MACHINE (K)NOT LEARNING



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Collaborators



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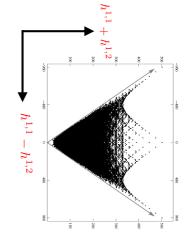
Arjun Kar



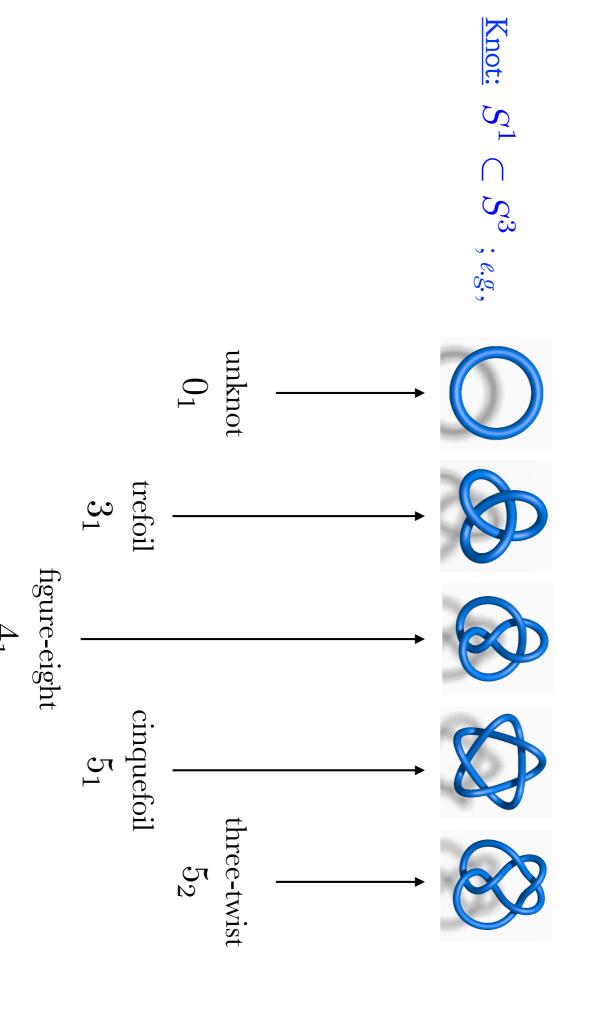
"Disentangling a Deep Learned Volume Formula" arXiv: 2012.03955

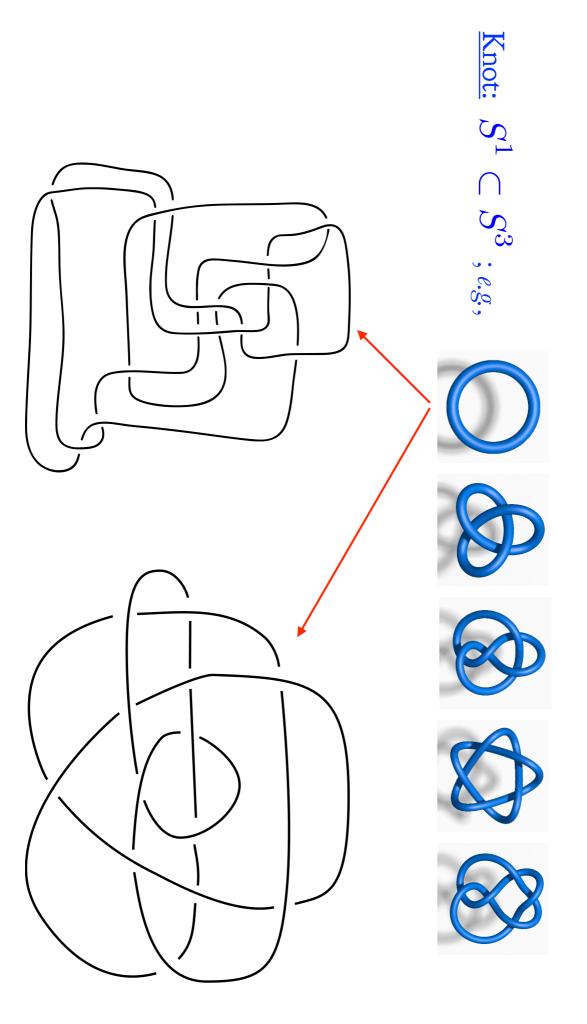
Mathematical Phenomenology

- Note patterns then look for an explanation
- Mirror symmetry is prototype example
- Knot theory provides another case study



- Use machine learning to train a computer to calculate in hep-th, math
- Black box gives **probably approximately correct** answers
- So far, we have mainly used ML to identify associations
- Want to bridge this success to new analytic results and methods
- Illustrate technology and then discuss this in a broader context





Thistlethwaite unknot

Ochiai unknot

Knot:
$$S^1 \subset S^3$$
; e.g.,











$$= q^{\frac{1}{4}}$$

w(K) = overhand - underhand

Jones (1985)

$$J(\bigcirc;q)=1$$

topological invariant: independent of how the knot is drawn

<u>Question:</u> how to calculate these:

Answer: quantum field theory!

Topological Invariants

On a manifold \mathcal{M} with metric $g_{\mu\nu}$, a topological invariant enjoys:

$$\frac{\delta}{\delta g_{\mu\nu}} \langle \mathcal{O}_1 \dots \mathcal{O}_n \rangle = 0$$

In <u>Chern-Simons theory</u>, the operators are Wilson loops

$$U_R(\gamma) = \operatorname{tr}_R \mathcal{P} \exp\left(i \oint_{\gamma} A\right)$$

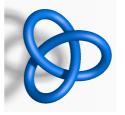
The colored Jones polynomial is a knot invariant:

$$J_n(K; q = e^{2\pi i/(k+2)}) = \frac{\int_{\mathcal{U}} [DA] \ U_n(K) e^{iS_{CS}(A)}}{\int_{\mathcal{U}} [DA] \ U_n(0_1) e^{iS_{CS}(A)}} = \frac{\langle U_n(K) \rangle}{\langle U_n(0_1) \rangle}$$

$$S_{\text{CS}}(A) = \frac{k}{4\pi} \int_{\mathcal{M}} \text{tr}\left(A \wedge dA + \frac{2}{3}A \wedge A \wedge A\right), \quad Z(\mathcal{M}) = \int_{\mathcal{U}} [DA] e^{iS_{\text{CS}}(A)}$$

