#### Machine-Learning Mathematical Structures

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# The String Landscape

#### • The Geometric Origin of our Universe

- String Theory (a unified ToE) exists in (9+1)-D; We live in (3+1)-D
- Extra dimension X = 6-dimensional manifold (10 4 = 6);
- Geometry (algebraic/differential geometry/topology) of X determines physics of our world.
- The Vacuum Degeneracy Problem TOO MANY possibilities for X
  - e.g., X Calabi-Yau 3-folds (topology/combinatorics tends to grow exponentially)
     Complex Dim 1 2 3 ... CY<sub>n</sub> T<sup>2</sup> T<sup>4</sup>, K3 > 10<sup>10</sup> ?
     see: YHH, The CY Landscape: from geometry, to physics, to ML, Springer LNM, 2021.

# The Typical Calculation: Inevitability of Algebraic Geometry

- Each X (+ bundles, discrete symmetries) gives a (3+1)-d universe
  - particles and interactions  $\sim$  cohomology theory; masses  $\sim$  metric; Yukawa  $\sim$ Triple intersections/integral of forms over X
  - $X \sim \text{algebraic variety} \sim \text{degree/coefficient data, numerical metrics}$



Ubi materia, ibi geometria

- Johannes Kepler (1571-1630)
- Our Universe:
   (1) probabilistic/anthropic?
   (2) Sui generis/selection rule?
   (3) one of multi-verse ?

  - cf. Exo-planet/Habitable Zone search
- cf. exact SM: Braun-YHH-Ovrut (2005), Candelas-de la Ossa-YHH-Szendroi

(2009), Anderson-Gray-Lukas-Ovrut-Palti (2012), ...,

# A Wild Question: NN Doesn't Care/Know about maths

• Typical Problem in String Theory:

$$\begin{array}{c|c} INPUT & OUTPUT \\\hline (integer, real) tensor & integer \\\end{array}$$

- Q: Can we "machine-learn the landscape?"
- [YHH 1706.02714] Deep-Learning the Landscape, *PLB* 774, 2017 ( *Science*, Aug, vol 365 issue 6452 )
  - Hodge Number of a Complete Intersection CY is the association rule, e.g.

CICY is  $12 \times 15$  integer matrix with entries  $\in [0, 5]$  is simply represented as a  $12 \times 15$  pixel image of 6 colours Proper Way; ML in matter of seconds/minutes

Major International Annual Conference Series

- 1986- First "Strings" Conference
- 2002- First "StringPheno" Conference
- 2006 2010 String Vacuum Project (NSF)
- 2011- First "String-Math" Conference
- 2014- First String/Theoretical Physics Session in SIAM Conference
- 2017- First "String-Data" Conference

YHH (1706.02714), Seong-Krefl (1706.03346), Ruehle (1706.07024),

Carifio-Halverson-Krioukov-Nelson (1707.00655) (A host of activity);

• • • • • • • • • • • •

# Machine Learning Mathematical Structures

Why stop at string/geometry?

q.v. Review Paper: YHH 2101.06317

Russell-Whitehead Principia Mathematica [1910s] programme (since at least Frege, even Leibniz) to axiomatize mathematics, but ...

Gödel [1931] Incompleteness ; Church-Turing [1930s] Undecidability

Automated Theorem Proving (ATP) The practicing mathematician hardly ever worries about Gödel

- Newell-Simon-Shaw [1956] Logical Theory Machine: proved subset of *Principia* theorems
- Type Theory [1970s] Martin-Löf, Coquand, ... Coq interactive proving system: 4-color (2005); Feit-Thompson Thm (2012); Lean (2013)
- Univalent Foundation / Homotopy Type Theory [2006-] Voevodsky

We can call this Bottom-up Mathematics

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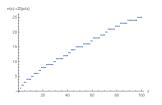
## How does one do mathematics, II ?

