Deep learning knot invariants and gauge theory

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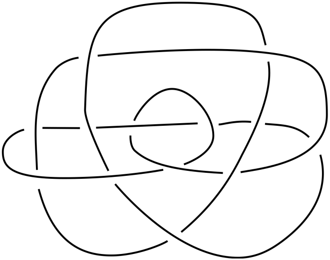
Motivation

Knots are embeddings of a circle S^1 in some 3-dimensional space.

A fundamental problem in knot theory is knot comparison. Given two 2d knot diagrams (projections to a plane), how can we tell if they represent the same knot?



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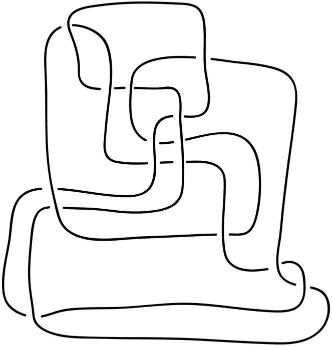
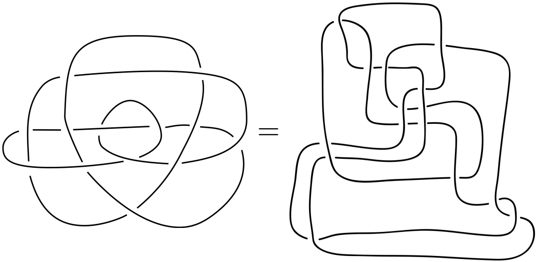
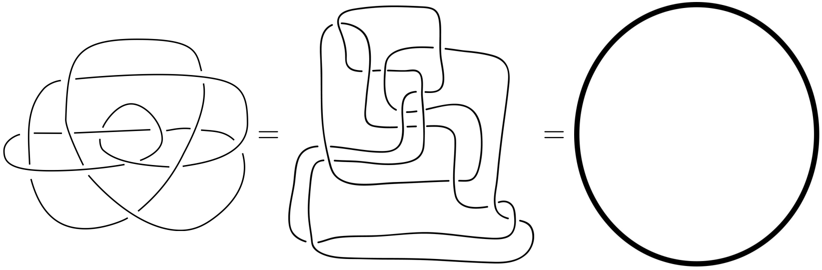


Motivation



Motivation



Motivation

To help identify knots, we compute topological invariants. If two diagrams yield different invariants, they represent different knots.

The knot complement manifold $S^3 \setminus K$, constructed by drilling out a solid torus neighborhood of K, is a knot invariant (though not a very useful one).

Motivation

Understanding relationships between invariants is an important question in knot theory, and such relationships are often associated with important open problems.

For instance, the volume conjecture relates a certain family of algebraic invariants to the hyperbolic volume of the knot complement. One approach to the smooth 4d Poincaré conjecture involves a knot invariant called the slice genus, a difficult-to-compute geometric quantity for which the existence of even a bound by an algebraic invariant is useful.

These relationships are also typically associated with subtle phenomena in topological field theory and string theory. Prior work demonstrated that, in some cases, they can be efficiently machine learned. [Hughes] [Craven, Jejjala, AK]

Outline

1. Review of relevant knot invariants and gauge theory
2. Machine learning correlations
3. Finding analytic explanations

Knots and gauge theory

The Jones polynomial $J(q)$ is a very useful and important knot invariant. [Jones]

It is a Laurent polynomial in q with integer coefficients obeying the recursion relation

$$qJ(\;;q) - q^{-1}J(\;;q) = (q^{1/2} - q^{-1/2})J(\;;q),$$

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

The simplest nontrivial knot, the trefoil knot, has Jones polynomial

$$J(\;;q) = q + q^3 - q^4.$$

Knots and gauge theory

The Jones polynomial and its generalizations are expectation values of a Wilson loop along the knot in $SU(2)$ Chern–Simons theory on S^3. [Witten 88]

$$W(A) = \frac{1}{4\pi} \int_{S^3} \left[A \wedge \mathrm{d}A + \frac{2}{3} A \wedge A \wedge A \right],$$

$$U_n(K) = \mathrm{tr}_n \, \mathcal{P} \exp \left(- \oint_K A \right),$$

$$J_n(e^{2\pi i/(k+2)}) = \frac{\int_{\mathcal{U}} [\mathcal{D}A] U_n(K) \exp[ikW(A)]}{\int_{\mathcal{U}} [\mathcal{D}A] U_n(\bigcirc) \exp[ikW(A)]}.$$

The original Jones polynomial corresponds to taking the Wilson loop trace in the fundamental representation with dimension $n = 2$.

