

## The AI Mathematician

## YANG-HUI HE

## 何楊輝

### London Institute of Mathematical Sciences, Royal Institution

Merton College, University of Oxford

University of Hertfordshire, Nov 2024

## The London Institute for Mathematical Sciences









- UK's only independent research institute for maths; modelled after IAS, Princeton
- Founded in 2011 by Dr. Thomas Fink
- Housed in the Faraday Suites of the Royal Institution of Great Britain
- 1 of 23 themes: AI for Maths Discovery

https://lims.ac.uk/event/ai-assisted-maths-discovery/

• 2022 Est: Arnold & Laudau Fellowships

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Hertfordshire, 2024 2 / 40



Bottom-Up as a formal logical system Top-Down as a creative/intuitive art Meta-Mathematics as a language

Review, YHH: A Triumvirate of AI Driven Theoretical Discovery, 2405.19973 Nature Rev. Phys, 2024

Review, YHH: Machine-Learning Mathematical Structures, 2101.06317 IJMSDS 2021



- speed-up in computations & modelling: goes without saying
- crucial to increasing number of important theorems
  - 4-color [Appel-Haken-Koch 1976]
  - Kepler Conjecture [Hales 1998, formal check + acceptance 2017]
  - Classification of Finite Simple Groups [ Galois 1832 Gorenstein et al. 2008]
  - . . .



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



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Automated Theorem Proving (ATP) a long tradition

- Newell-Simon-Shaw [1956] Logical Theory Machine  $\sim$  proved some Principia
- Type Theory [1970s] Martin-Löf, Coquand
- Univalent Foundation / Homotopy Type Theory [2006-] Voevodsky



- Coq interactive proving system: 4-color (2005); Feit-Thompson Thm (2012);
- Lean (2013-) all of undergraduate maths
- Davenport: ICM 2018 "Computer Assisted Proofs"
- Buzzard: ICM 2022: XenaProject (Lean)
- Gowers-Green-Manner-Tao (2023): Freiman-Rusza-Marton Conj (Lean Pf)
- Tao: Oxford/LMS public lecture 2024
- over-optimistic view Szegedy (DeepMind): computers > humans @ chess (1990s); @ Go (2018); @ Proving theorems (2030)



2018 [YHH-Jejjala-Nelson ] 1807.00735:  $\sim 10^6$  titles of hep-th, hep-ph, gr-qc, math-ph, hep-lat from ArXiv 1989-2017  $\Rightarrow$  Word2Vec LLM

- Subfields on ArXiv has own linguistic particulars
- Science (ArXiv) / Pseudo-science (viXra) syntactically distinguishable

2019 Tshitoyan et al., Nature July : 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

2022 ChatGPT has passed the Turing Test

2023-24 LLM for Maths: OpenAl's QStar, Meta-Al's LLama, EpochAi's FrontierMath, Meta's PatternBoost, RelationalAl's Graffiti Deepmind's FunSearch AlphaGeo (53%)

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### (Terence Tao, 28 points - Silver Medal; AlphaGeo2, 28 points - Silver Medal)





Graph showing performance of our AI system relative to human competitors at IMO 2024. We earned 28 out of 42 total points, achieving the same level as a silver medalist in the competition.

Score on IMO 2024 problems





• In practice, Maths is Top-Down: practice before (<) foundation Countless eg:

calculus < analysis; alg geometry < Bourbaki, permutations / Galois theory < abstract algebra  $\ldots$ 

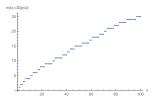
• The best neural network of C18-19th?



