Machine Learning for Knot Invariants.

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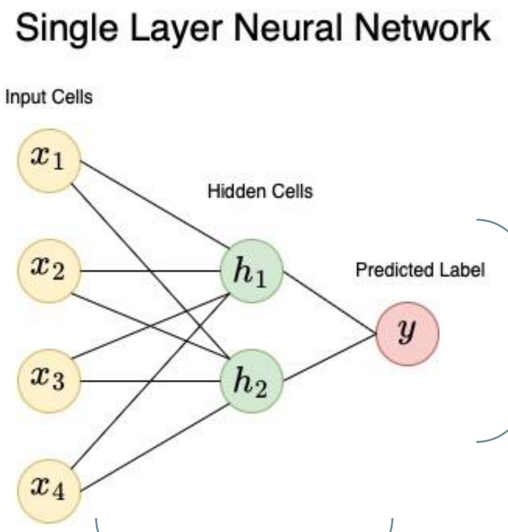
Summary.

- Machine Learning.
- Gaussian linking integral.
- Finite Type (Vassiliev) Knot Invariants.

Machine Learning.



Some choice of input data which has a true label.

Computation is iteratively improved until classification is as accurate as possible for given input.

Hidden computation: computer tries to accurately classify data.

Machine Learning for Knot Theory.

- M. Lackenby – finding relationships between different types of knot invariants[1].
  - Dataset: several knot invariants up to knots with 15 crossings.
    - Features: Knot Invariants.
    - Labels: Other Knot Invariants.

- O. Vandans – Classifying knot conformations in polymers[2].
  - Dataset: several thousand perturbed conformations of first 5 crossing knots (using coordinate data).
    - Features: XYZ coordinate data of knots
    - Labels: Knot type.

- Our Research – Classifying knot conformations.
  - Dataset: several thousand perturbed conformations knots.
    - Features: Geometric knot measures.

[1] Davies, A., Juhász, A., Lackenby, M., & Tomasev, N. (2021). The signature and cusp geometry of hyperbolic knots. *arXiv preprint arXiv:2111.15323*.
[2] Vandans, O., Yang, K., Wu, Z., & Dai, L. (2020). Identifying knot types of polymer conformations by machine learning. *Physical Review E*, *101*(2), 022502.

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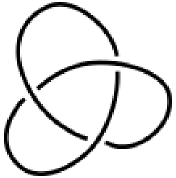
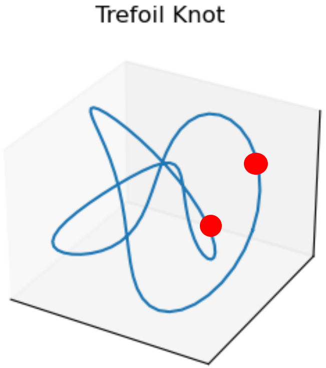
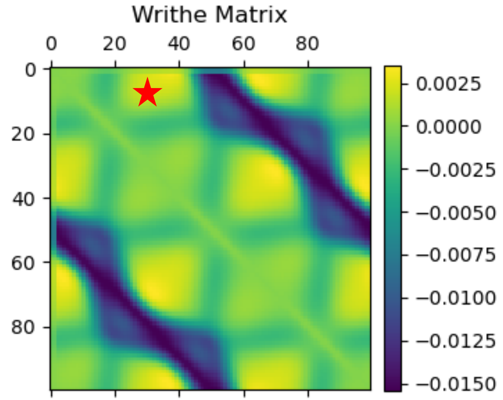
Feature: Gaussian Linking Integral[3].