- Late C20th increasing rôle of computers: 4-color [Appel-Haken-Koch 1976]; Classif. Finite Simple Groups [Galois 1832 - Gorenstein et al. 2008] ...
- Buzzard: "Future of Maths" 2019: already plenty of proofs unchecked (incorrect?) in the literature, MUST use computers for proof-checking; XenaProject, Lean establish database of mathematical statements
- Davenport: ICM 2018 "Computer Assisted Proofs".
- Hale & Buzzard: Foresee within 10 years AI will help prove "early PhD" level lemmas, all of undergrad-level maths formalized;
- Szegedy: more extreme view, computers > humans @ chess (1990s); @ Go (2018); @ Proving theorems (2030)

Image: A math a math

# How does one \*DO\* mathematics, III ?

- Historically, Maths perhaps more Top-Down: practice before foundation
  - Countless examples: calculus before analysis; algebraic geometry before Bourbaki, permutation groups / Galois theory before abstract algebra . .
  - A lot of mathematics starts with intuition, experience, and experimentation
- The best neural network of C18-19th? brain of Gauß ; e.g., age 16

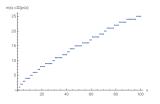


(w/o computer and before complex analysis [50 years before Hadamard-de la Vallée-Poussin's proof]): PNT  $\pi(x) \sim x/\log(x)$ 

• BSD computer experiment of Birch & Swinnerton-Dyer [1960's] on plots of rank  $r \& N_p$  on elliptic curves

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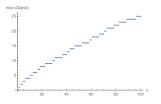


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- To extend the analogy: AlphaGo is top-down (need to see human games); even AlphaZero is not bottom-up (need to generate samples of games)
- In tandem with the bottom-up approach of Coq, Lean, Xena ... how to put in a little intuition and human results? If I gave you 100,000 cases of

), or, labeled data e.g.  $\begin{pmatrix} \frac{5}{2} 0 + \frac{3}{2} + \frac{2}{2} + \frac{3}{2} + \frac{3}{$ 

- Q: Is there a pattern? Can one conjecture & then prove a formula?
- Q: What branch of mathematics does it come from?
- Perfect for (unsupervised & supervised) machine-learning; focus on labeled

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e.g. 
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- Perfect for (unsupervised & supervised) machine-learning; focus on labeled case because it encodes WHAT is interesting to calculate (if not how).

e.

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- Mathematical Data is more structured than "real world" data, much less susceptible to noise; Outliers even more interesting, e.g. Sporadics, Exceptionals, ...
- Last 10-20 years: large collaborations of computational mathematicians, physicists, CS (cf. SageMATH, GAP, Bertini, MAGMA, Macaulay2, Singular, Pari, Wolfram, ...) computed and compiled vast data

o links

- Generic computation HARD
- mining provides some level of "intuition" & is based on "experience"

Bag of Tricks Hilbert's Programme of *Finitary Methods*, Landau's *theoretical minimum*, Migdal's *Mathmagics* . . .

IMO Grand Challenge (2020-) Good set of concrete problems to try on AI

Standard ML Regressor & Classifiers (w/ NO KNOWLEDGE of the maths) UAT

- NN: MLPs; CNNs; RNNs, ... (gentle tuning of architecture and hyper-parameters)
- SVM, Bayes, Decision Trees, PCA, Clustering, ...
- ML: emergence of complexity via connectivity ~> Intution (?)
- This Talk: Status Report of Experiments in the last couple of years
  - focus on supervised ML ("knows where to get to")
  - all standard methods  $\simeq$  same performance
  - ~ 20-80 split; training on 20 ( precision, Matthews'  $\phi$  or  $R^2$  )

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# Representation/Group Theory

- ML Algebraic Structures (GAP DB) [YHH-MH. Kim 1905.02263, ]
  - When is a Latin Square (Sudoku) the Cayley (multiplication) table of a finite group? Bypass quadrangle thm (0.95, 0.9)
  - Can one look at the Cayley table and recognize a finite simple group?
    - bypass Sylow and Noether Thm; (0.97, 0.95) rmk: can do it via character-table T, but getting T not trivial
    - SVM: space of finite-groups (point-cloud of Cayley tables) seems to exist a hypersurface separating simple/non-simple
- ML Lie Structure Chen-YHH-Lal-Majumder [2011.00871] Weight vector  $\rightarrow$  length

of irrep decomp / tensor product: (0.97, 0.93); (train on small dim, predict high dim: (0.9, 0.8))

