COLORED JONES POLYNOMIALS & THE VOLUME CONJECTURE



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Collaborators



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- <u>Knot:</u> $S^1 \subset S^3$
 - Organized by crossing number, a proxy for complexity



<u>Knot:</u> $S^1 \subset S^3$





8_2

8_3



8_4

8_5

8_6



8_7

8_8













8_9



8_11

8_12

8_13

8_14

8_15

8_16



8_17



8_18

8_19





8_21







<u>Knot:</u> $S^1 \subset S^3$

Reidemeister moves





Thistlethwaite unknot

Ochiai unknot

<u>Knot:</u> $S^1 \subset S^3$

Rolfsen table



 $10_{161} \quad \longleftarrow \quad \text{Perko pair (1973)} \longrightarrow \quad 10_{162}$

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

Jones polynomial:
$$J(K;q) = (-q^{\frac{3}{4}})^{w(K)} \frac{\langle K \rangle}{\langle O \rangle}$$
 $\langle \swarrow \rangle = q^{\frac{1}{4}} \langle \smile \rangle + \frac{1}{q^{\frac{1}{4}}} \langle)\langle \rangle$
 $w(K) = \text{overhand} - \text{underhand}$
 $J(O;q) = 1$

topological invariant: independent of how knot is drawn

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 in 3d:

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

$$S_{\mathrm{CS}}(A) = \frac{k}{2} \int_{\mathrm{CS}} tr \left(A \wedge dA + \frac{2}{2} A \wedge A \wedge A\right) = Z(AA) = \int_{\mathrm{CS}} [DA] e^{iS_{\mathrm{CS}}(A)}$$

$$S_{\rm CS}(A) = \frac{\kappa}{4\pi} \int_{\mathcal{M}} \operatorname{tr} \left(A \wedge dA + \frac{2}{3}A \wedge A \wedge A \right) , \quad Z(\mathcal{M}) = \int_{\mathcal{U}} [DA] \ e^{iS_{\rm CS}(A)} \\ k \in \mathbb{Z}$$
 Witten (1989)

Jones polynomial:
$$J(K;q) = (-q^{\frac{3}{4}})^{w(K)} \frac{\langle K \rangle}{\langle O \rangle}$$
 $\langle K \rangle = q^{\frac{1}{4}} \langle K \rangle + \frac{1}{q^{\frac{1}{4}}} \langle f \rangle \rangle$
 $w(K) = \text{overhand} - \text{underhand}$

vev of Wilson loop operator along K in \Box for SU(2) Chern-Simons on S^3

Jones (1985) Witten (1989)

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

Open question: Is unknot unique knot for which $J_2(q) = 1$? **Open question:** Unknot recognition problem — is this NP?

Dehn (1910) Turing (1954) Haken (1961) Lackenby (2021)

Knot:
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; e.g., $\left(\bigcup \right) \left(\bigcup \right) \left($

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Jones (1985) Witten (1989)

<u>Hyperbolic volume</u>: volume of $S^3 \setminus K$ is another knot invariant in 3d computed from tetrahedral decomposition of knot complement

Thurston (1978) Mostow (1968)





Table A1			
# Crossings	# Knots	# Torus	# Sat.
0	1		
3a	1	1	
4a	1		
5a	2	1	
6a	3		
7a	7	1	
8a	18		
8n	3	1	
9a	41	1	
9n	8		
10a	123		
10n	42	1	
11a	367	1	
11n	185		
12a	1,288		
12n	888		
13a	4,878	1	
13n	5,110		2
14a	19,536		
14n	27,436	1	2
15a	85,263	1	
15n	168,030	1	6
16a	379,799		
16n	1,008,906	1	10

1701936 knots up to 16 crossings

All but 32 are hyperbolic

Hoste, Thistlewaite, Weeks (1998)

Conjecture [Adams]: proportion of hyperbolic knots approaches 1 as crossing number goes to ∞





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Conjecture [Adams]: proportion of hyperbolic knots approaches 1 as crossing number goes to ∞

This conjecture is false!

 $\lim_{n \to \infty} \sup \, \frac{S_n}{P_n} > \frac{1}{2 \cdot 10^{17}}$

Malyutin (2018) Belousov, Malyutin (2019)

Volume conjecture:

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

Kashaev (1997) Murakami x 2 (2001) Gukov (2005)

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



Behavior is not monotonic!