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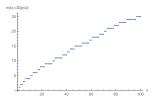
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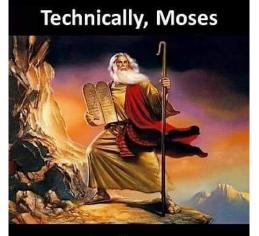
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• BSD computer experiment of Birch & Swinnerton-Dyer [1960's] on plots of rank r &  $N_p$  on elliptic curves



was the first person with a tablet downloading data from the cloud



The age of data science in mathematics/theoretical physics not as recent as you might think

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•  $[0, 0, 1, 0, 0, 1, 0, 0, 1, 0, 0, 1, \ldots]$ 



- [0, 0, 1, 0, 0, 1, 0, 0, 1, 0, 0, 1, . . .] multiple of 3 or not.
- - 0, 0, 0, 0, 1, 1, 0, 1, 1, 0 ...]



[0,0,1,0,0,1,0,0,1,0,0,1,...]
 multiple of 3 or not.

[1, 1, 1, 0, 1, 1, 0, 1, 1, 0, 1, 0, 0, 1, 1, 0, 0, 1, 0, 1, 1, 0, 1, 0, 0, 1, 0, 0, 1, 1, 0, 0, 1, 0, 1, 1, 0, 0, 1, 0, 1, 0, 0, 1, 0,

0, 0, 0, 0, 1, 1, 0, 1, 1, 0 ...]

Prime or Not for odd integers.

[1, 0, 0, 1, 0, 1, 0, 0, 1, 1, 0, 0, 0, 1, 1, 1, 0, 0, 0, 0, 1, 1, 0, 1, 1, 1, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 0, 1, 1, 1, 0, 0, 0, 0, 0, 0,

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1, 0, 1, 1, 1, 1, 0, 0, 0, 1, ...]

Even/Odd of number of prime factors (Liouville Lambda)



A mathematician, like a painter or a poet, is a maker of patterns. If his patterns are more permanent than theirs, it is because they are made with ideas... G. Hardy, A Mathematician's Apology



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One (only?) sure thing that AI can do better than humans is pattern detection.



• Binary Classification of a Binary Vector (sliding window of, say, length 100); supervised learning: predict next one, e.g., Prime/Not becomes:



• Binary Classification of a Binary Vector (sliding window of, say, length 100); supervised learning: predict next one, e.g., Prime/Not becomes:

- pass to standard classifiers: SVW, Bayes, Nearest Neighbour; NN of the form  $\mathbb{R}^{100} \xrightarrow{\text{linear}} \mathbb{R}^{20} \xrightarrow{\text{tanh}} \mathbb{R}^{20} \xrightarrow{\text{Round} \sum} \mathbb{Z}$ , your kitchen sink, ...
- take 50,000 samples, 20-80 cross-validation, record (precision, MCC)
- similar performance for most: Mod3: (1.0, 1.0); PrimeQ, after balancing: (0.8, 0.6); Liouville Λ: (0.5, 0.001)

Algebraic Geometry as Image Processing A stringy Origin

• A typical calculation:

• [YHH 1706.02714] Deep-Learning the Landscape, *PLB 774, 2017*; (cf. Feature in *Science*, Aug. vol 365 issue 6452, 2019): think of it as an image processing problem



# Thank you! Since 2017-





### fantastic students

Jiakang Bao, Elli Heyes, Ed Hirst, Tejas Acharya, Daatta Aggrawal, Malik Amir, Kieran Bull, Lucille Calmon, Siqi Chen, Suvajit Majumder, Maks Manko, Toby Peterken, Juan Pérez-Ipiña, Max Sharnoff, Yan Xiao

## wonderful collaborators

Physics: Guillermo Arias-Tamargo, David Berman, Heng-Yu Chen, Andrei Constantin, Sebastián Franco, Vishnu Jejjala, Seung-Joo Lee, Andre Lukas, Shailesh Lal, Brent Nelson, Diego Rodriguez-Gomez, Zaid Zaz