Knot: $S^1 \subset S^3$; e.g.,











$$\left\langle \right\rangle = q^{\frac{1}{4}} \left\langle \right\rangle + \frac{1}{q^{\frac{1}{4}}} \left\langle \right\rangle \left\langle \right\rangle$$

$$(\bigcup)$$
 $w(K) = \text{overhand} - \text{underhand}$

vev of Wilson loop operator along K in

$$\square$$
 for $SU(2)$ Chern–Simons on S^3

$$J_2(4_1;q) = q^{-2} - q^{-1} + 1 - q + q^2$$
, $q = e^{\frac{2\pi i}{k+2}}$

Hyperbolic volume: volume of $S^3 \setminus K$ is another knot invariant

computed from tetrahedral decomposition of knot complement

Topological Invariants

Volume appears as saddle point in $SL(2,\mathbb{C})$ Chern–Simons theory

$$\mathcal{Z}(\mathcal{M}) = \int_{\mathcal{U}_{\mathbb{C}}} [D\mathcal{A}][D\overline{\mathcal{A}}] \exp\left[\frac{it}{2}W(\mathcal{A}) + \frac{i\tilde{t}}{2}W(\overline{\mathcal{A}})\right]$$

$$W(A) = \frac{1}{4\pi} \int_{\mathcal{M}} \operatorname{tr}\left(A \wedge dA + \frac{2}{3}A \wedge A \wedge A\right)$$

$$t = \ell + is, \quad \tilde{t} = \ell - is, \quad \ell \in \mathbb{Z}, \quad s \in \mathbb{C}$$

$$\mathcal{Z}(S^3 \setminus K) \supset \exp\left[\frac{is}{2\pi} \operatorname{Vol}(S^3 \setminus K) + i\ell\pi \operatorname{CS}(S^3 \setminus K)\right]$$

The critical point responsible for this contribution is a flat $SL(2,\mathbb{C})$ valued connection \mathcal{A}_+ , the geometric conjugate connection:

$$W(\mathcal{A}_{+}) = -\frac{\imath}{2\pi} Vol(S^{3} \setminus K) + \pi \operatorname{CS}(S^{3} \setminus K)$$

Volume conjecture:

$$\lim_{n \to \infty} \frac{2\pi \log |J_n(K; \omega_n)|}{n} = \operatorname{Vol}(S^3 \setminus K)$$

$$K_{\mathrm{Ashaev}} (1997)$$

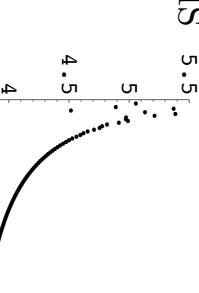
Murakami x 2 (2001)

Gukov (2005)

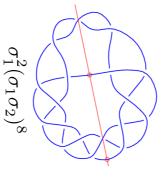
$$\omega_n = e^{\frac{2\pi i}{n}}$$

In fact, we take $n, k \to \infty$

SHI



Simplest hyperbolic non-two bridge knot, has 18 crossings



 $Vol(S^3 \setminus K_0) = 3.474247...$

ω 5

Behavior is not monotonic!

50

100

150

200

250 n

Volume conjecture:

$$\lim_{n \to \infty} \frac{2\pi \log |J_n(K; \omega_n)|}{n} = \text{Vol}(S^3 \setminus K)$$

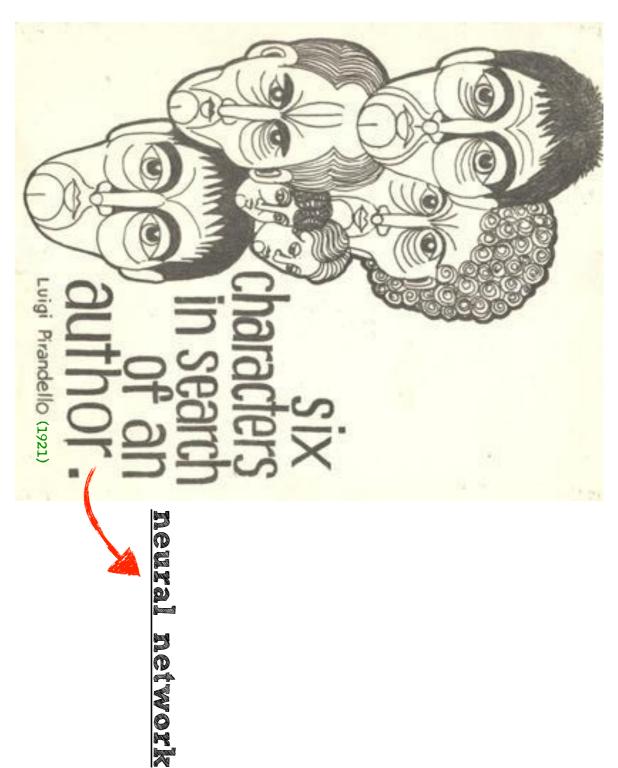
 $\omega_n=e^{rac{2\pi i}{n}}$ $\lim_{n\to\infty}$ $= \operatorname{Vol}(S^3 \setminus K)$ Kashaev (1997) Murakami x 2 (2001) Gukov (2005)

Khovanov homology: a homology theory \mathcal{H}_K whose graded Euler characteristic is $J_2(K;q)$; explains why coefficients are integers Khovanov (2000) Bar-Natan (2002)

 $\log |J_2(K;-1)|$, $\log(\operatorname{rank}(\mathcal{H}_K)-1) \propto \operatorname{Vol}(S^3 \setminus K)$

Dunfield Khovanov (2000) (2002)



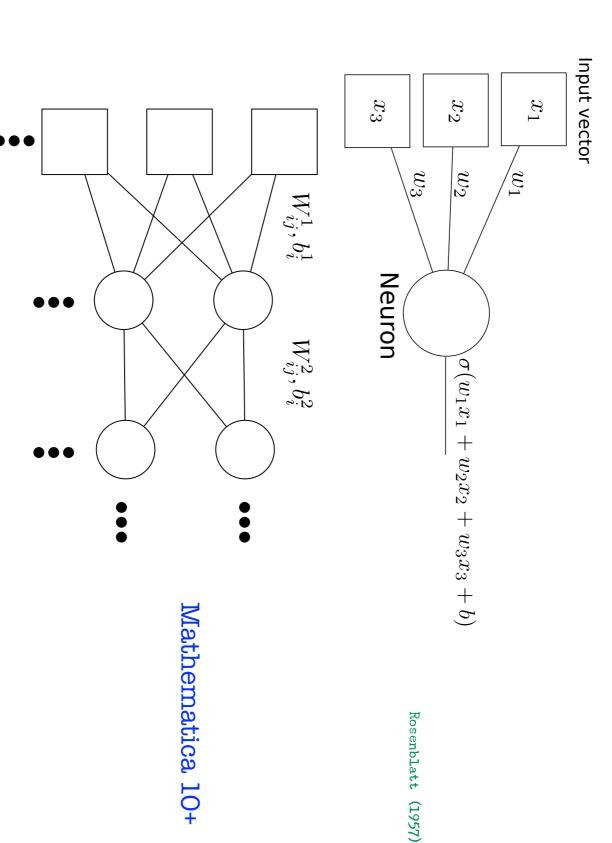


For other work on knots and machine learning, see Hughes (2016)

Levitt, Hajij, Sazdanovic (2019)