Garoufalidis, Lan (2004)

Volume conjecture:

$$\lim_{n \to \infty} \frac{2\pi \log |J_n(K;\omega_n)|}{n} = \operatorname{Vol}(S^3 \setminus K) \qquad \qquad \underset{\text{Gukov (2005)}}{\overset{\text{Kashaev (1997)}}{\underset{\text{Gukov (2005)}}{\overset{\text{Kashaev (1997)}}{\underset{\text{Gukov (2005)}}{\overset{\text{Kashaev (1997)}}{\underset{\text{Gukov (2005)}}{\overset{\text{Kashaev (1997)}}{\underset{\text{Gukov (2005)}}{\overset{\text{Kashaev (1997)}}{\underset{\text{Gukov (2005)}}{\overset{\text{Kashaev (1997)}}{\underset{\text{Gukov (2005)}}{\overset{\text{Kashaev (1997)}}{\overset{\text{Kashaev (1997)}}{\overset{\text{Kashaev (1997)}}{\overset{\text{Kashaev (1997)}}{\overset{\text{Kashaev (1997)}}{\overset{\text{Kashaev (1997)}}{\overset{\text{Kashaev (2001)}}{\overset{\text{Kashaev (2001)}}{\overset{\text{Kashaev (2001)}}{\overset{\text{Kashaev (2005)}}{\overset{\text{Kashaev (2005)}}{\overset{\text{Kaa$$

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 (2000) Khovanov (2002)







non-linearity



$$\mathbf{v}_{\ell} = f_{\ell}(f_{\ell-1}(\cdots(f_1(\mathbf{v}_0)\cdots))) , \qquad a_{\text{out}} := \sum_{m=1}^{n_{\ell}} \mathbf{v}_{\ell}^m$$



Hopfield (1982, 1984) Hinton (1986)





Neural Network



$$\begin{split} \{J_1, \dots, J_n\} &\longrightarrow \{v_1, \dots, v_n\} \\ J_i \in T \\ \{J'_1, \dots, J'_m\} &\longrightarrow ??? \\ J'_i \in T^c \end{split}$$



Jones polynomials are represented as 18-vectors

$$\vec{J}_K = (\min, \max, \text{coeffs}, 0, \dots, 0)$$

Two layer neural network in Mathematica

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

Logistic sigmoids for the hidden layers Mean squared loss function

VJ, Kar, Parrikar (2019)

Mathematica Code

```
• • •
                                              knot run.nb
                                                                                               200%
🚯 🗸 🏢 🗸 Input
                                                                                           In[•]:= f[frac] :=
         Module[{y, list, listcomp, joneslist, vollist, joneslistcomp, vollistcomp,
           test, aa, KnotNet0, TrainedKnotNet0},
          y = frac;
          list = Sort[RandomSample[Range[1, len], IntegerPart[len y]]];
          listcomp = Complement[Table[i, {i, 1, len}], list];
          joneslist = Table[joneses[list[i]], {i, 1, Length[list]}];
          vollist = Table[volumes[[list[[i]]], {i, 1, Length[list]}];
          joneslistcomp = Table[joneses[listcomp[i]], {i, 1, Length[listcomp]}];
          vollistcomp = Table[volumes[[listcomp[[i]]], {i, 1, Length[listcomp]}];
          KnotNet0 = NetChain[{LinearLayer[100], ElementwiseLayer[LogisticSigmoid],
             LinearLayer[100], ElementwiseLayer[LogisticSigmoid], SummationLayer[]},
            "Input" \rightarrow {maxlen}];
          TrainedKnotNet0 = NetTrain[KnotNet0, joneslist → vollist];
          test = TrainedKnotNet0[joneses];
          Show[ListPlot[Table[{test[i]], volumes[i]]}, {i, 1, len}],
            AxesLabel \rightarrow {"Predicted Volume", "Volume"}],
           Plot[x, \{x, 0, 40\}, PlotRange \rightarrow Full, PlotStyle \rightarrow \{Black, Dashed\}]
         ]
        f[.1]
```

Mathematica Code

```
✤ knot run.nb
                                                                                                         100% ∨
In[40]:= f[frac_] :=
     Module[{y, list, listcomp, joneslist, vollist, joneslistcomp, vollistcomp, test, aa,
        KnotNet0, TrainedKnotNet0},
      y = frac;
      list = Sort[RandomSample[Range[1, len], IntegerPart[leny]]];
      listcomp = Complement[Table[i, {i, 1, len}], list];
       joneslist = Table[joneses[[list[[i]]]], {i, 1, Length[list]}];
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       test = TrainedKnotNet0[joneses];
       Show[ListPlot[Table[{test[[i]], volumes[[i]]}, {i, 1, len}],
         AxesLabel → {"Predicted Volume", "Volume"}],
        Plot[x, {x, 0, 40}, PlotRange → Full, PlotStyle → {Black, Dashed}]]
     ]
    f[.1]
```

Volume from Jones



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

VJ, Kar, Parrikar (2019)

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 1,701,903 hyperbolic knots up to 16 crossings 841,139 unique polynomials (database compiled from Knot Atlas and SnapPy)

VJ, Kar, Parrikar (2019)

Result

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

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

Cybenko (1989) Hornik (1991)

• Surprise here is simplicity of architecture that does the job

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

Entr'acte

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

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

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

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!