# Combinatorics, Graph/Quivers

#### • [YHH-ST. Yau 2006.16619] Wolfram Finite simple graphs DB

• ML standard graph properties:

?acyclic (0.95, 0.96); ?planar (0.8, 0.6); ?genus >, =, < 0 (0.8, 0.7); ?∃</li>
Hamilton cycles (0.8, 0.6); ?∃ Euler cycles (0.8, 0.6)
(Rmk: NB. Only "solving" the likes of traveling salesman stochastically)

- spectral bounds  $(R^2 \sim 0.9) \dots$
- Recognition of Ricci-Flatness (0.9, 0.9) (todo: find new Ricci-flat graphs);
- [Bao-Franco-YHH-Hirst-Musiker-Xiao 2006.10783]: categorizing different quiver mutation (Seiberg-dual) classes (0.9 1.0, 0.9)

# Number Theory: A Classical Reprobate?

Arithmetic (prime numbers are Difficult!)

- [YHH 1706.02714, 1812.02893:]
  - Predicting primes  $2 \rightarrow 3, \ 2, 3 \rightarrow 5, \ 2, 3, 5 \rightarrow 7$ ; no way
  - fixed (or x/log(x)-scaled) window of (yes/no)<sub>1,2,...,k</sub> to (yes/no)<sub>k+i</sub> for some i (in binary); ML PRIMES problem (0.7, 0.8) NOT random! (prehaps related to AKS algorithm [2002], PRIMES is in P)
  - Sarnak's challenge: same window → Liouville Lambda (0.5, 0.001) Truly random (no simple algorithm for Lambda)
- [Alessandretti-Baronchelli-YHH 1911.02008]

ML/TDA@Birch-Swinnerton-Dyer III and  $\Omega$  ok with regression & decision trees: RMS < 0.1; Weierstrass  $\rightarrow$  rank: random

Arithmetic Geometry (Surprisingly Good)

- [Hirst-YHH-Peterken 2004.05218]: adjacency+permutation triple of dessin d'enfants (Grothendieck's Esquisse for Gal(Q/Q)); predicting transcendental degree (0.92, 0.9)
- YHH-KH Lee-Oliver arithmetic of curves
  - 2010.01213: Complex Multiplication, Sato-Tate  $(0.99 \sim 1.0, 0.99 \sim 1.0)$
  - 2011.08958: Number Fields: rank and Galois group (0.97, 0.9)
  - 2012.04084: BSD from Euler coeffs, integer points, torsion (0.99, 0.9); Tate-Shafarevich III (0.6, 0.8) [Hardest quantity of BSD]

• E an elliptic curve, local zeta-function & L-function:

$$Z(E/\mathbb{F}_p;T) = \exp\left(\sum_{k=1}^{\infty} \frac{\#E(\mathbb{F}_{p^k})T^k}{k}\right) = \frac{L_p(E,T)}{(1-T)(1-pT)};$$
  
$$L_p(E,T) = 1 - a_pT + pT^2; \quad a_p = p + 1 - \#E(\mathbb{F}_p).$$

Fix N and define vector  $v_L(E) = (a_{p_1}, \ldots, a_{p_N}) \in \mathbb{Z}^N$ ;

- $\sim 10^5$  balanced data from www.lmfdb.org; 50-50 cross validation.
- Labeled data:  $v_L(E) \longrightarrow \text{rank}$ , torsion, ... ([Birch-Swinnerton-Dyer: ])

$$L(E,s) := \prod_{p} L^{-1}(E,T) := p^{-s}; \quad \frac{L^{(r)}(E,1)}{r!} \stackrel{???}{=} \frac{|\mathrm{III}|\Omega \mathrm{Reg} \prod_{p} c_{p}}{(\#E(\mathbb{Q})_{\mathrm{tors}})^{2}},$$

r=rank; III=Shafarevich group; Reg=regulator;  $c_p$ =Tawagama; tors=Torsion

• Try generic ML algorithms on the data, record naive precision and Matthew's correlation coefficient/F1-Score

report (naive precision, Matthew's Correlation =  $\chi^2$ )

Rank 0 or 1 N = 300, conductor  $\in [1, 10^4]$ , Logistic regression: (0.991, 0.982) (Goldfield-Katz-Sarnak Conjecture: r=0 and 1 at 50% each)

Torsion Order = 1 or 2 N = 500, conductor  $\in [1, 3 \times 10^4]$ , naive Bayes: (0.9997, 0.9995) (Mordell-Weil, Faltings: max torsion = 16, but in LMFDB mostly 1 or 2)

 $\exists \mathbb{Z}$ -points (not just  $\mathbb{Q}$ ), N = 500, conductor range  $[1, 3 \times 10^4]$ , naive Bayes: (0.999, 0.998) (Siegel Thm: finite # integer points.)