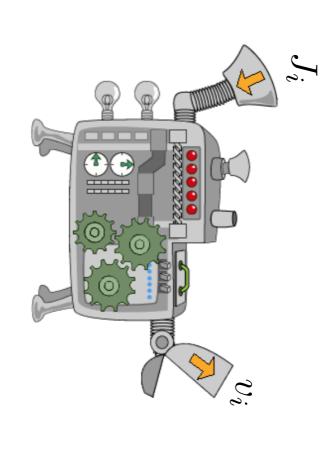
Gukov, Halverson, Ruehle, Sulkowski (2020)

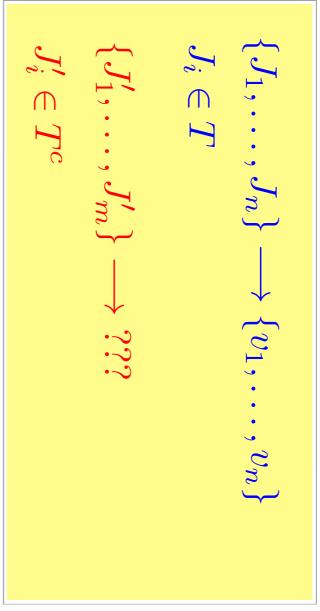
Feedforward Neural Networks



Schematic representation of feedforward neural network. The top figure denotes the perceptron (a single neuron), the bottom, the multiple neurons and multiple layers of the neural network.

Neural Network





Jones polynomials are represented as 18-vectors $J_K = (\min, \max, \text{coeffs}, 0, \dots, 0)$

Two layer neural network in Mathematica

$$f_{\theta}(\vec{J}_K) = \sum_{a} \sigma \left(W_{\theta}^2 \cdot \sigma(W_{\theta}^1 \cdot \vec{J}_K + \vec{b}_{\theta}^1) + \vec{b}_{\theta}^2 \right)^a$$

Input Layer

 100×18

 100×100

 $\sum_{a=1}^{100}$

Hidden Layer 1

Hidden Layer 2

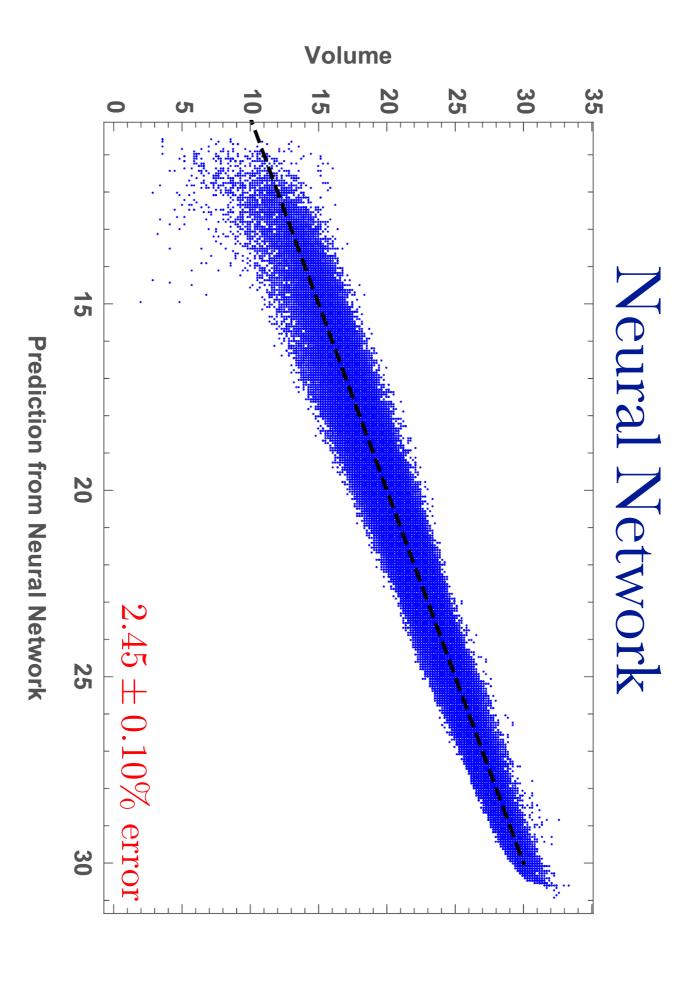
Output Layer

12000 hyperparameters

Logistic sigmoids for the hidden layers

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

VJ, Kar, Parrikar (2019)



trained on 10% of the 313,209 knots up to 15 crossings

Result

$$v_i = f(J_i) + \text{small corrections}$$

- J_i does not uniquely identify a knot e.g., 4_1 and K11n19 have same Jones polynomial, different volumes
- 174, 619 unique Jones polynomials 2.83% average spread in volumes for a Jones polynomial intrinsic mitigation against overfitting
- Same applies to 1,701,913 hyperbolic knots up to 16 crossings (database compiled from **Knot Atlas** and **SnapPy**)

Result

$$v_i = f(J_i) + \text{small corrections}$$

Neural network does better than more refined topological invariants

Beyond the volume conjecture in Chern-Simons Jones polynomial (quantum) \longleftrightarrow volume (classical) strong coupling limit of SU(2)weak coupling limit of $SL(2,\mathbb{C})$ Chern–Simons

something — maybe about the need for underlying homology theory Failed experiments (e.g., learning Chern-Simons invariant) also teach us

$$\lim_{n \to \infty} \frac{2\pi \log J_n(K; e^{2\pi i/n})}{n} = \operatorname{Vol}(S^3 \setminus K) + 2\pi^2 i \operatorname{CS}(S^3 \setminus K)$$

cf. Calabi—Yau Hodge numbers, line bundle cohomology, etc.

Result

$$v_i = f(J_i) + \text{small corrections}$$

activation function, single hidden layer with finite number of neurons can approximate continuous functions on compact subsets of \mathbb{R}^n Universal Approximation Theorem: feedforward neural network, sigmoid

Cybenko (1989) Hornik (1991)

Surprise here is simplicity of architecture that does the job

We want a **not** machine learning knot result

Entr'acte

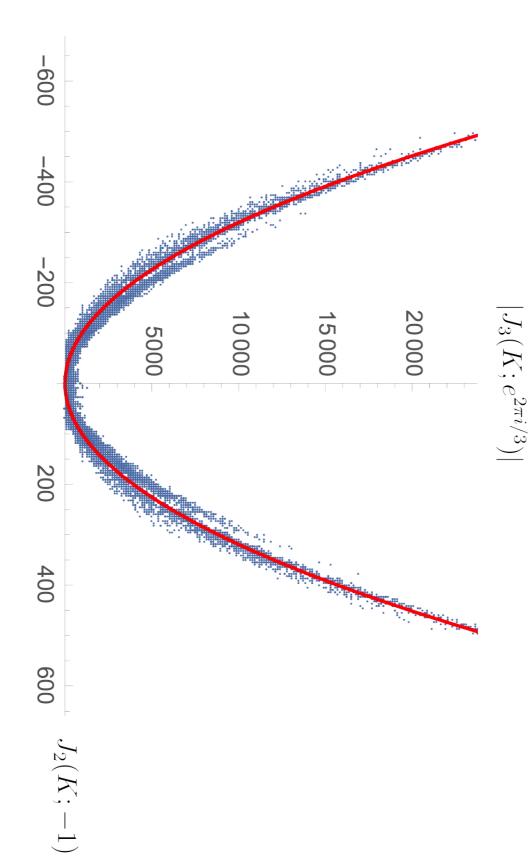
$$v_i = f(J_i) + \text{small corrections}$$

the volume as a function of the Jones polynomial We seek to reverse engineer the neural network to obtain an analytic expression for