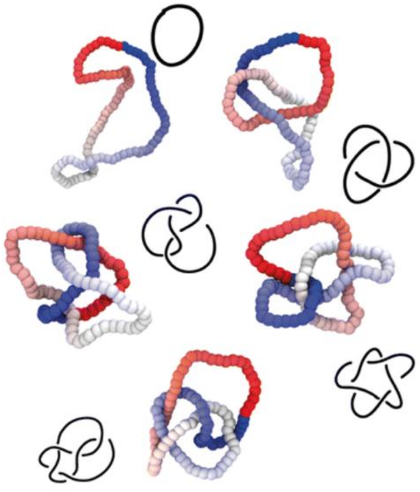


$$\omega(x, y) = \frac{\dot{r}(x) \times \dot{r}(y)) \cdot (r(x) - r(x))}{|r(x) - r(y)|^3}$$



[3] Sleiman, J. L., Conforto, F., Fosado, Y. A. G., & Michieletto, D. (2024). Geometric learning of knot topology. *Soft Matter*, *20*(1), 71-78.

Dataset[3].



⋯ 100, 000 different configurations per knot.

⋮

Up to 10 crossing knots.

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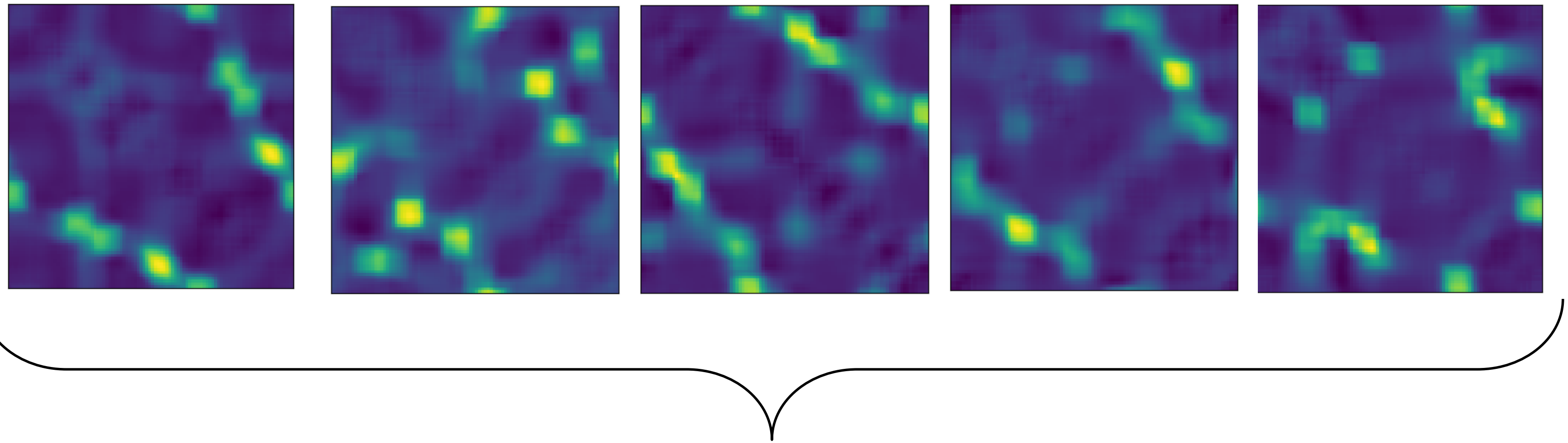

Some 5_1 configurations in the dataset (substantial variation).

