### Knot theory and machine learning

Marc Lackenby Joint work with Alex Davies, András Juhász, Nenad Tomasev

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# The branches of knot theory

Knot theory is divided into three quite distinct subfields:

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- hyperbolic knot theory
- gauge/Floer theory
- quantum topology

#### Invited speakers

- Ian Agol (U. C. Berkeley)
- Martin Bridson (Oxford U.)
- Jeff Brock (Yale U.)
- Ted Chinburg (U. Pennsylvania)
- Michelle Chu (U.I. Chicago)
- Jeff Danciger (U.T. Austin)
- Cameron Gordon (U.T. Austin)
- Ursula Hamenstadt (U. Bonn)
- Neil Hoffman (O.S.U.)
- Autumn Kent (U.W. Madison)
- Darren Long (U.C. Santa Barbara)
- Alex Lubotzky (Hebrew U.)
- Bruno Martelli (U. Pisa)
- Gaven Martin (Massey U.)
- Priyam Patel (U. Utah)
- Kate Petersen (U.M. Duluth)
- Jessica Purcell (Monash U.)
- Peter Sarnak (Princeton U.)
- Matt Stover (Temple U.)
- Sam Taylor (Temple U.)
- Genevieve Walsh (Tufts U.)
- Will Worden (Rice U.)

#### Alan Reid's conference

#### **Topics:**

- Interplay of 3-dimensional and 4-dimensional Topology
- · Floer homology theories and associated invariants
- · Khovanov homology
- · Geometric and analytic aspects of gauge theoretic equations

#### Speakers:

D. GABAI, Princeton University, USA L. GOETTSCHE, ICTP, Italy L. GUTH, MIT, USA J. HOM, Georgia Tech, USA C. HUGELMEYER, Princeton University, USA \*P. KRONHEIMER, Harvard University, USA F. LIN, Princeton University, USA R. LIPSHITZ, University of Oregon, USA P. LISCA, Università di Pisa, Italy C. MANOLESCU, Stanford University, USA G. MATIC, University of Georgia, USA R. MAZZEO, Stanford University, USA M. MILLER, Stanford University, USA E. MURPHY, Princeton University, USA \*J. PARDON, Princeton University, USA L. PICCIRILLO, MIT, USA J. PINZON CAICEDO, University of Notre Dame, USA J. RASMUSSEN, Cambridge, UK D. RUBERMAN, Brandeis University, USA A. STIPSICZ, Central European University, Hungary Z. SZABO, Princeton University, USA \*C.TAUBES, Harvard University, USA D. WANG SUNY, Stony Brook, USA J. WANG, Harvard University, USA C. ZIBROWIUS, University of Regensburg, Germany

#### Trieste conference

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Each field has plenty of knot invariants:

Hyperbolic invariants:

3/4-dimensional invariants:

- Volume
- Cusp shape and volume
- Length spectrum
- ► Trace field ...

- Heegaard Floer homology
- Instanton Floer homology

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3/4-dimensional invariants:

signature

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Goal: Find new connections between these invariants

## Knot signature

The 3/4-dimensional invariant that we focused on was the signature.

This is defined by starting with a Seifert surface S for the knot K. The symmetrised Seifert form for S is the bilinear form

$$egin{aligned} &\mathcal{H}_1(\mathcal{S}) imes \mathcal{H}_1(\mathcal{S}) 
ightarrow \mathbb{Z} \ & (\ell_1,\ell_2) \mapsto \mathrm{lk}(\ell_1,\ell_2^+) + \mathrm{lk}(\ell_2,\ell_1^+) \end{aligned}$$

where  $\ell_2^+$  is the push-off of  $\ell_2$  in the positive normal direction from *S*.

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The signature  $\sigma(K)$  is the signature of this bilinear form.

# Connections with dimension 4

View  $\mathbb{R}^3$  as the boundary of  $\mathbb{R}^4_+ = \{(x_1, x_2, x_3, x_4) : x_4 \ge 0\}.$ 



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The 4-ball genus of a knot K is the minimal genus of a (topological locally-flat) surface in  $\mathbb{R}^4_+$  with boundary equal to K.