To interpret the formula, we use machinery of analytically continued Chern-Simons theory

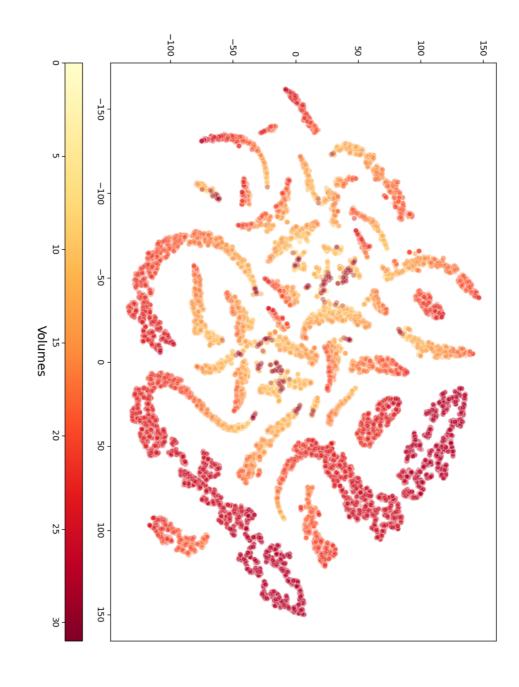
Towards the Volume Conjecture

The volume conjecture:
$$\lim_{n \to \infty} \frac{2\pi \log |J_n(K; \omega_n)|}{n} = \operatorname{Vol}(S^3 \setminus K)$$



11,921 colored Jones polynomials at n=3

t-SNE

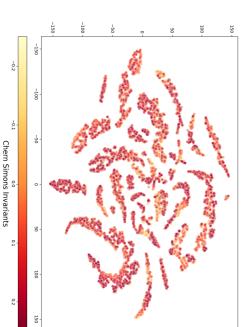


Volume is learnable from coefficients

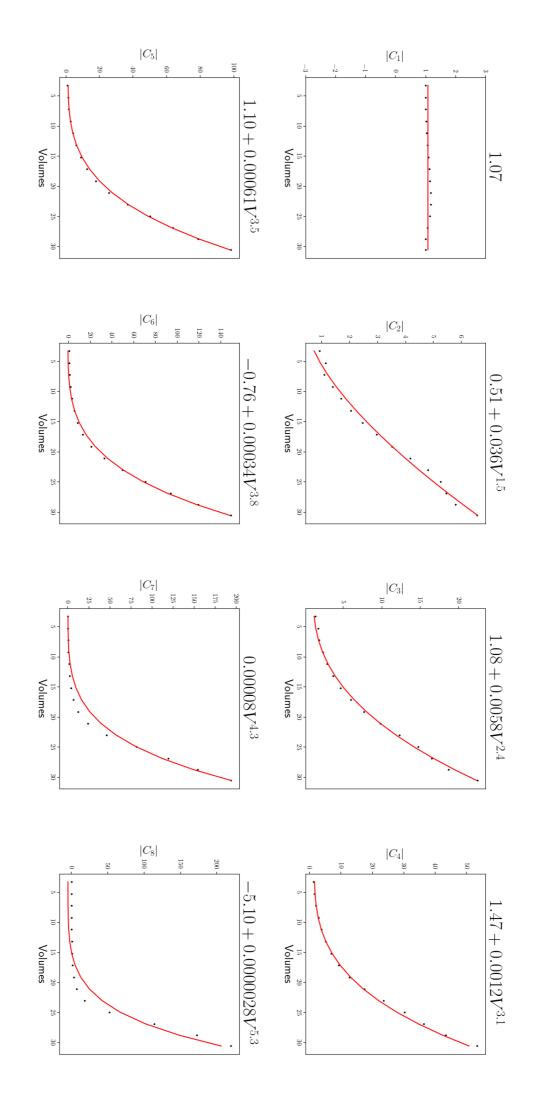
Chern-Simons invariant probably is not

$$\lim_{n \to \infty} \frac{2\pi \log J_n(K; \omega_n)}{n}$$

$$= \operatorname{Vol}(S^3 \setminus K) + 2\pi^2 i \operatorname{CS}(S^3 \setminus K)$$



Coefficients

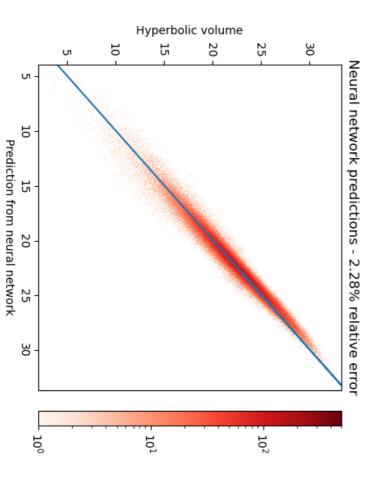


Coefficients scale with volume as power law

 $|C_n| \sim |C_{-n}|$

No Degrees Needed

- Suppose we drop the degrees and provide only the coefficients; Jones polynomial is no longer recoverable from the input vector
- Results are unchanged!



N.B.: we have switched to Python 3 using GPU-Tensorflow with Keras wrapper two hidden layers, 100 neurons/layer, ReLu activation, mean squared loss, Adam optimizer

Jones Evaluations

- be responsible for information in $J_2(K;q)$ Physics in Chern-Simons theory that leads to volume conjecture may also
- Consider evaluations of Jones polynomial at roots of unity
- In particular, fix $r \in \mathbb{Z}$ and evaluate $j_p^r := J_2(K; e^{2\pi i p/(r+2)})$
- The input vector

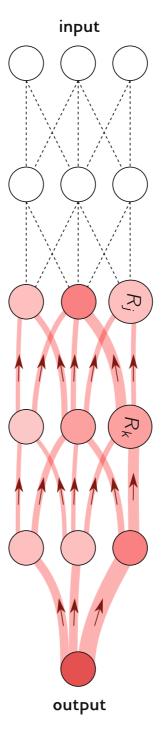
$$\mathbf{v}_{\text{in}} = (\text{Re}(j_0^r), \text{Im}(j_0^r), \dots, \text{Re}(j_{\lfloor (r+2)/2 \rfloor}^r), \text{Im}(j_{\lfloor (r+2)/2 \rfloor}^r))$$

does not degrade neural network performance

Consistent with degrees not mattering In fact, we only need to feed in the magnitudes: $\mathbf{v}_{\text{in}} = (|j_0^r|, \dots, |j_{\lfloor (r+2)/2 \rfloor}|)$

