarization: $x^{\mathsf{T}}y = \frac{1}{2} \left(\|x + y\|^2 - \|x\|^2 - \|y\|^2 \right).$
- This implies efficient approximation of polynomials; can we do more?

Let dimension d and smoothness order r be given. Given $f:[0,1]^d\to\mathbb{R}$, all rth order derivatives bounded by 1, exists a network g

with $C_{d,r} \ln(e/\epsilon)$ layers and $C_{d,r} \epsilon^{-d/r} \ln(e/\epsilon)$ nodes so that

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Proof.

Conditions imply accurate local Taylor expansions. Therefore can write f as a linear combination of this basis: polynomials multiplied by local bumps.

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$$\sup_{x \in [0,1]^d} |f(x) - g(x)| \le \epsilon.$$

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- There is depth, but it is function independent: only the basis coefficients use f.
- This is a shallow representation: only the basis coefficients
- ▶ Lipschitz constant is possibly bad: Δ^{1/ε} is ¹/ε-Lipschitz, the bumps are ¹/ε^{d/r}-Lipschitz.

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Remarks.

- There is parallel and subsequent work with similar proof ideas and Lipschitz constants: (Safran-Shamir '16), (Petersen-Voigtlaender '17), (Schmidt-Hieber '17).
- Another appearance of polynomials in DN: Sum-product networks.

These were the first to have depth separation (Delalleau-Bengio '11).

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- DN can approximate polynomials efficiently, but the reverse is false: a single ReLU requires degree ¹/ε.
- Polynomials can not handle flat regions well; this is used above, and in approximated rational functions (T '17).
Theorem (Yarotsky '16).

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Remarks.

▶ Corresponding lower bounds indicate depth is needed.

Interlude: three questions

- 1. Are fixed DN architectures closed under addition? No, add together perturbed copies of Δ^k .
- 2. Can RNNs model Turing Machines?



- **Hint.** ReLU networks can do exact Boolean formulae. Set f to state transition table, encode tape on s.
- 3. Given continuous $g : \mathbb{R}^d \to \mathbb{R}$, can we construct custom univariate activations so that

$$g(x) \stackrel{!}{=} \sum_{i=0}^{2d} f_i\left(\sum_{j=1}^d h_{i,j}(x_j)\right)?$$

Hint? Contradicts a Hilbert problem?



Typical setup: pushforward measure $g#\mu$, meaning

sample $x \sim \mu$, output g(x).

Many easy constructions have bad/ ∞ Lipschitz constants! E.g., mapping uniform into [0, 1/2], (3/2, 2].

Some literature: (Arora-Ge-Liang-Ma-Zhang '17, BT '18, Bai-Ma-Risteski '19, Elchanan's talk this week!) Randomly *initialized* networks

Approximation fact in recent optimization papers: a small perturbation of random initialization gives any function you want!(Du-Lee-Li-Wang-Zhai '18, AllenZhu-Li-Song '18).

There is residual error from the noise approximating high-Lipschitz functions is problematic! (BJTX '19.) Randomly *sampled* networks

Theorem. With probability $\geq 1 - \frac{1}{e}$,

$$\begin{split} \sup_{\|x\|_2 \le 1} \left| \int \sigma_{\mathbf{r}}(a^{\mathsf{T}}x - b) \, \mathrm{d}\mu(a, b) - \frac{\|\mu\|_1}{N} \sum_{i=1}^N \sigma_{\mathbf{r}}(a_i^{\mathsf{T}}x - b_i) \right| \\ \le \mathcal{O}\left(\frac{B\|\mu\|_1}{\sqrt{N}}\right), \end{split}$$

where support of μ has $||(a, b)|| \leq B$.

Randomly *sampled* networks

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where support of μ has $||(a, b)|| \leq B$.

Proof. Invoke Rademacher complexity, but swap inputs and parameters.

(Koiran-Gurvits '97, Sun-Gilbert-Tewari '18, BJTX '19.) Also Maurey's Lemma (Barron '93). Adversarial stability



Adversarial examples lower bound the Lipschitz constant...

Adversarial stability



Adversarial examples lower bound the Lipschitz constant...

... but a bad Lipschitz constant can be good for adversarial examples! Adversarial stability



Adversarial examples lower bound the Lipschitz constant...

... but a bad Lipschitz constant can be good for adversarial examples!

Given the existence of adversarial examples, uniform approximation too stringent?

Turing machines and RNNs



Make f the TM state transition table, s the tape. Turing machines and RNNs



- Make f the TM state transition table, s the tape.
- ▶ $x \mapsto \mathbb{1}[x \ge 0]$ is **not computable**; bits need a special encoding within *s*.

Turing machines and RNNs



- Make f the TM state transition table, s the tape.
- ▶ $x \mapsto \mathbb{1}[x \ge 0]$ is **not computable**; bits need a special encoding within *s*.
- ► Use a robust "cantor-like" encoding.

(Siegelmann-Sontag '94.)

There exist continuous $((h_{i,j})_{i=0}^{2d})_{j=1}^d : \mathbb{R} \to \mathbb{R}$, so that for any continuous $g : \mathbb{R}^d \to \mathbb{R}$, there exist continuous $(f_i)_{i=0}^{2d} : \mathbb{R} \to \mathbb{R}$ with

$$g(x) = \sum_{i=0}^{2d} f_i \Big(\sum_{j=1}^d h_{i,j}(x_j) \Big).$$

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Step 1. Fix target accuracy $\epsilon > 0$.

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Step 2. Choose $f : \mathbb{R} \to \mathbb{R}$, nearly injective $Q : \mathbb{R}^d \to \mathbb{R}$, $g \approx f(Q(x))$



There exist continuous $((h_{i,j})_{i=0}^{2d})_{j=1}^d : \mathbb{R} \to \mathbb{R}$, so that for any continuous $g : \mathbb{R}^d \to \mathbb{R}$, there exist continuous $(f_i)_{i=0}^{2d} : \mathbb{R} \to \mathbb{R}$ with

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Step 3.

Replace near-injection $Q : \mathbb{R}^d \to \mathbb{R}$ with $\sum_j h_j(x_j)$.



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Step 4. Replace $f(\sum_j h_j(x_j))$ with staggered versions $\sum_i f_i(\sum_j h_{i,j}(x_j))$; for any $x \in [0, 1]^d$, \geq half are correct.



There exist continuous $((h_{i,j})_{i=0}^{2d})_{j=1}^d : \mathbb{R} \to \mathbb{R}$, so that for any continuous $g : \mathbb{R}^d \to \mathbb{R}$, there exist continuous $(f_i)_{i=0}^{2d} : \mathbb{R} \to \mathbb{R}$ with

$$g(x) = \sum_{i=0}^{2d} f_i \Big(\sum_{j=1}^d h_{i,j}(x_j) \Big).$$

Step 5. Embed the solutions for infinitely many ϵ into one.



Main story.

- ► Can fit continuous functions in various ways; the size is bad $((d \cdot \text{Lip}/\epsilon)^{\mathcal{O}(d)})$.
- Composition and depth bring some concrete benefits; exponential reductions in width!
- Polynomials may be efficiently approximated, but also some non-polynomials (Sobolov balls, rational functions, flat regions, ...).

Remarks.

- Refined depth separations (e.g., a single new layer) and practical depth separations are still elusive.
- ▶ Refined, average-case complexity measures are elusive.