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The 4-ball genus of a knot K is the minimal genus of a (topological locally-flat) surface in  $\mathbb{R}^4_+$  with boundary equal to K. <u>Theorem</u>: [Murasugi 1965]  $g_4(K) \ge |\sigma(K)|/2$ .

Goal: can we predict the signature from hyperbolic invariants?

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- ► This was the Regina census of 1,700,000 knots with ≤ 16 crossings plus 1,000,000 randomly chosen knots with ≤ 80 crossings.

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- We then tested this network using the test set.
- The network could predict the signature with impressive accuracy.

# Saliency

The main hyperbolic invariants that were used to predict signature:



# Hyperbolic structures

A hyperbolic structure on a knot complement is a complete finite-volume Riemannian metric of constant curvature -1.

By Mostow rigidity, if such a metric exists, it is a unique up to isometry.

<u>Thurston's theorem</u>: The complement of a non-trivial knot K has a hyperbolic structure if and only if K is not a torus knot or a satellite knot.



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# Cusp geometry

Any knot complement has an end of the form  $\mathcal{T}^2\times [1,\infty).$ 

When the knot is hyperbolic, this has a canonical geometry and is called a cusp.

Let  $\mathbb{H}^3$  be upper-half space  $\{(x, y, z) : z > 0\}$ . Let H be the horoball  $\{z \ge 1\}$ .

Then the cusp is formed  $H/\langle \text{group of Euclidean translations} \rangle$ .



# The cusp boundary

The boundary of the cusp is a Euclidean torus  $\mathbb{C}/\Lambda$  for a lattice  $\Lambda$ . We normalise  $\Lambda$  so that the longitude  $\lambda$  is real and positive, and the meridian  $\mu$  has positive imaginary part.





Cusp torus for  $6_1$ 

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Cusp torus for  $6_1$ 

The three main features that the machine learning algorithms used to predict signature were  $\lambda$ ,  $\operatorname{Re}(\mu)$  and  $\operatorname{Im}(\mu)$ .

#### Signature and cusp geometry



#### A plot of signature against $\operatorname{Re}(\mu)$ coloured by $\lambda$

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#### Signature and cusp geometry



A plot of signature against  $\operatorname{Re}(\mu)$  coloured by  $\lambda$ 

<u>Initial observation</u>: the signs of the signature and  $\operatorname{Re}(\mu)$  are highly correlated.

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# The natural slope

#### The natural slope

Pick a geodesic representative μ for the meridian.



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- Fire a geodesic µ<sup>⊥</sup> orthogonally from it.
- Eventually, it will return to the meridian.
- In that time, it will have gone along one longitude and some number s of meridians.

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- Eventually, it will return to the meridian.
- In that time, it will have gone along one longitude and some number s of meridians.
- Define the natural slope to be -s.

 $\operatorname{slope}(K) = \operatorname{Re}(\lambda/\mu).$ 

# Slope and signature



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#### First conjectures

#### <u>Conjecture</u>: There is a constant $c_0$ such that

 $\sigma(K) \simeq c_0 \operatorname{slope}(K).$ 

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<u>Conjecture</u>: There are constants  $c_0$  and  $c_1$  such that

$$|\sigma(K) - c_0 \operatorname{slope}(K)| \le c_1 \operatorname{vol}(K).$$

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# Highly twisted knots

<u>Theorem</u>: Let K be a knot, and let  $C_1, \ldots, C_n$  be curves in the complement that bound disjoint discs in  $S^3$ . Suppose  $K \cup C_1 \cup \cdots \cup C_n$  is hyperbolic. Let  $K(q_1, \ldots, q_n)$  be the knot obtained from K by adding  $q_i$  full twists along each  $C_i$ .

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$$\left|\operatorname{slope}(\mathcal{K}(q_1,\ldots,q_n))+\sum_{i=1}^n\ell_i^2q_i
ight|\leq k$$

$$igg| \sigma(\mathcal{K}(q_1,\ldots,q_n)) + \left(rac{1}{2}\sum_{i=1}^m \ell_i^2 q_i + rac{1}{2}\sum_{i=m+1}^n (\ell_i^2 - 1)q_i
ight) igg| \leq k \ \mathrm{vol}(\mathcal{K}(q_1,\ldots,q_n)) \leq k.$$

So the conjectures are false!