Knots and gauge theory

The Jones polynomial can be categorified: there is a bigraded cohomology theory $\mathcal{H}(K) = \oplus_{m,n}\mathcal{H}^{m,n}(K)$ for which $J(q)$ is the graded Euler characteristic: [Khovanov]

$$(q+q^{-1})J(q^2) = \sum_{m,n} \dim \mathcal{H}^{m,n}(K)(-1)^m q^n.$$

$\mathcal{H}(K)$ is often presented in a tabular form. For the trefoil, $\mathcal{H}($$)$ is

$n \setminus m$	0	1	2	3
1	$\mathbb{Q}$			
3	$\mathbb{Q}$			
5			$\mathbb{Q}$	
7				
9				$\mathbb{Q}$

Knots and gauge theory

While it is not proven that $\mathcal{H}(K)$ may be computed using gauge theory, there is a proposal that $\mathcal{H}(K)$ is the cohomology of a supercharge Q in the 6d (0,2) theory on a certain Cauchy slice with a surface operator Σ_K whose topology is set by K. [Witten 11]

The space $\mathcal{H}(K)$ also has a (non-UV-complete) description as the Q-cohomology in the Hilbert space of 5d super-Yang-Mills theory, where the bigrading is generated by a $U(1) \times U(1)$ symmetry associated to fermion and instanton number operators. [Witten 11]

For the specialization yielding $J(q)$, there is an equivalent 4d super-Yang-Mills path integral which counts classical supersymmetric solutions weighted by $(-1)^F q^P$ where F and P are the fermion and instanton numbers. This gives a 4d interpretation of the Jones polynomial, originally a 3d invariant. [Gaiotto, Witten]

Knots and gauge theory

Two other knot invariants, which (in a certain sense) are naturally defined in 4d, are the Rasmussen s-invariant and smooth slice genus g.

The s-invariant is defined using a certain spectral sequence which collapses $\mathcal{H}(K) \Rightarrow \mathbb{Q} \oplus \mathbb{Q}$, and the two remaining factors have instanton grading $s \pm 1$. [Lee] [Rasmussen]

The smooth slice genus of a knot K is the least integer g for which there is a smooth surface $\Sigma \subset B^4$ with genus g that has $K = \partial\Sigma \subset \partial B^4$.

The trefoil has $s(☘) = 2$ and $g(☘) = 1$.

Knots and gauge theory

Neither s nor g have simple gauge theory interpretations, though s may be accessible through certain supercharge deformations.

[Kronheimer, Mrowka] [Gukov et al]

There is sometimes a more direct connection between Khovanov homology and s than the spectral sequence. Though false in general, the knight move conjecture provides a formula for s in terms of the Khovanov polynomial $\mathrm{Kh}(q,t)$ for many knots.

[Manolescu, Marengon]

The Khovanov polynomial is defined as

$$\mathrm{Kh}(q,t) \equiv \sum_{m,n} \dim \mathcal{H}^{m,n} t^m q^n.$$

The knight move conjecture states

$$\mathrm{Kh}(q,-q^{-4}) = q^s(q+q^{-1}).$$

Knots and gauge theory

It is worthwhile to understand what sort of information is contained in the Jones polynomial and Khovanov homology. Rasmussen proved

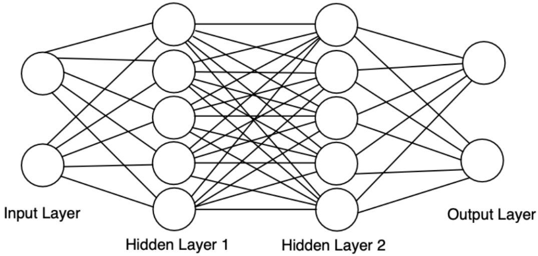
$$|s| \leq 2g,$$

relating the s-invariant to the slice genus. But perhaps $J(q)$ and $\mathcal{H}(K)$ know more about s and g than is obvious?

