# Machine-Learning Mathematical Structures 

## YANG-HUI HE

Dept of Mathematics, City, University of London
Merton College, University of Oxford
School of Physics, NanKai University

String Data 2020

## How does one *DO* mathematics, I ?

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


## How does one *DO* mathematics, I ?

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

## 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)


## 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

- BSD computer experiment of Birch \& Swinnerton-Dyer [1960's] on plots of rank $r$ \& $N_{p}$ on elliptic curves


## 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

- BSD computer experiment of Birch \& Swinnerton-Dyer [1960's] on plots of rank $r$ \& $N_{p}$ on elliptic curves


## 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


## Question

- 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
- 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 case because it encodes WHAT is interesting to calculate (if not how)


## Question

- 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

- 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 case because it encodes WMIAT is interesting to calculate (if not how)


## Question

- 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

- 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 case because it encodes WHAT is interesting to calculate (if not how)


## Question

- 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
- 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 case because it encodes WHAT is interesting to calculate (if not how).


## Mathematical Data: perfect for mining

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


## Methodology

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 Supervised ML Methods Regressor \& Classifiers

- NN: MLPs; CNNs; RNNs, ... (gentle tuning of architecture and hyper-parameters)
- SVM, Bayes, Decision Trees, PCA, Clustering, ...
- ML: emergence of complexity via connectivity $\leadsto$ Intution (?)

This Talk: Status Report of Experiments in the last couple of years

- all standard methods $\simeq$ same performance
- ~20-80 split; training on 20 ( precision, Matthews' $\phi$ or $R^{2}$ )


## String/Algebraic Geometry

- CICY configuration $\rightarrow$ Hodge Numbers: YHH (1706.02714) Bull-YHH-Jejjala-Mishra (1806.03121, 1903.03113), Krippendorf-Syvaeri [2003.13679] Erbin-Finotello (2007.13379; : $(0.99,0.9)$ 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


## String/Algebraic Geometry: 2018-

- 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: $N N=R G$;
Vanchurin 2008: Universe $=$ NN.

## 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: $(0.9,0.8)$ )
- [Chen-YHH-Lal-Zas 2006.16114]: even/odd/reflection sym (>0.99); distinguishing CFT 3 pt functions ( $>0.99$ ); Fourier coefficients / conformal block presence ( $>0.97$ ) ...
(q.v. [Krippendorf-Syvaeri 2003.13679])


## 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 $>,=,<0(0.8,0.7) ; ? \exists$
Hamilton cycles ( $0.8,0.6$ ); ? $\exists$ Euler cycles $(0.8,0.6)$
(Rmk: NB. Only "solving" the likes of traveling salesman stochastically)
- spectral bounds ( $R^{2} \sim 0.9$ ) ...
- 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 window of (yes/no $)_{1,2, \ldots, k}$ to (yes/no) $)_{k+i}$ for some $i$; ML PRIMES problem (0.7, 0.8) NOT random! (prehaps related to AKS algorithm [2002], PRIMES is in P )
- Sarnak's challenge: same window $\rightarrow$ Liouville Lambda (0.5, 0.001) Truly random (no simple algorithm for Lambda)
- [Alessandretti-Baronchelli-YHH 1911.02008]

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

## Number Theory: A Modern Hope?

## Arithmetic Geometry (Surprisingly Good)

- [Hirst-YHH-Peterken 2004.05218]: adjacency+permutation triple of dessin d'enfants (Grothendieck's Esquisse for $\operatorname{Gal}(\overline{\mathbb{Q}} / \mathbb{Q})$ ) ; 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 Ш $(0.6,0.8)$ [Hardest quantity of BSD]


## Clearly useful for maths and physics

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; proved.
- '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


## The other Extreme (?) View-Point

On the other hand, what is analyticity?