#### Theorems

<u>Theorem 1</u>: There is a constant  $c_1$  such that

$$|\sigma(\mathcal{K}) - (1/2)\operatorname{slope}(\mathcal{K})| \le c_1 \operatorname{vol}(\mathcal{K})\operatorname{inj}(\mathcal{K})^{-3}.$$

Here,  $\operatorname{inj}(K)$  is  $\inf\{\operatorname{inj}_x(S^3 - K) : x \in (S^3 - K) - \operatorname{cusp}\}.$ 

#### Theorems

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Here,  $\operatorname{inj}(\mathcal{K})$  is  $\operatorname{inf}\{\operatorname{inj}_{X}(S^{3} - \mathcal{K}) : x \in (S^{3} - \mathcal{K}) - \operatorname{cusp}\}$ . <u>Theorem 2</u>:  $\sigma(\mathcal{K})$  and

$$(1/2)$$
 slope $(K) + \sum_{\gamma \in \text{OddGeo}} \kappa(\gamma)$ 

differ by at most  $c_2 \operatorname{vol}(K)$  for some constant  $c_2$ .

Here, OddGeo is the set of geodesics with length at most 0.1 and that have odd linking number with K, and  $\kappa(\gamma)$  is a correction term defined in terms of the complex length of  $\gamma$ .

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Consequence: 4-ball genus

Corollary:

$$g_4(K) \geq |\operatorname{slope}(K)|/4 - (c_1/4)\operatorname{vol}(K)\operatorname{inj}(K)^{-3}.$$

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The slopes on  $\partial N(K)$  are parametrised by fractions q/p. Let K(q/p) be the manifold obtained by Dehn filling along q/p.

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Let K(q/p) be the manifold obtained by Dehn filling along q/p.

The filling is exceptional if K(q/p) does not have a hyperbolic structure.

Each slope q/p has a length  $\ell(q/p)$  as measured in the Euclidean metric on the torus.

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<u>Theorem</u>: [Agol, L] If  $\ell(q/p) > 6$ , then q/p is not exceptional.

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<u>Theorem</u>: [Agol, L] If  $\ell(q/p) > 6$ , then q/p is not exceptional.

Lemma:  $\ell(q/p) > |p\operatorname{slope}(K) + q|$ . Hence if q/p is exceptional, then

$$q/p \in [-\operatorname{slope}(K) - 6/p, -\operatorname{slope}(K) + 6/p].$$

#### Exceptional slopes and signature

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## Exceptional slopes and signature

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Hence, q/p is 'close' to  $-2\sigma(K)$ .

Example: (-2,3,7) pretzel knot.

Its exceptional slopes are 16, 17, 18, 37/2, 19, 20. slope(K)  $\simeq -18.215$   $\sigma(K) = -8.$ 



## Signature and spanning surfaces

Let S be an unoriented spanning surface for K. Its Goeritz form is

$$egin{aligned} G_S\colon H_1(S) imes H_1(S) o \mathbb{Z}\ (\ell_1,\ell_2)\mapsto \mathrm{lk}(\ell_1,\ell_2') \end{aligned}$$

where  $\ell'_2$  is the double push-off of  $\ell_2$ . <u>Theorem:</u> [Gordon-Litherland]

$$\sigma(K) = \sigma(G_S) + e(S)/2,$$

where e(S) is the framing of  $\partial S$ .

## Building a triangulation

<u>Theorem</u>: [Thurston] Any closed hyperbolic 3-manifold M has a triangulation where the number of tetrahedra is at most  $O(\text{vol}(M)\text{inj}(M)^{-3})$ .

# Building a triangulation

<u>Theorem</u>: [Thurston] Any closed hyperbolic 3-manifold M has a triangulation where the number of tetrahedra is at most  $O(\text{vol}(M)\text{inj}(M)^{-3})$ .



Form the associated Voronoi domain.

Add a vertex to each face and cone off the face. Triangulate each polyhedron of the domain as a cone on its boundary.

<u>Theorem</u>: Any cusped hyperbolic 3-manifold M has a triangulation where the number of tetrahedra is at most  $O(vol(M)inj(M)^{-3})$ .