Machine learning

We performed four classes of experiments using a simple two-layer neural network with 100 hidden units per layer.

The input to the network was one of $\{J(q), \mathrm{Kh}(q,t)\}$ and the output was one of $\{s, g\}$. As the outputs are integer-valued, we set up a classification problem with a number of classes equal to the number of possibilities in the dataset.



Machine learning

The dataset consists of roughly 500,000 knots. Due to the difficulty of computing the slice genus, the data generation process was complicated.

We began with two groups of seed braids: the KnotInfo dataset (1200 knots of known slice genus) and random quasipositive or quasinegative braids (of the form $\alpha\sigma_i^{\pm}\alpha$, known slice genus by the slice-Bennequin inequality).

Given a seed braid β, we randomly inserted words of the form $\gamma\sigma_i^{\pm}\gamma^{-1}$ into β. Each such insertion changes the slice Euler characteristic by ± 1 or 0, which together with the known initial slice genus gives upper and lower bounds on the final slice genus. A final sequence of Markov moves further randomized the dataset.

Machine learning

Computation of other invariants was enough to completely fix the slice genus for many knots.

For instance, using the software KnotJob, we computed s-invariants and used $|s| \leq 2g$. [Schütz]

A smaller dataset was generated using the random petal permutation model, but the slice genus for these is hard to compute and we excluded them from slice genus experiments.
[Adams et al]

Machine learning

In total, we used a dataset of 535,239 knots with known $J(q)$, $\mathrm{Kh}(q, t)$, and s. We know g exactly for 438,295 of these.

Despite the careful construction, there are no known exact relationships between these invariants in our dataset other than the knight move conjecture, which holds for the vast majority of our knots.

$$\mathrm{Kh}(q, -q^{-4}) = q^s(q + q^{-1}).$$

Machine learning

The network predicts s and g with 98.3% and 98.6% accuracy from $\mathrm{Kh}(q,t)$ when trained on 25% of the data, but these do not drop below 94% when the training fraction is 1% of the total.

We obtain the following accuracies for predicting s or g from specializations $\mathrm{Kh}(q,-q^n)$ of the Khovanov polynomial:

n	s-invariant accuracy	slice genus accuracy
-5	0.9567 ± 0.0024	0.9700 ± 0.0021
-4	0.9977 ± 0.0010	0.9452 ± 0.0007
-3	0.9791 ± 0.0043	0.9716 ± 0.0068
-2	0.9988 ± 0.0005	0.9456 ± 0.0002
-1	0.9771 ± 0.0054	0.9751 ± 0.0051
0	0.9480 ± 0.0021	0.9720 ± 0.0016

Machine learning

When trained on the same fraction, the network achieves 95% and 96% accuracy in predicting s or g respectively from $J(q)$. When the fraction is decreased to 1%, the accuracies are still close to 89%.

We also evaluate $J(q = e^{\pi in/(k+2)})$ and assemble a vector for each k with values $n \in [0, k+1]$.

k	Rasmussen accuracy	Slice genus accuracy
3	0.9314 ± 0.0013	0.9672 ± 0.0017
4	0.9186 ± 0.0009	0.9601 ± 0.0010
5	0.9650 ± 0.0006	0.9826 ± 0.0009
6	0.9674 ± 0.0007	0.9828 ± 0.0008
7	0.9676 ± 0.0007	0.9825 ± 0.0008
8	0.9673 ± 0.0005	0.9825 ± 0.0006
9	0.9669 ± 0.0011	0.9814 ± 0.0014
10	0.9680 ± 0.0006	0.9826 ± 0.0008

Machine learning

The upshot of these experiments (see the paper for more) is that a robust correlation exists between $J(q)$ or $\mathrm{Kh}(q,t)$ and the s-invariant or slice genus.

The slice genus correlation is very difficult to explain, as there is no known simple formula to extract g from the Khovanov homology. On the other hand, the s-invariant has a clear definition from Khovanov homology, so we can look for analytic explanations of this correlation.