Algebraic Geometry: Anthony Ashmore, Challenger Mishra, Rehan Deen, Burt Ovrut

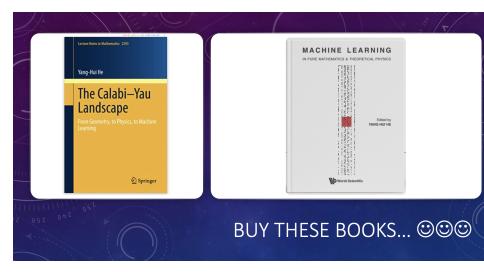
Number Theory: Laura Alessandretti, Andrea Baronchelli, Kyu-Hwan Lee, Tom Oliver, Alexey Pozdnyakov, Drew Sutherland, Eldar Sultanow

Representation Theory: Mandy Cheung, Pierre Dechant, Minhyong Kim, Jianrong Li, Gregg Musiker

Combinatorics: Johannes Hofscheier, Alexander Kasprzyk, Shiing-Tung Yau

## Please buy









### Programme theme

Defining a theory of quantum govery sensitive one of the most challenging problems at the outling edge of meanth is methemotion and Preceded physics. Unlocating this problem implies constructing a quantum field benefits description of gover which July elacisities from a quantum field theory moved granitational protection budgeture disalization.

Nuch of the progress is shaping the language and the framework of this problem owes its genesis to a specific subset of problems in quantum gravity, namely those dealing with understanding the organisation of information in black holes.

These problems is tark can be neady divided into two streams of research, each dealing with a different class of black hales as systems of interest

1. The examenation of the quantum microsolities of a special state of black holes, called BPS. Much holes, in supershifts benches, fronge Moch moduler form and automorphic forms. This has led to successing a consceptiol of exoting connections between they there gave particular statements, such as the setting microsolities and Moch moduler is more statement. The statement of BPS black holes and Moch moduler is more, the statement of BPS statements, such as the setting microsolities of BPS black holes and Moch moduler is more, the statement of BPS black holes and Moch moduler is more than the filter of Black holes and Moch moduler is more than the statement of BPS.



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YHH, M. Burtsev, Nature, Jan 2024.



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• (Automaticity) be generated by AI



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#### garasers

 Appendix Carlin Likewaldy of Cardinoppe Soloof In Michael Course Likewaldy Tang-Ini He Condon-Anthina Kowaldy Mang-Ini He Condon-Anthina Kowaldy Markan Calago Markan Calago

- (Automaticity) be generated by AI
- (Interpretability) concrete enough to be a conjecture



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- (Automaticity) be generated by AI
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- (Non-Triviality) for the community to work on it



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- (Automaticity) be generated by AI
- (Interpretability) concrete enough to be a conjecture
- (Non-Triviality) for the community to work on it
- make Birch happy





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2022 Murmuration Phenomenon A new pattern in the primes, relation to BSD and a bias in L-coefficients of elliptic curves [YHH-Lee-Oliver-Podznyakov, 2022, YHH-Lee-Oliver-Podznyakov-Sutherland, 2024] made Buzzard/Birch almost happy (still not completely: human intervention was needed)



2017-8 YHH (1706.02714, 1812.02893)

- Predicting primes  $2 \rightarrow 3, 2, 3 \rightarrow 5, 2, 3, 5 \rightarrow 7$ ; no way
- PrimeQ: (0.7, 0.8); Sarnak's Challenge of Liouville Lambda (0.5, 0.001)

# 2019 (Alessandretti-Baronchelli-YHH 1911.02008) ML/TDA@BSD from Weierstrass represenation; naive attempt

2020-21 (YHH-KH Lee-Oliver):

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]

# Al-Driven Mathematical Discovery: Murmuration





2022 - YHH, Kyu-Hwan Lee, Tom Oliver, Alexey Pozdnyakov (2204.10140)

Quanta Feature 2024:





Diophatine Equations (rational  $\mathbb{Q}$  solutions to polynomials)

• quadratic (Pythagoras)  $x^2 + y^2 = 1$ , many e.g.  $(x, y) = (\frac{3}{5}, \frac{4}{5})$ 



