## Approximation power of deep networks

Matus Telgarsky [mjt@illinois.edu](mailto:mjt@illinois.edu) (with help from many friends!)

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Primary setting: statistical learning theory, thus

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

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we make this small everywhere (universal/uniform/ $L_{\infty}(P) \mathbf{a p x}$, or in $L_{1}(P)$.
- 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}\left(A_{1} x+b_{1}\right) \cdots\right)+b_{L},
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There are many conventions; we will briefly discuss others.

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

Elementary universal approximation.


Classical universal approximation.


Benefits of depth.


Sobolev spaces.


Odds \& ends.

Univariate functions via step activations


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$$
x \mapsto 2 \cdot \mathbb{1}[x-3 \geq 0]+\mathbb{1}[x-5 \geq 0]+2 \cdot \mathbb{1}[x-7 \geq 0]-\mathbb{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^{\prime}(b) \mathrm{d} b=f(0)+\int_{0}^{\infty} \mathbb{1}[x-b \geq 0] f^{\prime}(b) \mathrm{d} b .
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Remarks.

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




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Need to sample avg smooth $/ \epsilon^{2}$ ReLU!
(In some sense optimal (Savarese-Evron-Soudry-Srebro '19).)
$\square$




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## Caveats:

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

Approximate a multivariate box.



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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?

Approximate a multivariate ball.


Fix \#3: add all the hyperplanes!


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Resulting radial function is constant within ball, attenuates away from it.


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Resulting radial function is constant within ball, attenuates away from it.

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

Combinations of radial bumps.


Normalize bumps/RBFs into density $p$; convolve with $f$.


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\begin{aligned}
& \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| \leq \int|f(x)-f(x-z)| p(z) \mathrm{d} z
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which is small if $p(z) \approx 0$ for large $\|z\|$.
Size estimate: $(d \cdot \operatorname{Lip} / \epsilon)^{\mathcal{O}(d)}$.
(Mhaskar-Michelli '92, BJTX '19.)

So far:

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


## Remarks.

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

$$
\mathbb{E} \sigma_{\mathrm{r}}\left(a^{\top} x\right)=\frac{1}{2} \mathbb{E}\left|a^{\top} x\right|=\frac{\|x\|}{\sqrt{2 \pi}}
$$

- Poor complexity measures outside univariate!

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

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

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

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


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$$

To remove the product:

$$
\begin{aligned}
\cos (x) \cos (x) & =\frac{1}{2}(\cos (2 x)+1) \\
2 \cos \left(x_{1}\right) \cos \left(x_{2}\right) & =\cos \left(x_{1}+x_{2}\right)+\cos \left(x_{1}-x_{2}\right)
\end{aligned}
$$

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.

Theorem (Hornik-Stinchcombe-White '89).
Let $\sigma: \mathbb{R} \rightarrow \mathbb{R}$ be given with

$$
\lim _{z \rightarrow-\infty} \sigma(z)=0, \quad \lim _{z \rightarrow+\infty} \sigma(z)=1
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and define $\mathcal{H}_{\sigma}:=\left\{x \mapsto \sigma\left(a^{\top} x-b\right):(a, b) \in \mathbb{R}^{d+1}\right\}$.
Then $\operatorname{span}\left(\mathcal{H}_{\sigma}\right)$ uniformly approximates continuous functions on compact sets.

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continuous functions on compact sets.

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

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

Now uniformly approximate fixed $\mathcal{H}_{\text {cos }}$ with $\operatorname{span}\left(\mathcal{H}_{\sigma}\right)$. (Univariate fitting.)

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

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Remarks.

- $\operatorname{ReLU}$ is fine: use $\sigma(z):=\sigma_{\mathrm{r}}(z)-\sigma_{\mathrm{r}}(z-1)$.
- Size estimate: expanding terms, seem to get $(\operatorname{Lip} / \epsilon)^{\Omega(d)}$.
- Best conditions on $\sigma$ (Leshno-Lin-Pinkus-Schocken '93): theorem holds iff $\sigma$ not a polynomial.
- Inner hint about DN: no need for explicit multiplication?
- (Cybenko '89.)

Assume contradictorily you miss some functions.
By duality, $0=\int \sigma\left(a^{\top} x-b\right) \mathrm{d} \mu(x)$
for some signed measure $\mu$, all $(a, b)$.
Using Fourier, can show this implies $\mu=0 \ldots$

- (Leshno-Lin-Pinkus-Schocken '93.)

If $\sigma$ a polynomial, ...;
else can (roughly) get derivatives of all orders, polynomials of all orders.