- $n$-th pime $=\left\lfloor\frac{n!\bmod (n+1)}{n}\right\rfloor(n-1)+2$ (not efficient)
- bundle-cohomology:

e.g. $(2,4)$-CY3 hypersurface:

$$
h^{q}\left(X, \mathcal{O}_{X}(-k, m)\right)=
$$

$$
\begin{cases}(k+1)\binom{m}{3}-(k-1)\binom{m+3}{3} & q=0 \quad k<\frac{(1+2 m)\left(6+m+m^{2}\right)}{3(2+3 m(1-m))} \\ (k-1)\binom{m+3}{3}-(k+1)\binom{m}{3} & q=1 \quad k>\frac{\left.(1+2 m)(6+m+m)^{2}\right)}{3(2+3 m(1-m))} \\ 0 & \text { otherwise }\end{cases}
$$

- better suited for a computer programme any way


## An Inherent Hierarchy?

- In decreasing precision/increasing difficulty:


## numerical

string theory $\rightarrow \quad$ algebraic geometry over $\mathbb{C} \sim$ arithmetic geometry algebra string theory $\rightarrow \quad$ combinatorics analytic number theory

## - Categorical Theory

- suggested by \& in prog. w/ B. Zilber, Merton Prof. of Logic, Ox
- major part of Model Theory: Morley-Shelah Categoricity Thm
- Hart-Hruskovski-Laskowski Thm: 13 classes (levels) of iso-classes $I(T, k)$ of a theory $T$ in first order logic over some cardinality $k$.


## Thank you!

| 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 AI 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)

## Various Databases

- 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

## A Prototypical Question

- Hand-writing Recognition, e.g., my 0 to 9 is different from yours:

$$
1234567890
$$

- How to set up a bijection that takes these to $\{1,2, \ldots, 9,0\}$ ? Find a clever Morse function? Compute persistent homology? Find topological invariants? ALL are inefficient and too sensitive to variation.
- What does your iPhone/tablet do? What does Google do? Machine-Learn
- Take large sample, take a few hundred thousand (e.g. NIST database)

$$
\begin{aligned}
& 6 \rightarrow 6,8 \rightarrow 8,2 \rightarrow 2,4 \rightarrow 4,8 \rightarrow 8, \boldsymbol{y} \rightarrow 7,8 \rightarrow 8, \\
& 0 \rightarrow 0,4 \rightarrow 4,2+2,5+5,6 \rightarrow 6,3 \rightarrow 3,2 \rightarrow 2,
\end{aligned}
$$

$$
\mathbf{9}+\mathbf{9}, \mathbf{O}+8, \mathbf{3}+3, \mathbf{8}+8, \mathbf{8}+8, \mathbf{(}+1, \mathbf{O}+0, \ldots \quad 28 \times 28 \times(R G B)
$$

## A Single Neuron: The Perceptron

- began in 1957 (!!) in early AI experiments (using CdS photo-cells)
- DEF: Imitates a neuron: activates upon certain inputs, so define
- Activation Function $f\left(z_{i}\right)$ for input tensor $z_{i}$ for some multi-index $i$;
- consider: $f\left(w_{i} z_{i}+b\right)$ with $w_{i}$ weights and $b$ bias/off-set;
- typically, $f(z)$ is sigmoid, Tanh, etc.
- Given training data: $D=\left\{\left(x_{i}^{(j)}, d^{(j)}\right\}\right.$ with input $x_{i}$ and known output $d^{(j)}$, minimize

$$
S D=\sum_{j}\left(f\left(\sum_{i} w_{i} x_{i}^{(j)}+b\right)-d^{(j)}\right)^{2}
$$

to find optimal $w_{i}$ and $b \leadsto$ "learning", then check against Validation Data

- Essentially (non-linear) regression


## The Neural Network: network of neurons $\sim$ the "brain"

- DEF: a connected graph, each node is a perceptron (Implemented on Mathematica $\geq 11.1$ / TensorFlow-Keras on Python)
(1) adjustable weights/bias;
(2) distinguished nodes: 1 set for input and 1 for output;
(3) iterated training rounds.
input layer


Simple case: forward directed only, called multilayer perceptron

Many Layers: DEEP Learning
Connectivity $\leadsto$ Emergence of Complexity

- Essentially how brain learns complex tasks; apply to our Landscape Data

Back to Landscape