Layer-wise Kelevance Propagation

starting from output layer employing a conservation property To determine which inputs carry the most weight, propagate backward

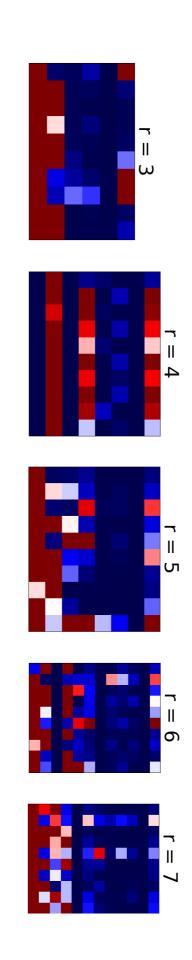


Montavon et al. (2019)

Compute relevance score for a neuron using activations, weights, and biases

$$R_{j}^{m-1} = \sum_{k} rac{a_{j}^{m-1}W_{jk}^{m} + N_{m-1}^{-1}b_{k}^{m}}{\sum_{l} a_{l}^{m-1}W_{lk}^{m} + b_{k}^{m}} R_{k}^{m}$$
 , $\sum_{k} R_{k}^{m} = 1$ $j^{ ext{th}}$ neuron in layer $m-1$

Layer-wise Kelevance Propagation



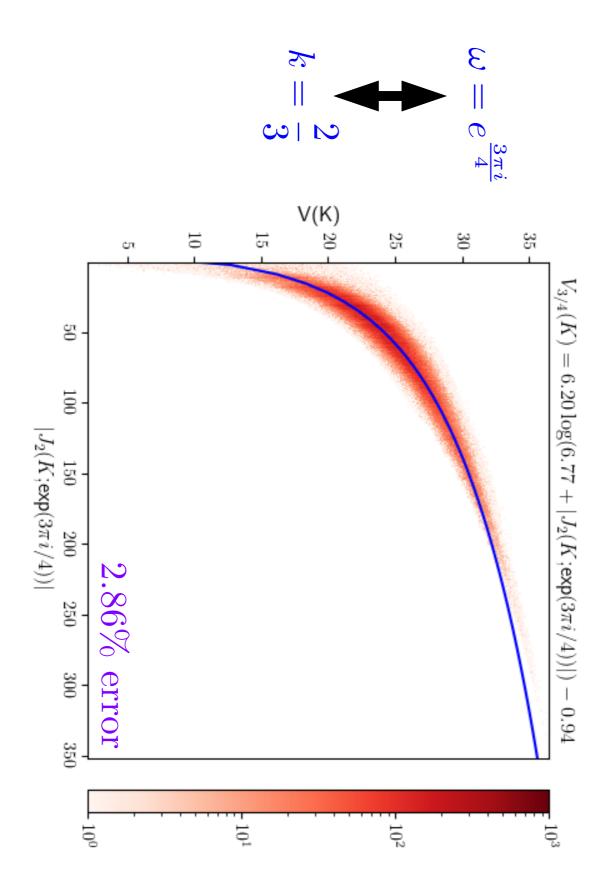
- Each column is a single input corresponding to evaluations of the Jones polynomial at phases $e^{\frac{2\pi ip}{r+2}}$, $0 \le 2p \le r+2$, $p \in \mathbb{Z}$
- Ten different knots
- features light up We show the relevances (red is most relevant) and notice that the same input

Relevant Phases

4 3 7	Error 3.48% 6.66%	Relevant roots $e^{4\pi i/5}$ -1	Fractional levels $\frac{1}{2}$
4	6.66%	— <u>1</u>	0
Ŋ	3.48%	$e^{6\pi i/7}$	$\overline{3}$
6	2.94%	$e^{3\pi i/4}, -1$	$\frac{2}{3}$, 0
7	5.37%	$e^{8\pi i/9}$	4
∞	2.50%	$e^{3\pi i/5}, e^{4\pi i/5}, -1$	$\frac{4}{3}, \frac{1}{2}, 0$
6	2.74%	$e^{8\pi i/11}, e^{10\pi i/11}$	$\frac{3}{4}, \frac{1}{5}$
10	3.51%	$e^{2\pi i/3}, e^{5\pi i/6}, -1$	$1, \frac{2}{5}, 0$
11	2.51%	$e^{8\pi i/13}$, $e^{10\pi i/13}$, $e^{12\pi i/13}$	$\frac{5}{4}, \frac{3}{5}, \frac{1}{6}$
12	2.39%	$e^{5\pi i/7}, e^{6\pi i/7}, -1$	$\frac{4}{5}, \frac{1}{3}, 0$
13	2.52%	$e^{2\pi i/3},e^{4\pi i/5},e^{14\pi i/15}$	
14	2.58%	$e^{3\pi i/4}, e^{7\pi i/8}, -1$	$\frac{2}{3}, \frac{2}{7}, 0$
15	2.38%	$e^{12\pi i/17}$, $e^{14\pi i/17}$, $e^{16\pi i/17}$	$\frac{5}{6}, \frac{3}{7}, \frac{1}{8}$
16	2.57%	$e^{2\pi i/3}$, $e^{7\pi i/9}$, $e^{8\pi i/9}$, -1	, <u>1</u>
17	2.65%	$e^{14\pi i/19}$, $e^{16\pi i/19}$, $e^{18\pi i/19}$,	$\frac{5}{7}, \frac{3}{8}, \frac{1}{9}$
18	2.49%	$e^{4\pi i/5}, e^{9\pi i/10}, -1$	$\frac{1}{2}, \frac{2}{9}, 0$
19	2.45%	$e^{2\pi i/3}$, $e^{16\pi i/21}$, $e^{6\pi i/7}$, $e^{20\pi i/21}$	 $1, \frac{5}{8}, \frac{1}{3}, \frac{1}{10}$
20	2.79%	$e^{8\pi i/11}, e^{9\pi i/11}, e^{10\pi i/11}, -1$	$\frac{3}{4}, \frac{4}{9}, \frac{1}{5}, 0$