Diophatine Equations (rational  $\mathbb{Q}$  solutions to polynomials)

- quadratic (Pythagoras)  $x^2 + y^2 = 1$ , many e.g.  $(x,y) = (\frac{3}{5}, \frac{4}{5})$
- cubic (Elliptic Curve) HARD!!!!
  - e.g.,  $E: x^3 + y^2 = 1$  (Thm: Weierstrass form  $y^2 = x^3 g_2 x g_4$ )
  - has enormous implications: e.g. Fermat's Last Theorem
  - Thm:  $E(\mathbb{Q}) \simeq \mathbb{Z}^r \times Z_{tor}$  (*r* rank = # infinite families of solutions)
  - Work modulo prime p, e.g.,  $2^3+4^2\equiv 1(\bmod 23), \ 3^3+2^2\equiv 1(\bmod 5)$
  - Euler Coeffcients  $a_p = p + 1 \#E(\mathbb{F}_p)$

### ML on 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;  $c_p$ =Tamagawa; tors=Torsion



### Importance of Representation

(Alessandretti-Baronchelli-YHH 1911.02008, *New Scientist* feature 2019 used Weierstrass coefficients of elliptic curves: useless in predicting any of the BSD quantities

needed insights from Oliver+Lee to use  $a_p$  coefficients

### Importance of Human Interpretation

Murmurations of elliptic curves: YHH, Lee, Oliver, Pozdnyakov, 2204.10140 A new mathematical phenomenon



Q: YHH, Lee, Oliver, Pozdnyakov on HLOP results from 2020 - 22: WHY is ML so good at telling ranks apart by looking at  $a_p$  coefficients?? e.g., PCA:

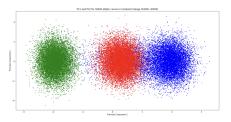
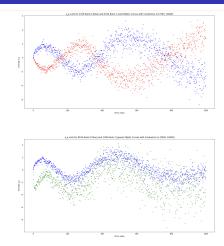


Figure 2: A plot of PC1 (*x*-axis) against PC2 (*y*-axis) for elliptic curves in the balanced dataset of 36,000 randomly chosen elliptic curves with rank  $r_E \in \{0, 1, 2\}$  and conductor  $N_E \in [1000, 4000]$ . The blue (resp. red, green) points are the images of the vectors  $v_L(E)$  corresponding to the elliptic curves in our dataset with rank 0 (resp. 1, 2) under a map  $\mathbb{R}^{100} \rightarrow \mathbb{R}^2$  onstructed using PCA.

# Murmuration function





construct a vertical average (rank r, conductor range  $[N_1, N_2]$ , n-th prime  $p_n$ )

$$f_r(n) := \frac{1}{\#\mathcal{E}_r[N_1, N_2]} \sum_{E \in \mathcal{E}_r[N_1, N_2]} a_{p_n}(E)$$

Figure 1: (Top) Plots of the functions  $f_0(n)$  (blue) and  $f_1(n)$  (red) for  $1\leq n\leq 1000$  and  $[N_1,N_2]=(7500,10000]$ . (Bottom) Plots of the functions  $f_0(n)$  (blue) and  $f_2(n)$  (green) for  $1\leq n\leq 1000$  and  $[N_1,N_2]=[5000,10000]$ . Further details are given in Example 1.