- (Barron '93.)

Consider activation $x \mapsto \exp \left(i a^{\top} x\right)$,
infinite width form $\int \exp \left(i a^{\top} x\right) \widetilde{f}(a) \mathrm{d} a$.
Take real part and sample (Maurey) to get $g \in \operatorname{span}\left(\mathcal{H}_{\mathrm{cos}}\right)$; convert to $\operatorname{span}\left(\mathcal{H}_{\sigma}\right)$ 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 $\mathcal{H}_{\text {cos }}$ or $\mathcal{H}_{\exp }$ (Hornik-Stinchcombe-White, '89).
- Proof with size estimates beating $(\operatorname{Lip} / \epsilon)^{d}$, 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").

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Odds \& ends.

Radial functions are easy with two ReLU layers

Consider $f\left(\|x\|^{2}\right)$ with Lipschitz constant Lip.

- Pick $h(x) \approx_{\epsilon}\|x\|_{2}^{2}=\sum_{i} x_{i}^{2}$ with $d \cdot$ Lip $/ \epsilon$ ReLU.

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\left|f\left(\|x\|^{2}\right)-g(h(x))\right| & \leq\left|f\left(\|x\|^{2}\right)-f(h(x))\right|+|f(h(x))-g(h(x))| \\
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## Remarks.

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


## Theorem (Eldan-Shamir, 2015).

There exists a radial function $f$,
expressible with two ReLU layers of width $\operatorname{poly}(d)$, and a probability measure $P$
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 $\left(x, x^{\prime}\right) \sim P$ be uniform on two sphere surfaces, define $h\left(x, x^{\prime}\right)=\sin \left(\pi d^{3} x^{\top} x^{\prime}\right)$.
For any $g$ with a single ReLU layer of width $d^{\mathcal{O}(d)}$ and weight magnitude $\mathcal{O}\left(2^{d}\right)$,

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and $h$ can be approximated to accuracy $\epsilon$ by $f$ with two $\operatorname{ReLU}$ layers of size $\operatorname{poly}(d, 1 / \epsilon)$.

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## Proof hints.

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

(A radial function contour plot.)
If we can approximate each shell, we can approximate the overall function.


Let's approximate a single shell; consider

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x \mapsto \mathbb{1}[\|x\| \in[1-1 / d, 1]],
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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?

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One weakness: their complexity scales with \#bumps.

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


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What is the effect of composition?

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f(\Delta(x))=\left\{\begin{array}{lll}
x \in[0,1 / 2) & \Longrightarrow \quad f(2 x)=f \text { squeezed into [0, } 1 / 2] \\
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$$

## Proof.

1. $g$ with few oscillations can't apx oscillatory regular $f$.
2. There exists a regular, oscillatory $f$. $\left(f=\Delta^{k^{2}+3}\right.$. $)$
3. Width $m$ depth $L \Longrightarrow$ few $\left(\mathcal{O}\left(m^{L}\right)\right)$ 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 $\quad \stackrel{?}{\Longrightarrow} \quad \int_{[0,1]}|g-f|$ large.



$$
\text { Let's use } f=\Delta^{k^{2}+3}
$$



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$g$ with few oscillations;
$f$ highly oscillatory, regular $\Longrightarrow \quad \int_{[0,1]}|g-f|$ 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.
- $\Delta^{k^{2}+3}$ can be written with $\mathcal{O}\left(k^{2}\right)$ depth and $\mathcal{O}(1)$ width, requires width $\Omega\left(2^{k}\right)$ if depth $\mathcal{O}(k)$.

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## Remarks.

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

Elementary universal approximation.


Classical universal approximation.


Benefits of depth.


Sobolev spaces.


Odds \& ends.
$h_{k}:=$ piecewise-affine interpolation of $x^{2}$ at $\left\{0, \frac{1}{2^{k}}, \frac{2}{2^{k}}, \ldots, \frac{2^{k}}{2^{k}}\right\}$.

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$$
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Thus $h_{k}(x)=x-\sum_{i \leq k} \Delta^{i}(x) / 4^{i}$.
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$h_{1}$.

$h_{2}$.

Thus $h_{k}(x)=x-\sum_{i \leq k} \Delta^{i}(x) / 4^{i}$.

- $h_{k}$ needs $k=\mathcal{O}(\ln (1 / \epsilon))$ to $\epsilon$-apx $x \mapsto x^{2}$ (Yarotsky, '16), with matching lower bounds.
- Squaring implies multiplication via polarization:

$$
x^{\top} y=\frac{1}{2}\left(\|x+y\|^{2}-\|x\|^{2}-\|y\|^{2}\right) .
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- This implies efficient approximation of polynomials; can we do more?