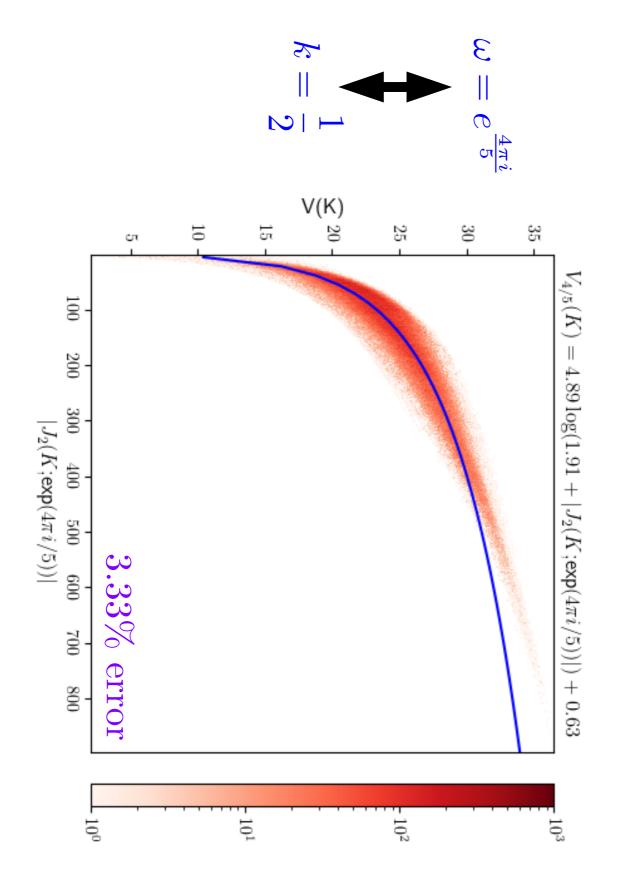
 $e^{ix} = e^{\frac{2\pi i}{k+2}}$

Phenomenological Function



Parameters fixed via curve fitting routines in Mathematica

Phenomenological Function



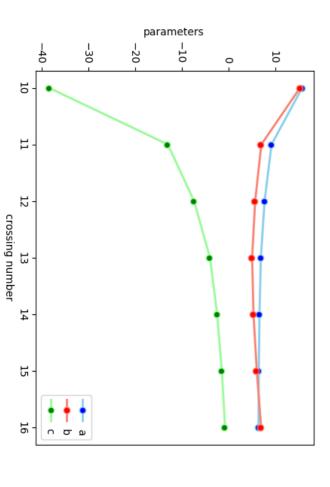
Parameters fixed via curve fitting routines in Mathematica

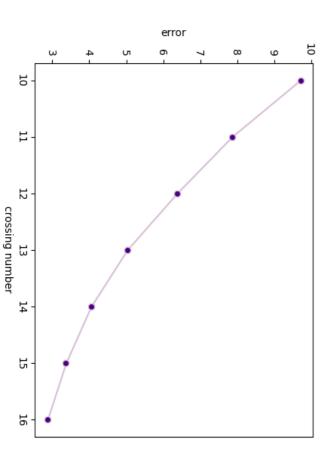
Phenomenological Function

$$V_{3/4}(S^3 \setminus K) = 6.20 \log(|J_2(K; e^{\frac{3\pi i}{4}})| + 6.77) - 0.94$$

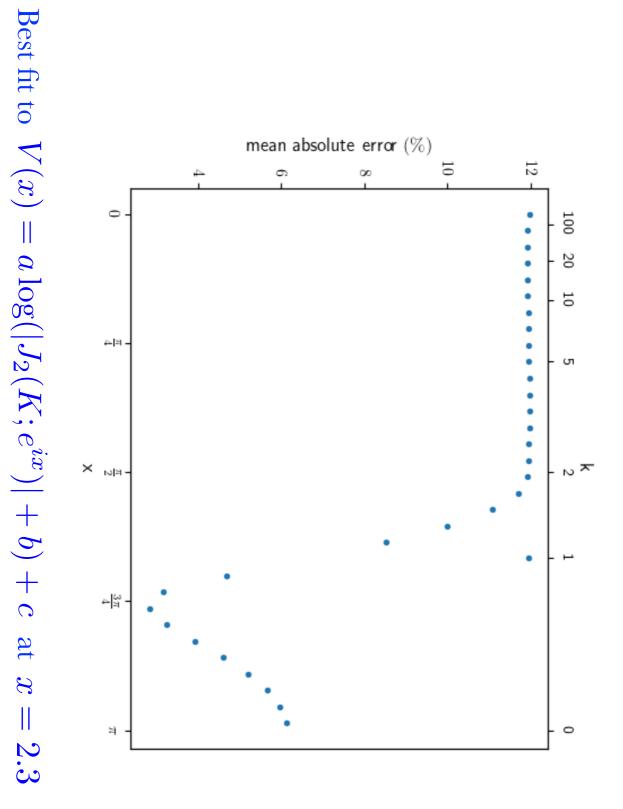
2.86% error compared to 2.28% error for neural network corresponds to Chern–Simons level $k = \frac{2}{3}$