- To appear [HLOP + Sutherland]
  - Does not work if ordered by height (Weierstrass coef)
  - Take dyadic conductor range:  $[N^x, N^{x+1}]$  : scale invariant (indep of x)
  - Taking more data  $(10^{7\sim8})$  at high N: converges to oscillatory curve
- A General Phenomenon that reflects biases in distribution of primes
  - L-function for Dirichlet characters (Lee-Oliver-Podznyakov 2023)
  - Zubrilina, Cowan: for weight 2 modular forms (2023)
  - conference at ICERM in July

https://icerm.brown.edu/events/htw-23-ma/



### **Conjecture Formulation**

- C19th Gauss's eyes on  $\pi(x) \sim \int_2^x rac{dx}{\ln(x)}$
- C20th Birch + Swinnerton-Dyer on the EDSAC-2 computer@Cambridge
- C21st AI guided human intuition:

Knots ~> New Expressions for Invariants (DeepMind)

LMFdD ~> Murmuration Conjectures (YHH-Lee-Oliver-Poznyakov)

New Matrix Multiplication (DeepMind)



### **Conjecture Formulation**

- C19th Gauss's eyes on  $\pi(x) \sim \int_2^x rac{dx}{\ln(x)}$
- C20th Birch + Swinnerton-Dyer on the EDSAC-2 computer@Cambridge
- C21st AI guided human intuition:

Knots ~> New Expressions for Invariants (DeepMind)

LMFdD  $\sim$  Murmuration Conjectures (YHH-Lee-Oliver-Poznyakov)

New Matrix Multiplication (DeepMind)

- The future of mathematics is a combination of
  - Bottom-up ATP using AI
  - Top-Down machine-guided human intuition using AI
  - Mathematics as LLM using AI

## THANK YOU





"I have often wondered over the roles of knowledge or experience, on the one hand, and imagination or intuition, on the other, in the process of discovery. I believe that there is a certain fundamental conflict between the two, and knowledge, by advocating caution, tends to inhibit the flight of imagination. Therefore, a certain naivete, unburdened by conventional wisdom, can sometimes be a positive asset."

- Harish-Chandra Mehrotra



- $\bullet\,$  Trichtomy classification of (connected compact orientable) surfaces  $\Sigma\,$ 
  - Euler: topological classification of  $\dim_{\mathbb{R}} = 2$  Euler number  $\chi(\Sigma)$ , genus  $g(\Sigma)$
  - Gauss: relates topology to metric geometry
  - Riemann: complexify  $\rightsquigarrow$  Riemann surfaces or complex curves:  $\dim_{\mathbb{C}} = 1$

		<b>20</b> do 88		
$g(\Sigma) = 0$	$g(\Sigma) = 1$	$g(\Sigma) > 1$		
$\chi(\Sigma) = 2$	$\chi(\Sigma) = 0$	$\chi(\Sigma) < 0$		
Spherical	Ricci-Flat	Hyperbolic		
+ curvature	$0 \ {\rm curvature}$	— curvature		



$\chi(\Sigma) = 2 - 2g(\Sigma) =$	$= [c_1(\Sigma)] \cdot [\Sigma] =$	$=rac{1}{2\pi}\int_{\Sigma} R=$	$=\sum_{i=0}^{2}(-1)^{i}h^{i}(\Sigma)$
Topology	Algebraic Geometry	Differential Geometry	Index Theorem (co-)Homology
Invariants	Characteristic classes	Curvature	Betti Numbers



- $\bullet \ \dim_{\mathbb{R}} > 2$  manifolds extremely complicated
- Luckily, for a special class of complex manifolds called Kähler

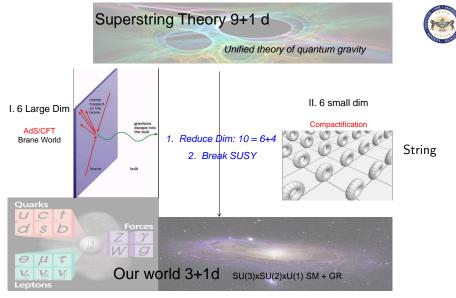
$$g_{\mu\bar{\nu}} = \partial_{\mu}\partial_{\bar{\nu}}K(z,\bar{z})$$

all  $\Sigma$  in  $\dim_{\mathbb{C}}=1$  automatically Kähler

• CONJECTURE [E. Calabi, 1954, 1957]: M compact Kähler manifold  $(g, \omega)$ and  $([R] = [c_1(M)])_{H^{1,1}(M)}$ . Then  $\exists ! (\tilde{g}, \tilde{\omega})$  such that  $([\omega] = [\tilde{\omega}])_{H^2(M;\mathbb{R})}$  and  $Ricci(\tilde{\omega}) = R$ .