## Theorem (Yarotsky '16).

Let dimension $d$ and smoothness order $r$ be given. Given $f:[0,1]^{d} \rightarrow \mathbb{R}$, all $r$ th 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

$$
\sup _{x \in[0,1] d}|f(x)-g(x)| \leq \epsilon
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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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$$

## Remarks.

- 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:
$\Delta^{1 / \epsilon}$ is $1 / \epsilon$-Lipschitz, the bumps are $1 / \epsilon^{d / r}$-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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## Remarks.

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


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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 $\Delta^{k}$.
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 $g: \mathbb{R}^{d} \rightarrow \mathbb{R}$, can we construct custom univariate activations so that

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

Hint? Contradicts a Hilbert problem?

Elementary universal approximation.


Classical universal approximation.


Benefits of depth.


Sobolev spaces.


Odds \& ends.

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

$$
\text { sample } x \sim \mu, \quad \text { output } g(x)
$$

Many easy constructions have bad/ $\infty$ 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!)

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.)

Theorem. With probability $\geq 1-1 / e$,

$$
\begin{aligned}
& \sup _{\|x\|_{2} \leq 1}\left|\int \sigma_{\mathrm{r}}\left(a^{\top} x-b\right) \mathrm{d} \mu(a, b)-\frac{\|\mu\|_{1}}{N} \sum_{i=1}^{N} \sigma_{\mathrm{r}}\left(a_{i}^{\top} x-b_{i}\right)\right| \\
& \quad \leq \mathcal{O}\left(\frac{B\|\mu\|_{1}}{\sqrt{N}}\right)
\end{aligned}
$$

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

## Randomly sampled networks

Theorem. With probability $\geq 1-1 / e$,

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& \sup _{\|x\|_{2} \leq 1}\left|\int \sigma_{\mathrm{r}}\left(a^{\top} x-b\right) \mathrm{d} \mu(a, b)-\frac{\|\mu\|_{1}}{N} \sum_{i=1}^{N} \sigma_{\mathrm{r}}\left(a_{i}^{\top} x-b_{i}\right)\right| \\
& \quad \leq \mathcal{O}\left(\frac{B\|\mu\|_{1}}{\sqrt{N}}\right)
\end{aligned}
$$

where support of $\mu$ 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 examples lower bound the Lipschitz constant...


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


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

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


- Make $f$ the TM state transition table, $s$ the tape.

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- $x \mapsto \mathbb{1}[x \geq 0]$ is not computable; bits need a special encoding within $s$.

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- $x \mapsto \mathbb{1}[x \geq 0]$ is not computable; bits need a special encoding within $s$.
- Use a robust "cantor-like" encoding.
(Siegelmann-Sontag '94.)

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

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g(x)=\sum_{i=0}^{2 d} f_{i}\left(\sum_{j=1}^{d} h_{i, j}\left(x_{j}\right)\right) .
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## Step 1.

Fix target accuracy $\epsilon>0$.

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


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$$

## Step 3.

Replace near-injection $Q: \mathbb{R}^{d} \rightarrow \mathbb{R}$ with $\sum_{j} h_{j}\left(x_{j}\right)$.

| $4 \sqrt{2}$ |  |  |  |
| :---: | :---: | :---: | :---: |
| $3 \sqrt{2}$ |  |  |  |
| $2 \sqrt{2}$ |  |  |  |
| 1 | 2 | 3 | 4 |

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

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g(x)=\sum_{i=0}^{2 d} f_{i}\left(\sum_{j=1}^{d} h_{i, j}\left(x_{j}\right)\right) .
$$

Step 4.
Replace $f\left(\sum_{j} h_{j}\left(x_{j}\right)\right)$
with staggered versions $\sum_{i} f_{i}\left(\sum_{j} h_{i, j}\left(x_{j}\right)\right)$; for any $x \in[0,1]^{d}$,
$\geq$ half are correct.


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

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## Step 5.

Embed the solutions for infinitely many $\epsilon$ into one.


## Main story.

- Can fit continuous functions in various ways; the size is $\operatorname{bad}\left((d \cdot \operatorname{Lip} / \epsilon)^{\mathcal{O}(d)}\right)$.
- 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.

Elementary universal approximation.


Classical universal approximation.

Benefits of depth.
$\downarrow$ Sobolev spaces.


Elementary universal approximation.


Classical universal approximation.