Parameters of fit robust as a function of crossing number

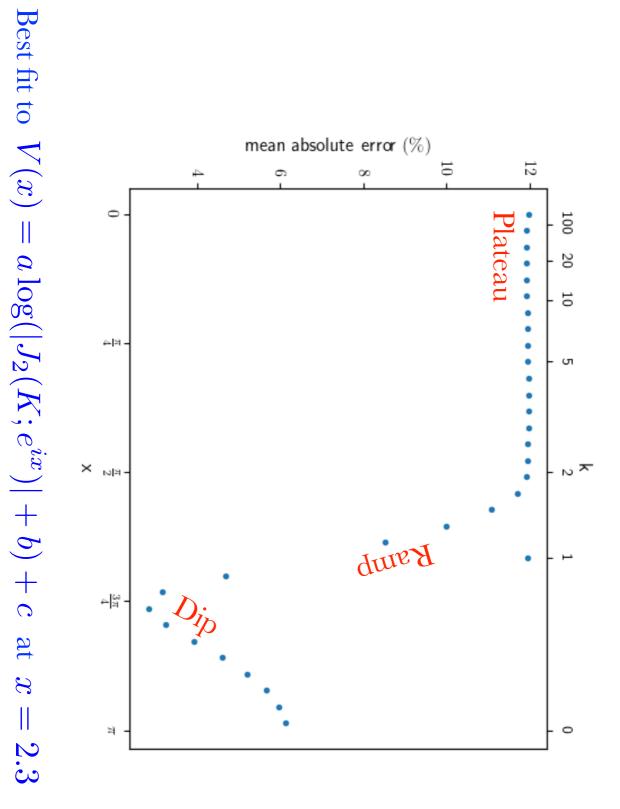




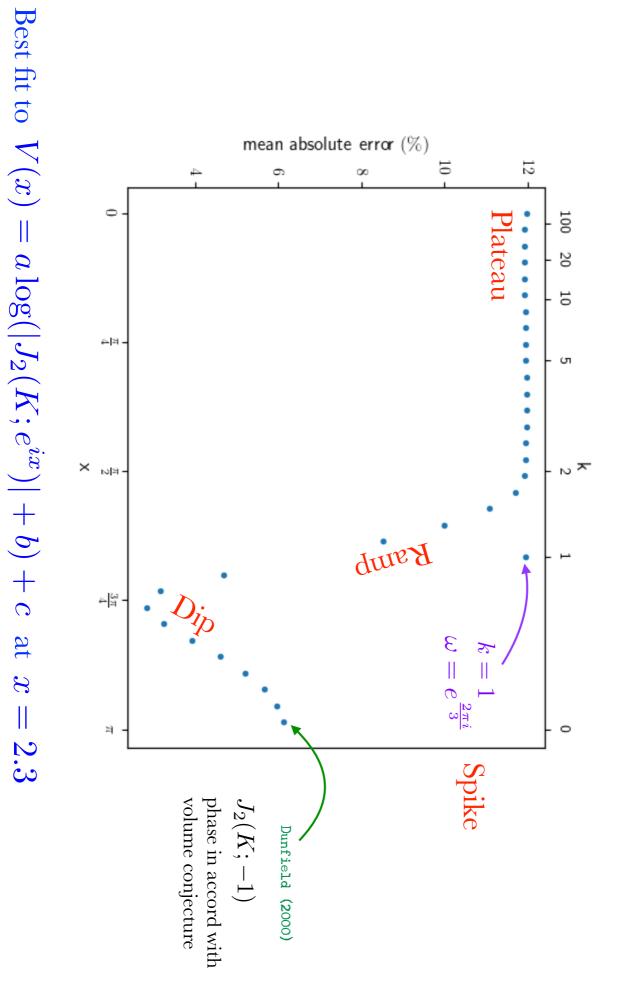
Best Phase



Best Phase



Best Phase



Chern—Simons Theory

- Recall that $S_{CS} = \frac{k}{4\pi} \int_{\mathcal{M}} \operatorname{tr} \left(A \wedge dA + \frac{2}{3} A \wedge A \wedge A \right)$
- Under the gauge transformation $A_{\mu} \mapsto g^{-1}A_{\mu}g + g^{-1}\partial_{\mu}g$,

$$\Delta S_{\rm CS} = \frac{k}{4\pi} \int d^3x \ \epsilon^{\mu\nu\rho} \left(\partial_{\mu} {\rm tr} \left((\partial_{\nu} g) g^{-1} A_{\rho} \right) + \frac{1}{3} {\rm tr} \left(g^{-1} \partial_{\mu} g g^{-1} \partial_{\nu} g g^{-1} \partial_{\rho} g \right) \right)$$

Associated to large gauge transformations, we recognize the winding

$$w(g) = \frac{1}{24\pi^2} \int d^3x \ \epsilon^{\mu\nu\rho} \mathrm{tr} \left(g^{-1} \partial_{\mu} g g^{-1} \partial_{\nu} g g^{-1} \partial_{\rho} g \right) \in \mathbb{Z}$$

- This implies that the level $k \in \mathbb{Z}$
- So what does fractional level mean?
- In Abelian Chern–Simons theory, can make sense of $k = \frac{1}{2}$

Analytic Continuation

- We can analytically continue the level
- Appeal to Morse theory; the integration cycle \mathcal{C} used to compute path integral is decomposed in terms of Lefschetz thimbles
- neighborhood of $\gamma = \frac{n-1}{k} = 1$ at large kThe validity of the volume conjecture amounts to statement that geometric conjugate connection A_{+} contributes to SU(2) path integral in

<u>N.B.</u>: for the Jones polynomial, n=2, $\gamma=k^{-1}$

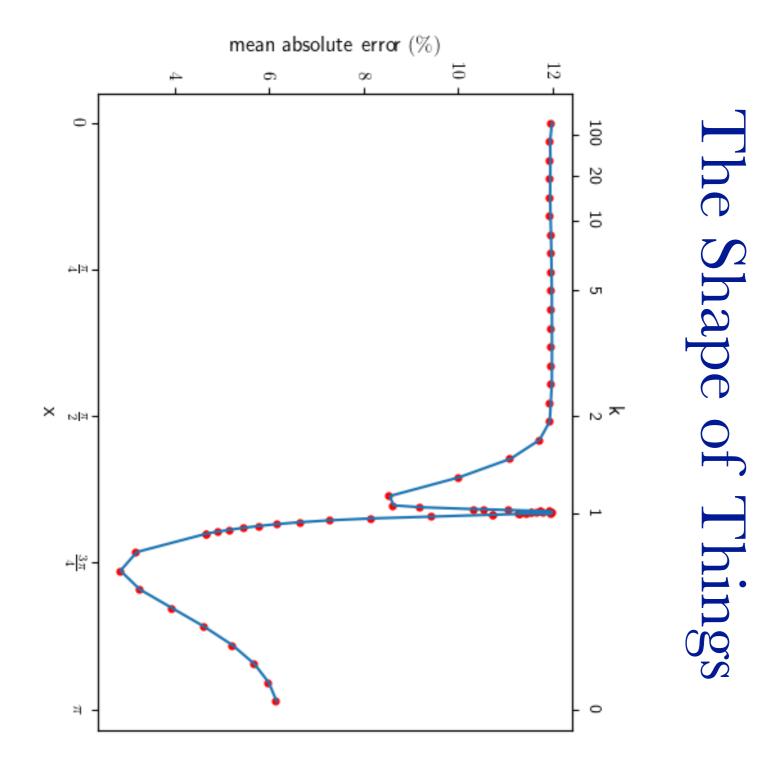
As 7 is varied, analytically continued integration cycle can pick up phenomena that occur along Stokes lines in complex $\, \gamma \,$ plane contributions from new critical points or lose current ones; these are Stokes

Analytic Continuation

- For integer k, even if A_+ saddle is present in integration cycle, it cancels with another saddle
- For general k, the leading contribution of the two saddles is $e^{iW(A_+)}(1-e^{2\pi ik})$
- This survives in semi-classical limit $\gamma \to 1$, $k \to \infty$
- i.e., $e^{iW(\mathcal{A}_+)}(1-e^{2\pi ik})$ to path integral from pair of $SL(2,\mathbb{C})$ critical points after analytic continuation
- conjugate connection for every knot at n = k + 2Volume conjecture essentially states that this behavior occurs for geometric

Hypothesis

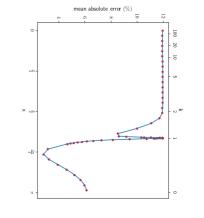
The approximation formula works well for levels kChern–Simons path integral, and its accuracy for which \mathcal{A}_+ makes a contribution to the increases with fraction of knots in dataset that receive such a contribution



The Shape of Things

$$Vol(S^3 \setminus K) = \langle Vol(S^3 \setminus K) \rangle$$

this gives 11.97% error for knots up to 16 crossings



corresponds to latent correlations in the dataset

near
$$k = \frac{2}{3}$$
 or $\gamma = \frac{3}{2}$

connection we expect in semiclassical limit for most knots Lefschetz thimbles contain geometric conjugate $SL(2,\mathbb{C})$

$$0 < k < \frac{2}{3}$$

knots retain geometric conjugate connection even as $k \ll 1$ or $\gamma \gg 1$

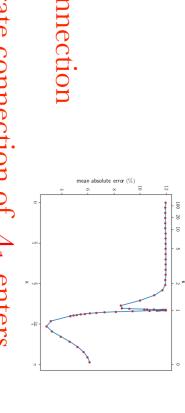
this is explanation for observation that $\log |J_2(K;-1)| \propto \operatorname{Vol}(S^3 \setminus K)$