Tate-Shafarevich group nothings gets better than 0.6; hardest part of BSD

looking for new conjectures e.g.,

- '19 YHH-Kim: separating hyperplane simple/non-simple groups; open
- '19 Brodie-Constantin-Lukas: exact formulae for cohomo surf.; proved.
- '20 YHH-Lee-Oliver: L-coefs and integer pt./torsion on ell; Known.
- '20 Craven-Jejjala-Par: Jones poly best-fit function; open
- . . .

speed up computations and accuracies e.g.,

- computing/estimating (top.inv., charges, etc) MUCH FASTER
- '19 Ashmore-YHH-Ovrut: speed up Donaldson alg@CY metric 10-100
- '20 Douglas et al., Anderson et al. accuracy improvement on Donaldson 10-100 times

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On the other hand, what is analyticity?

• prime generator =  $\left\lfloor \frac{n! \mod (n+1)}{n} \right\rfloor (n-1) + 2$  (not efficient)

• bundle-cohomology: Bott for Projective space:  $h^{q}(\mathbb{P}^{n}, (\wedge^{p}T\mathbb{P}^{n}) \otimes \mathcal{O}(k)) = \begin{cases} \binom{(k+n+p+1)\binom{k+n}{n-p}}{q} = 0 & k > -p-1, \\ 1 & q=n-p & k=-n-1, \\ \binom{-k-p-1}{k-n-1}\binom{-k-n-2}{p} & q=n & k < -n-p-1, \\ 0 & \text{otherwise} \end{cases}$ e.g. (2, 4)-CY3 hypersurface:  $h^{q}(X, \mathcal{O}_{X}(-k, m)) = \begin{cases} \binom{(k+n+p+1)\binom{k+n}{n-p}}{q} & q=0 & k < \frac{(1+2m)(6+m+m^{2})}{3(2+3m(1-m))} \\ \binom{(k+1)\binom{m+3}{3} - (k+1)\binom{m}{3}}{q} & q=0 & k < \frac{(1+2m)(6+m+m^{2})}{3(2+3m(1-m))} \\ 0 & \text{otherwise} \end{cases}$ • ...

• better suited for a computer programme any way

# An Inherent Hierarchy?

• In decreasing precision/increasing difficulty:

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\begin{array}{rl} \mbox{numerical} \\ \mbox{string theory} \rightarrow & \mbox{algebraic geometry over } \mathbb{C} \sim \mbox{arithmetic geometry} \\ & \mbox{algebra} \\ \mbox{string theory} \rightarrow & \mbox{combinatorics} \\ & \mbox{analytic number theory} \end{array}
```

Categorical Theory

- $\bullet\,$  suggested by & in prog. w/ B. Zilber, Merton Prof. of Logic, Oxford
- major part of Model Theory: Morley-Shelah Categoricity Thm
- Hart-Hrushovski-Laskowski Thm: 13 classes (levels) of iso-classes I(T,k) of a

theory T in first order logic over some cardinality k.

- Special Collection in AACA, Birkhäuser, *Dechant, YHH, Kaspryzyk, Lukas, ed*: https://www.springer.com/journal/6/updates/18581430
- Special Volume in JSC, Springer, *Hauenstein, YHH, Kotsireas, Mehta, Tang, ed.* https://www.journals.elsevier.com/journal-of-symbolic-computation/ call-for-papers/algebraic-geometry-and-machine-learning
- ML in theoretical physics & pure maths, Book, WS, YHH, ed.
- Int. J. Data Science in the Mathematical Sciences, WS, YHH et al., ed.

#### [YHH-Jejjala-Nelson ] "hep-th" 1807.00735

Word2Vec: [Mikolov et al., '13] NN which maps words in sentences to a vector space by context (much better than word-frequency, quickly adopted by Google); maximize (partition function) over all words with sliding window (W<sub>1,2</sub> weights of 2 layers, C<sub>α</sub> window size, D # windows )

$$Z(W_1, W_2) := \frac{1}{|D|} \sum_{\alpha=1}^{|D|} \log \prod_{c=1}^{C_{\alpha}} \frac{\exp([\vec{x}_c]^T \cdot W_1 \cdot W_2)}{\sum_{j=1}^{V} \exp([\vec{x}_c]^T \cdot W_1 \cdot W_2)}$$

We downloaded all ~ 10<sup>6</sup> titles of hep-th, hep-ph, gr-qc, math-ph, hep-lat from ArXiv since the beginning (1989) till end of 2017 (word cloud) (rmk: Ginzparg has been doing a version of linguistic ML on ArXiv) (rmk: abs and full texts in future)

ML Mathematical Structures

# Subfields on ArXiv has own linguistic particulars

• Linear Syntactical Identities

*bosonic* + *string-theory* = *open-string* 

holography + quantum + string + ads = extremal-black-hole

string-theory + calabi-yau = m-theory + g2

space + black-hole = geometry + gravity ...

- binary classification (Word2Vec + SVM) of formal (hep-th, math-ph, gr-qc) vs phenomenological (hep-ph, hep-lat) : 87.1% accuracy (5-fold classification 65.1% accuracy). ArXiv classifications
- Cf. Tshitoyan et al., "Unsupervised word embeddings capture latent knowledge from materials science literature", Nature July, 2019: 3.3. million materials-science abstracts; uncovers structure of periodic table, predicts discoveries of new

thermoelectric materials years in advance, and suggests as-yet unknown materials

# Merci!

	Syntax		Semantics
•	Alpha Go	$\rightarrow$	Alpha Zero
	ML Patterns	$\rightarrow$	Auto Thm Pf&Chk

• Renner et al., PRL/Nature News, 2019:

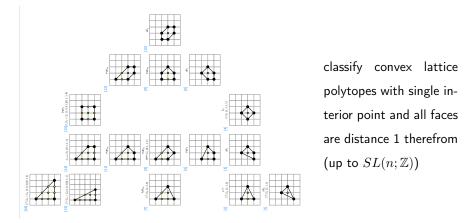
ML (SciNet, autoencoder)

- Lample-Charton, 2019: ML Symolic manipulations in mathematics
- Tegmark et al., 2019 Al Feynman, symb regressor
- Raayoni et al. 2020 Ramanujan-Machine
- Barbaresco-Nielson 2021 Infor Geom/ML



Sophia (Hanson Robotics, HK) 1st non-human citizen (2017, Saudi) 1st non-human with UN title (2017) 1st String Data Conference (2017)

## 16 Reflexive Polygons Back to Reflexives



Kreuzer-Skarke: 4319 reflexive polyhedra, 473,800,776 reflexive 4-polytopes, Skarke: next number is at least 185,269,499,015.

# Computing Hodge Numbers $\mathcal{O}(e^{e^d})$

• Recall Hodge decomposition  $H^{p,q}(X) \simeq H^q(X, \wedge^p T^\star X) \leadsto$ 

 $H^{1,1}(X) = H^1(X, T_X^*), \qquad H^{2,1}(X) \simeq H^{1,2} = H^2(X, T_X^*) \simeq H^1(X, T_X)$ 