Analytic explanations

The correlations between $\mathrm{Kh}(q,t)$ or $\mathrm{Kh}(q,-q^{-4})$ and s are simply explained using the knight move conjecture. However, the strong performance of $\mathrm{Kh}(q,-q^{-2})$ is more mysterious.

We found that $\mathrm{Kh}(q,-q^{-2})$ often takes a form which is completely fixed by s. For instance, nearly every knot in the dataset obeys a relation similar to

$$\mathrm{Kh}(q,-q^{-2}) = q^s \left(-\left(\tfrac{s}{2}-1\right) q + \left(\tfrac{s}{2}+1\right) q^{-1}\right).$$

There are also cases with three or more terms:

$$\mathrm{Kh}(q,-q^{-2}) = -q^{s-1} + \left(5+\tfrac{s}{2}\right) q^{s+1} - \left(2+\tfrac{s}{2}\right) q^{s+3}.$$

Analytic explanations

In these formulas, we know how to explain for a given knot which powers of q will appear and how many terms the formula will have. This comes from a substitution $\mathrm{Kh}(q, tq^{-2})$ to "renormalize" the fermion grading before sending $t = -1$, which fixes the powers and number of terms that can appear in terms of the instanton gradings at t^0, which are related directly to s.

The coefficients, on the other hand, cannot be so simply explained. Their complete determination by s suggests that perhaps Rasmussen's invariant is encoded in Khovanov homology in more than one way. Specifically, it is not just the instanton number which may yield s, but also the total (appropriately graded) number of supersymmetric ground states in the 5d super-Yang–Mills theory.

Analytic explanations

The correlation of the Jones polynomial with s is even less understandable. It is common lore in knot theory that the s-invariant captures information which is distinct from $J(q)$. Indeed, there are knots with identical $J(q)$ but different s, so there can be no precise formula for s which uses only $J(q)$.

The gauge theory statement of this connection, which we are currently exploring, is as follows. The correspondence between Khovanov homology and the supercharge cohomology in 5d super-Yang–Mills arises by applying stringy dualities to the 4d $\mathcal{N} = 4$ theory on $\mathbb{R}_+ \times \mathbb{R}^3$ with a knot defect on the boundary. This 4d path integral is equal by supersymmetric localization to the 3d Chern–Simons path integral on its boundary, possibly with an exotic integration cycle. [Witten 10] [Gaiotto, Witten]

Analytic explanations

The correlation between $J(q)$ and s points to an appearance in 3d Chern–Simons theory of some specific information about approximate supersymmetric ground states of the 5d theory which arises by looking for a Hilbert space formulation of the 4d path integral.

The conjecture we would like to make is that the space of exotic integration cycles in 3d Chern–Simons theory has privileged access to the instanton numbers of approximate supersymmetric ground states in the 5d theory with fermion number zero, and in favorable cases may actually determine these instanton numbers completely.

We are currently exploring this conjecture by trying to understand the necessary deformation of Khovanov homology to derive s in the 5d language.

Conclusions

We have trained a neural network to learn robust correlations between the Jones or Khovanov polynomials and the Rasmussen s-invariant or slice genus. These correlations persist even when training on 1% of the dataset.

We have partial analytic explanations for the Khovanov correlation with the s-invariant, and a rough conjecture for a gauge theory story approximately relating $J(q)$ and s.

The correlations with g remain mysterious, and perhaps suggest some kind of algebraic formula for the slice genus.

Outlook

In previous work, a similar correlation between $J(q)$ and the hyperbolic volume was explained using exotic integration cycles in Chern–Simons theory. [Craven, Jejjala, AK]

Though the volume is also not determined by $J(q)$, understanding the gauge theory mechanism leads one immediately to the celebrated volume conjecture relating the colored Jones polynomials to the hyperbolic volume.

If we can find a similar gauge theory mechanism here, whether through gauge symmetry breaking, supercharge deformation, etc., will we be led to a "slice genus conjecture" or "s-invariant conjecture", this time relating some similar 3d algebraic invariant to a geometric 4d invariant?