<u>N.B.</u>: 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

Layer-wise Relevance Propagation

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



Montavon et al. (2019)

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

$$R_{j}^{m-1} = \sum_{k} \frac{a_{j}^{m-1} W_{jk}^{m} + N_{m-1}^{-1} b_{k}^{m}}{\sum_{l} a_{l}^{m-1} W_{lk}^{m} + b_{k}^{m}} R_{k}^{m} , \qquad \sum_{k} R_{k}^{m} = 1$$

$$j^{\text{th}} \text{ neuron in layer } m - 1$$

Layer-wise Relevance Propagation



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

Phenomenological Function



- Use layerwise relevance propagation to determine best phase
- Approximation formula works almost as well as neural network

Craven, VJ, Kar (2020)

The Shape of Things



Analytic Continuation

- We can analytically continue the level
- Appeal to Morse theory; the integration cycle C used to compute path integral is decomposed in terms of Lefschetz thimbles
- Path integral evaluated on flat connections depends on one parameter, $\gamma \equiv \frac{n-1}{k}$; the semiclassical limit is $n, k \to \infty$

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

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

The Shape of Things

<u>Plateau:</u> k > 2

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

this gives 11.97% error for knots up to 16 crossings

corresponds to latent correlations in the dataset

Minimum:

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

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

Dip: $0 < k < \frac{2}{3}$ knots retain geometric conjugate connection even as $k \ll 1$ or $\gamma \gg 1$ this is explanation for observation that $\log |J_2(K; -1)| \propto \operatorname{Vol}(S^3 \setminus K)$ Dunfield (2000)



The Shape of Things



<u>Ramp:</u> $\frac{2}{3} < k < 2$ 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

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

i.e., no analytic continuation is necessary

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

geometric conjugate connection is crucial to success of Conclusion: approximation formula

Explanation

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

$$Z \sim e^{iS(\mathcal{A}_+)} \left(1 - e^{2\pi ik}\right)$$

Polynomials from Braids

• Braid group has generators that satisfy algebra

$$b_i b_{i+1} b_i = b_{i+1} b_i b_{i+1}$$
, $1 \le i < n-1$;
 $[b_i, b_j] = 0$ if $|i-j| > 1$

• Two closed braids equivalent iff related by Markov moves $AB \rightarrow BA$ for $A, B \in B_n$;

- $A \to Ab_n^{\pm 1}$ for $A \in B_n$, $b_n \in B_{n+1}$ and inverse move
- Obtain invariant polynomials by constructing representation of braid group and then defining Markov move independent polynomials
- Yang–Baxter equation as braid relation $F: X \times X \to X \times X$

 $F_{12} \circ F_{13} \circ F_{23} = F_{23} \circ F_{13} \circ F_{12}$



Exactly Solvable Models

- Let G_i be representation of $b_i \in B_n$
- Suppose we have $\phi(AB) = \phi(BA)$ for $A, B \in B_n$;

 $\phi(AG_n) = \tau \phi(A) , \quad \phi(AG_n^{-1}) = \overline{\tau} \phi(A) \quad \text{for} \quad A \in B_n , \quad G_n \in B_{n+1}$ $\tau = \phi(G_i) , \quad \overline{\tau} = \phi(G_i^{-1}) \quad \forall i$

- Invariant polynomial is $\alpha(A) = (\tau \overline{\tau})^{-(n-1)/2} \left(\frac{\overline{\tau}}{\tau}\right)^{e(A)/2} \phi(A)$ $A \in B_n$, e(A) is sum of exponents of b_i in A
- Can compute these in N-state vertex model

$$\phi(A) = \operatorname{Tr}(H \cdot A) \qquad h = \tau \operatorname{diag}(1, q, \dots, q^{N-1})$$
$$\tau(q) = \left(\sum_{m=0}^{N-1} q^m\right)^{-1}, \quad \overline{\tau} = \tau(q^{-1}) \qquad H = \underbrace{h \otimes \cdots \otimes h}_{n}$$
$$G_i = \mathbf{1}_1 \otimes \cdots \otimes \mathbf{1}_{i-1} \otimes R_{i,i+1} \otimes \mathbf{1}_{i+1} \otimes \cdots \otimes \mathbf{1}_n$$

Akutsu, Wadati (1987)

R-matrix

- N = 2, six-vertex model computes Jones polynomials
- N = 3, nineteen-vertex model computes adjoint Jones polynomials
- n strand braid corresponds to a $N^n \times N^n$ *R*-matrix satisfying Yang-Baxter equation
- We have computed:

11,941 $J_3(q)$ up to 13 crossings (92%)18,353 $J_3(q)$ at 14 crossings (39%)147,022 $J_3(q)$ at 15 crossings (58%)