Rmk:  $c_1(M) = 0 \Leftrightarrow$  Ricci-flat (rmk: Ricci-flat familiar to physicists through GR)

• THEOREM [S-T Yau, 1977-8; Fields 1982] Existence Proof



Phenomenology [Candelas-Horowitz-Strominger-Witten]: 1985

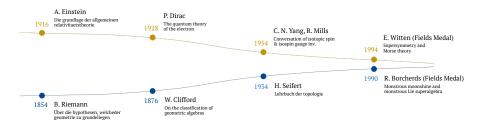
simplest solution of 6 extra dimensions: Ricci-Flat, Kähler  $\dim_{\mathbb{C}} = 3$ 



- Strominger was next door to Yau in 1986 at the IAS, physicists called Ricci-Flat, Kähler manifolds, CHSW called these Calabi-Yau manifolds
- GEOMETRIZATION PROGRAMME: Historically, the right language of physics is increasingly geometrical:
  - $\bullet \ \ {\sf Gravity}/{\sf Space-time} \rightsquigarrow {\sf GR} \rightsquigarrow {\sf Differential geometry};$
  - Particle physics/Standard Model → Gauge Theory/Yang-Mills → Algebraic geometry (bundles/connections) + group theory (Lie and Finite groups);
  - Condensed matter physics of topological insulators  $\sim$  algebraic topology;  $\dots$
  - String theory is a brain-child of this tradition
- TAKE-HOME MESSAGE: Whenever physics and maths converge and generate new ideas, the right things are happening



### Physics



#### Mathematics



### 1959

### 2010

The Unreasonable Effectiveness of Mathematics in the Natural Sciences

Richard Courant Lecture in Mathematical Sciences delivered at New York University, May 11, 1939

> EUGENE P. WIGNER Princeton University

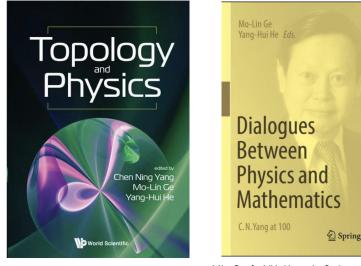
Phil. Trans. R. Soc. A (2010) 368, 913-926

#### Geometry and physics

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"One may be tempted to invert Wigner's comment and marvel at 'the unreasonable effectiveness of physics in mathematics.""



CN Yang, ML Ge & YH He, ed, World Scientific, 2019 contributions: Atiyah, Dijkgraaf, Kim, Penrose, Witten, et al.

D Springer ML Ge & YH He, ed, Springer-Nature,

2022 contributions: Drinfeld, Leggett, Manin, Penrose, Polyakov, Wilczek, Wit-

ten. et al.



- 1986- "Strings" Conference
- 2002- "StringPheno" Conference
- 2006 2010 String Vacuum Project (NSF)
- 2008 ISGT Integrability in String/Gauge
- 2011- "String-Math" Conference (2020 , M-theory & Maths Workshop)
- 2012- "Amplitudes"
- 2014- String/Theoretical Physics Session in SIAM Conference
- 2017- "String-Data" Conference

Back to ML for Maths

# Computing Hodge Numbers: Sketch (Back to AG)



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

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

• 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:



- Bijection from 1234567890 to  $\{1, 2, \dots, 9, 0\}$ ?
- Take large sample, take a few hundred thousand (e.g. NIST database)



• Data = Training Data ⊔ Validation Data

Test trained NN on validations data to see accuracy performance



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 NN@Alg Geo