The Shape of Things

Ramp:

$$\frac{2}{3} < k < 2$$
 interpolating regime

knots lose access to geometric conjugate connection



at $k=\frac{3}{2}$ or $\gamma=\frac{2}{3}$, the geometric conjugate connection of 4_1 enters

Witten (2010)

Spike:

near k=1

contributions only from SU(2) valued critical points at integer values of level with $k+1 \geq n$, the path integral receives

i.e., no analytic continuation is necessary

the error becomes high because we lose knowledge of the geometric conjugate connection,

Conclusion:

geometric conjugate connection is crucial to success of approximation formula

A Better Formula

- Our reverse engineered function gave 2.86% error compared to 2.28% error for neural network; the latter is essentially intrinsic
- Can we do better with a formula? If so, how much better?
- Define a new error measure

$$\sigma = \frac{\text{variance of (actual volume - predicted volume)}}{\text{variance of volumes in dataset}}$$

σ-measure is shift/rescaling invariant [suggested to us in correspondence with Fischbacher, Münkler]

Can ask what fraction of variance is left unexplained

A Better Formula

variance of (actual volume – predicted volume) variance of volumes in dataset

By this measure, the neural network gives $\sigma=0.033$ while our functional approximation gives $\sigma = 0.068$

- If we just assign the average volume to every knot in the dataset, $\sigma=1$; this corresponds to plateau
- There is room for improvement, but it is remarkable that a function with only three fit parameters works so well

Other Experiments

- Different representations of Jones polynomial work just as well
- Khovanov polynomial predicts volume with 97.2% accuracy; $m HOMFLY ext{-}PT$ polynomial does less well with 93.9% accuracy

$$J_2(K;q) = \frac{Kh(K;-1,q)}{q+q^{-1}} = P(K;q^{-1},q^{1/2}-q^{-1/2})$$

- Chern-Simons invariant does not look to be learnable from Jones polynomial in various experiments
- Symbolic regression using PySR gives formulae with 96.6% accuracy, but not so interpretable Cranmer, et al. (2020)

Prospectus

- Simons theory; investigate this for higher colors as well Inequalities à la volume-ish theorem using analytically continued Chern-
- Use numerics to study Stokes phenomena in Chern-Simons theory
- Monotonic version of the volume conjecture
- Relations between other topological invariants
- Better understanding of what problems are machine learnable in mathematics and physics — failed experiments may teach us something!
- Keverse engineer other machine learned results

Smooth Poincaré in 4d

- <u>Conjecture</u>: A four manifold with homotopy type S^4 is diffeomorphic to S^4
- Freedman proved it is homeomorphic
- Does S^4 admit exotic smooth structures?
- The Rasmussen s-invariant cannot be used to detect counterexamples
- Find topologically slice knots that are not slice

Freedman, Gompf, Morrison, Walker (2010)
Manolescu, Piccirillo (2021)

Perhaps ML can assist in identifying further interesting knots

A View to Holography

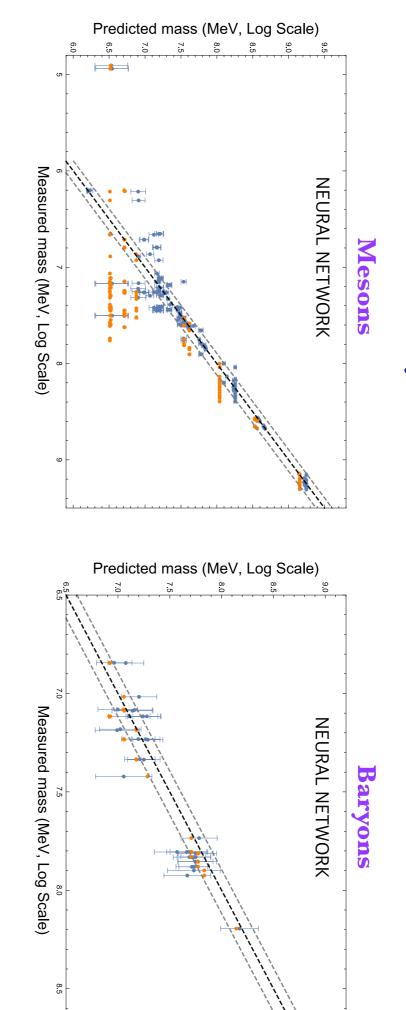
- Beautiful recent work by Hashimoto, et al.
- Train on lattice data for chiral condensate vev vs. quark mass
- dictionary despite not being in large-N limit Obtain metric from parameters in neural network and follow AdS/QCD
- Predict form of quark—antiquark potential
- Hashimoto, Sugishita, Tanaka, Tomiya (2018) Hashimoto (2019) Akutagawa, Hashimoto, Sugimoto (2020)

Investigations in CFT

Chen, He, Lal, Zaz (2020) 10, Seif, Lundgren, Whitsitt, Hafezi (2021) Kántor, Niarchos, Papageorgakis (2021)

Look at interesting black hole datasets

Baryons and Mesons



13.0% error

39.3% error

9.7% error

8.7% error

 $u:336~{
m MeV}$

 $d:340~{
m MeV}$

 $s:486~{
m MeV}$

 $c:1550~{
m MeV}$

 $b:4730~{
m MeV}$

Constituent quark mass = QCD binding energy

amount of energy to add to spontaneously emit meson containing given valence quark



The Future

Machine learning identifies associations

Want to convert this to analytics — i.e., how does a machine learn?

What problems in physics and mathematics are machine learnable?

• Can a machine do interesting science?

hep-th

- Use machine learning to classify papers into arXiv categories
- 65% success at exact subject, 87% success at formal vs. phenomenology
- Mapping words to vectors contextually, we discover syntactic identities

Paris – France + Italy = Rome

$$king - man + woman = queen$$

hep-th

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An idea generating machine for hep-th:

$$\label{eq:symmetry+black} symmetry + black \ hole = Killing \\ symmetry + algebra = group \\ black \ hole + QCD = plasma \\ spacetime + inflation = cosmological \ constant \\ string \ theory + Calabi-Yau = M-theory + G_2$$

String Data

- string_data 2017 (Northeastern)
- string_data 2018 (LMU, Munich)
- Physics () ML (Microsoft)
- string_data 2020 (CERN)
- Interactions, 2020-present (Harvard, MIT, Northeastern, Tufts) NSF Institute for Artificial Intelligence and Fundamental
- string_data 2021 (Wits)
- string_data 2022 (Turing Institute)

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