• Euler Sequence for subvariety  $X \subset A$  is short exact:

$$0 \to T_X \to T_M|_X \to N_X \to 0$$

Induces long exact sequence in cohomology:

• Need to compute Rk(d), cohomology and  $H^i(X, T_A|_X)$  (Cf. Hübsch)

Back to ML

# String/Algebraic Geometry: 2017-

- CICY configuration → Hodge Numbers: YHH (1706.02714)
   Bull-YHH-Jejjala-Mishra (1806.03121, 1903.03113), Krippendorf-Syvaeri
   [2003.13679] Erbin-Finotello (2007.13379; '21) : (0.99, 0.9) YHH-Lukas
   [2009.02544] CICY4: (0.98, 0.9)
- Elliptic fibrations (from CICYs): YHH-SJ Lee (1904.08530) (0.99,0.9)
- Distinguishing Heterotic SMs from the sum-line-bundle database (Anderson-Constantin-Gray-Lukas-Palti) and extrapolating beyond Deen-YHH-Lee-Lukas (2003.13339): (0.98, 0.99)
- Calabi-Yau metric: improves Donaldson alg. for numerical CY metric by 10-100 times Ashmore–YHH–Ovrut '19, q.v. Anderson, Gray, Krippendorf, Raghuram, Ruehle; Douglas–Lakshminarasimhan–Qi, '20,

Jejjala-Pena-Kaloni-Mishra, '21

YANG-HUI HE (London/Oxford/Nankai)

ML Mathematical Structures

- q.v., Bundle Cohomology (Ruehle, Brodie-Constantin-Lukas, Larfors-Schneider, Otsuka-Takemoto, Klaewer-Schlechter)
- q.v., Kreuzer-Skarke Dataset (Halverson, Long, Nelson; McCallister-Stillman)
- q.v., Calabi-Yau volumes in AdS/CFT (Krefl-Seong)
- q.v., MSSM from orbifold models (Parr-Vaudrevange-Wimmer)
- q.v. Particle Masses Gal-Jejjala-Pena-Mishra ....
- q.v. Knot invariants: Jejjala-Kar-Parrikar, Craven-Jejjala-Kar Gukov-Halverson-Ruehle-Sułkowski, using NLP
- YHH-Jejjala-Nelson NLP on ArXiv sections
- q.v. DEEP CONNECTIONS K. Hashimoto: AdS/CFT = Boltzmann
   Machine; Halverson-Maiti-Stoner: QFT = NN; de Mello-Koch: NN = RG;
   Vanchurin 2008: Universe = NN. Back to ML Maths YHH, 2011.14442 Review

- Kreuzer-Skarke: http://hep.itp.tuwien.ac.at/~kreuzer/CY/
  - new PALP: Braun-Walliser: ArXiv 1106.4529
  - Triang: Altmann-YHH-Jejjala-Nelson: http://www.rossealtman.com/
- CICYs: resurrected Anderson-Gray-YHH-Lukas, http://www-thphys. physics.ox.ac.uk/projects/CalabiYau/cicylist/index.html
- q.v. other databases of interesting to the math/physics community: Graded Rings/Varieties: Brown, Kasprzyk, et al. http://www.grdb.co.uk/ Finite Groups/Rings: GAP https://www.gap-system.org/ Modular Forms: Sutherland, Cremona et al. https://www.lmfdb.org/ Knots & Invariants: KnotAtlas http://katlas.org/ Return

. . .

Large Depth Thm: (Cybenko-Hornik) For every continuous function  $f : \mathbb{R}^d \to \mathbb{R}^D$ , every compact subset  $K \subset \mathbb{R}^d$ , and every  $\epsilon > 0$ , there exists a continuous function  $f_\epsilon : \mathbb{R}^d \to \mathbb{R}^D$  such that  $f_\epsilon = W_2(\sigma(W_1))$ , where  $\sigma$  is a fixed continuous function,  $W_{1,2}$  affine transformations and composition appropriately defined, so that  $\sup_{x \in K} |f(x) - f_\epsilon(x)| < \epsilon$ .

Large Width Thm: (Kidger-Lyons) Consider a feed-forward NN with n input neurons, m output neuron and an arbitrary number of hidden layers each with n + m + 2 neurons, such that every hidden neuron has activation function  $\varphi$  and every output neuron has activation function the identity. Then, given any vector-valued function f from a compact subset  $K \subset \mathbb{R}^m$ , and any  $\epsilon > 0$ , one can find an F, a NN of the above type, so that  $|F(x) - f(x)| < \epsilon$  for all  $x \in K$ .

**ReLU Thm:** (Hanin) For any Lebesgue-integral function  $f : \mathbb{R}^n \to \mathbb{R}$  and any  $\epsilon > 0$ , there exists a fully connected ReLU NN F with width of all layers less than n + 4 such that  $\int_{\mathbb{R}^n} |f(x) - F(x)| dx < \epsilon$ .

Back to Landscape

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