• calculations up to 7 strands

Zeroes

 $J_2(q)$



Zeroes





Minimum Degree



Maximum Degree





Length



 $|J_3(e^{2\pi i/3})|$ vs. $J_2(-1)$



Jones to Volume



Adjoint Jones to Volume



Phase Evaluations

Evaluations of J_3



Best Phase

- The best phase for evaluating the adjoint Jones polynomial is $e^{8\pi i/15}$
- This corresponds to Chern–Simons level $k = \frac{7}{4}$ (or $\gamma = \frac{8}{7}$)

Best Phase Conjecture

- The best phase for evaluating the adjoint Jones polynomial is $e^{8\pi i/15}$
- This corresponds to Chern–Simons level $k = \frac{7}{4}$ (or $\gamma = \frac{8}{7}$)
- Since we have two data points, we can guess a formula for higher colors

$$\frac{x}{x_{vc}} = \frac{n+1}{n+2} \qquad n \to \infty: \qquad \frac{x}{x_{vc}} \to 1 - \frac{1}{n}$$

$$q = \exp\left(2\pi i \frac{n+1}{n(n+2)}\right) \qquad q \to \exp\left(2\pi i (\frac{1}{n} - \frac{1}{n^2})\right)$$

$$k = \frac{n^2 - 2}{n+1} \qquad k \to (n-1) - \frac{1}{n}$$

$$\gamma = \frac{n^2 - 1}{n^2 - 2} \qquad \gamma \to 1 + \frac{1}{n^2}$$

Best Phase Conjecture



Best Phase Conjecture



Summary

- Calculated a large (though incomplete) dataset of adjoint Jones polynomials
- Consistent with the naïve expectation of the volume conjecture, adjoint polynomials predict the volume better than fundamental polynomials
- Non-trivial because convergence at large color not necessarily monotonic
- Increasing crossing number improves prediction
- Conjectured color dependent best phase for prediction

Prospectus

- Complete calculation of adjoint polynomials
- Calculate datasets of polynomials for higher colors
- Check volume conjecture: do predictions hold?

is convergence monotonic?

A better organizing principle for (hyperbolic) knots
 e.g., minimum number of ideal tetrahedra needed to compute volume

Organizing Principle



Other Experiments



• Obtain a theorem in knot theory from saliency analysis of ML experiments

Theorem: There exists a constant *c* such that for every hyperbolic knot, $|2\sigma(K) - \operatorname{slope}(K)| \le c \operatorname{Vol}(K) \operatorname{inj}(K)^{-3}$



• See also: Hughes (2016)

Levit, Hajij, Sazdanovic (2019) Gukov, Halverson, Ruehle, Sulkowski (2020) Craven, Hughes, VJ, Kar (2021, 2022) Gukov, Halverson, Manolescu, Ruehle (2023)

Poincaré Conjecture

- A homotopy *n*-sphere has the same homotopy and homology groups as S^n
- **Conjecture:** Any homotopy *n*-sphere is homeomorphic, PL-isomorphic, diffeomorphic to S^n
 - homeomorphic is always true
 - piecewise linear isomorphic is true for $n \neq 4$
 - -n=1 is trivial
 - n = 2 proved by Poincaré (1907) and Koebe (1907)
 - $n \ge 5$ wins Fields Medal for Smale (1966); cf. Newman (1966)
 - n = 4 wins Fields Medal for Freedman (1986)
 - n = 3 wins Fields Medal for Perelman (2006, declined)

SPC4

• **Conjecture:** Any manifold homotopy equivalent to S^n is also diffeomorphic to S^n

isomorphism of smooth manifolds, *i.e.*, f, f^{-1} continuously differentiable

- False generally, but true if n = 1, 2, 3, 5, 6, 12, 56, 61
- n = 7: 28 different smooth structures on the sphere
 Milnor (1956)
 Remark: These are interpreted as gravitational instantons
 Witten (1985)



SPC4

- **Conjecture:** Any manifold homotopy equivalent to S^n is also diffeomorphic to S^n isomorphism of smooth manifolds, *i.e.*, f, f^{-1} continuously differentiable
- False generally, but true if n = 1, 2, 3, 5, 6, 12, 56, 61
- n = 7: 28 different smooth structures on the sphere
 Milnor (1956)
 Remark: These are interpreted as gravitational instantons
 Witten (1985)
- n = 4: answer unknown; equivalent to PL-isomorphic statement [also unknown for n = 126, conjectured to be false for even dimensions $n \ge 64$]
- If certain knots have certain topological invariants, this supplies counterexamples to SPC4
 - $S^3 = \partial B_4 , \quad K = \partial \Sigma$ $K \subset S^3 , \quad \Sigma \subset B_4$
- **SPC4:** Any smooth manifold B with $\partial B = S^3$ homotopy equivalent to B_4 is also diffeomorphic to B_4

THANK YOU



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