<u>Theorem</u>: Any cusped hyperbolic 3-manifold M has a triangulation where the number of tetrahedra is at most  $O(vol(M)inj(M)^{-3})$ . Furthermore, if  $M = S^3 - K$  and n is a closest even integer to slope(K), then the slope  $\lambda - n\mu$  is represented by a normal curve that intersects each triangle in  $\partial M$  in at most one arc.

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Start with a maximal set of points in  $\partial(\text{cusp})$ , no two of which are closer than  $\epsilon/4$ , and then extend this to a maximal set in M - int(cusp).



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<u>Lemma:</u> Let *C* be a normal curve in  $\partial M$  that intersects each triangle in at most one arc and that is trivial in  $H_1(M; \mathbb{Z}_2)$ . Then *C* extends to a normal surface *F* in *M* that intersects each tetrahedron in at most one triangle or square.

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Join these points.



<u>Theorem 1</u>: There is a constant  $c_1$  such that

 $|\sigma(\mathcal{K}) - (1/2)\operatorname{slope}(\mathcal{K})| \le c_1 \operatorname{vol}(\mathcal{K})\operatorname{inj}(\mathcal{K})^{-3}.$ 

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Gordon-Litherland:  $\sigma(K) = \sigma(G_F) + n/2$ .  
So  $|\sigma(K) - \operatorname{slope}(K)/2| \leq |\sigma(G_F)| + 1 \leq O(\operatorname{vol}(M)\operatorname{inj}(M)^{-3})$ .

<u>Theorem 2</u>:  $\sigma(K)$  and (1/2) slope $(K) + \sum_{\gamma \in OddGeo} \kappa(\gamma)$  differ by at most  $c_2$  vol(K) for some constant  $c_2$ .

<u>Theorem 2</u>:  $\sigma(K)$  and (1/2) slope $(K) + \sum_{\gamma \in OddGeo} \kappa(\gamma)$  differ by at most  $c_2$  vol(K) for some constant  $c_2$ .

Proof outline:



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#### Proof outline:

Margulis: There is a universal  $\epsilon>0.1$  such that the points x with  $\mathrm{inj}_x\leq\epsilon/2$  form cusps and regular neighbourhoods of short geodesics.

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## Proof of Theorem 2

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## Proof of Theorem 2

<u>Theorem 2</u>:  $\sigma(K)$  and (1/2) slope $(K) + \sum_{\gamma \in OddGeo} \kappa(\gamma)$  differ by at most  $c_2$  vol(K) for some constant  $c_2$ .

#### Proof outline:

Margulis: There is a universal  $\epsilon > 0.1$  such that the points x with  $inj_x \le \epsilon/2$  form cusps and regular neighbourhoods of short geodesics. The rest is the thick part of M. Triangulate the thick part using O(vol(M)) tetrahedra. Form a spanning surface F that intersects each tetrahedron in at most one triangle or square and with boundary slope equal to  $\lambda - n\mu$ , where n is closest even integer to slope(K). Carefully specify F in N(short geodesics).

$$\sigma(G_F) = O(\operatorname{vol}(M)) + \sum_{\gamma \in \operatorname{OddGeo}} \kappa(\gamma)$$

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<u>Theorem 2</u>:  $\sigma(K)$  and (1/2) slope $(K) + \sum_{\gamma \in OddGeo} \kappa(\gamma)$  differ by at most  $c_2$  vol(K) for some constant  $c_2$ .

#### Proof outline:

Margulis: There is a universal  $\epsilon > 0.1$  such that the points x with  $inj_x \le \epsilon/2$  form cusps and regular neighbourhoods of short geodesics. The rest is the thick part of M. Triangulate the thick part using O(vol(M)) tetrahedra. Form a spanning surface F that intersects each tetrahedron in at most one triangle or square and with boundary slope equal to  $\lambda - n\mu$ , where n is closest even integer to slope(K). Carefully specify F in N(short geodesics).

$$egin{aligned} \sigma(\mathcal{G}_{\mathcal{F}}) &= \mathcal{O}(\mathrm{vol}(\mathcal{M})) + \sum_{\gamma \in \mathrm{OddGeo}} \kappa(\gamma) \ &\\ \sigma(\mathcal{K}) &= \sigma(\mathcal{G}_{\mathcal{F}}) + n/2. \end{aligned}$$

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# The machine knew all along!



Items 4 and 5 are the terms appearing in Theorems 1 and 2.

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