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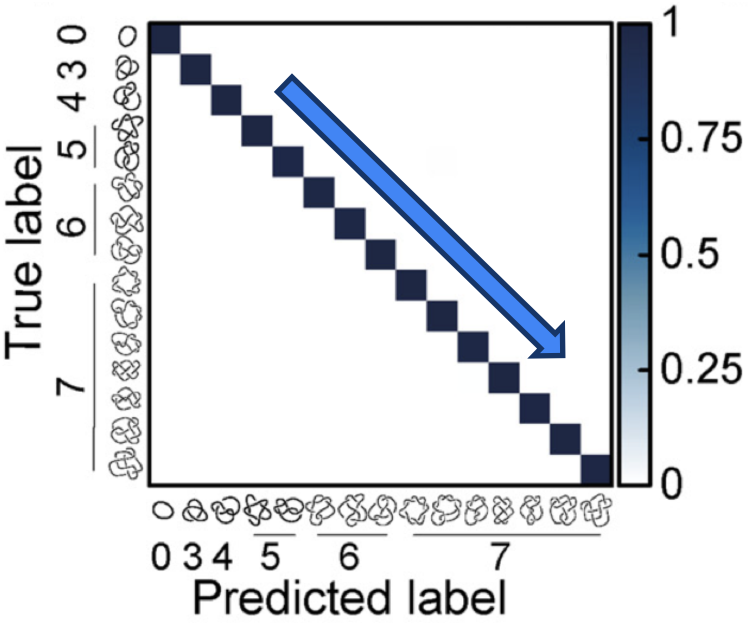
Predicting Knot Type Using Writhe Matrix[3].

7 Class: classification of first 7 crossing knots.

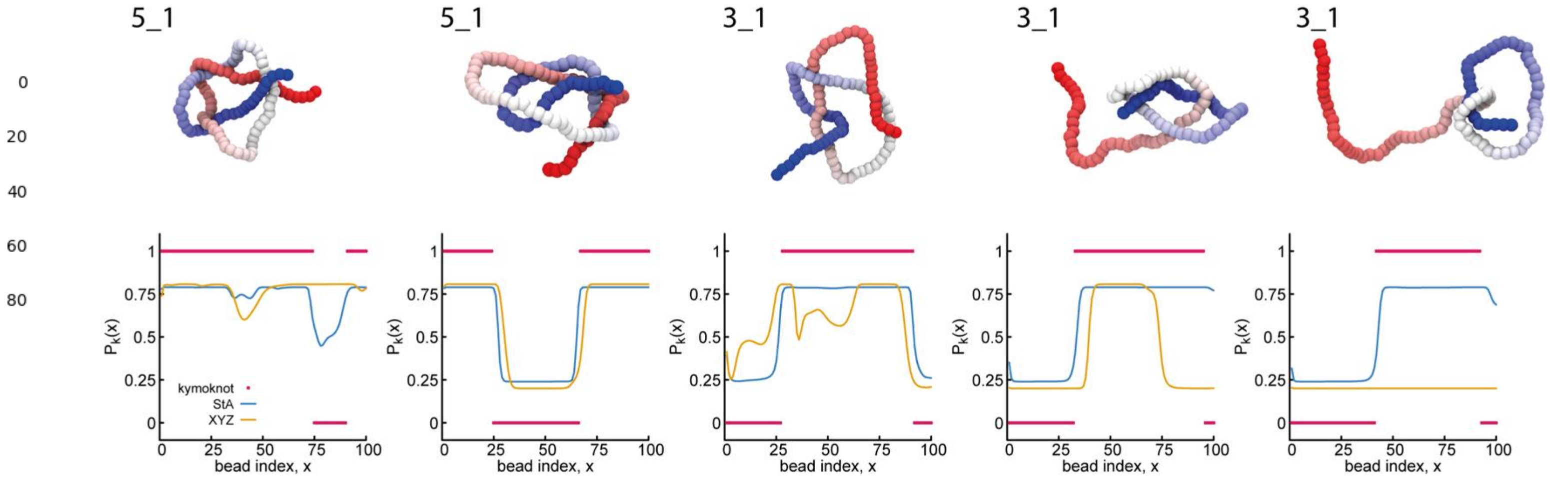


- 5 Class: ~99.9%
- 7 Class: ~99.8%
- 10 (>250 knots) Class: ~95%

[3] Sleiman, J. L., Conforto, F., Fosado, Y. A. G., & Michieletto, D. (2024). Geometric learning of knot topology. *Soft Matter*, *20*(1), 71-78.

Knot Localization[3].

Integral measure over writhe matrix provides classification of knot localization – naturally extends to knots on open curves.



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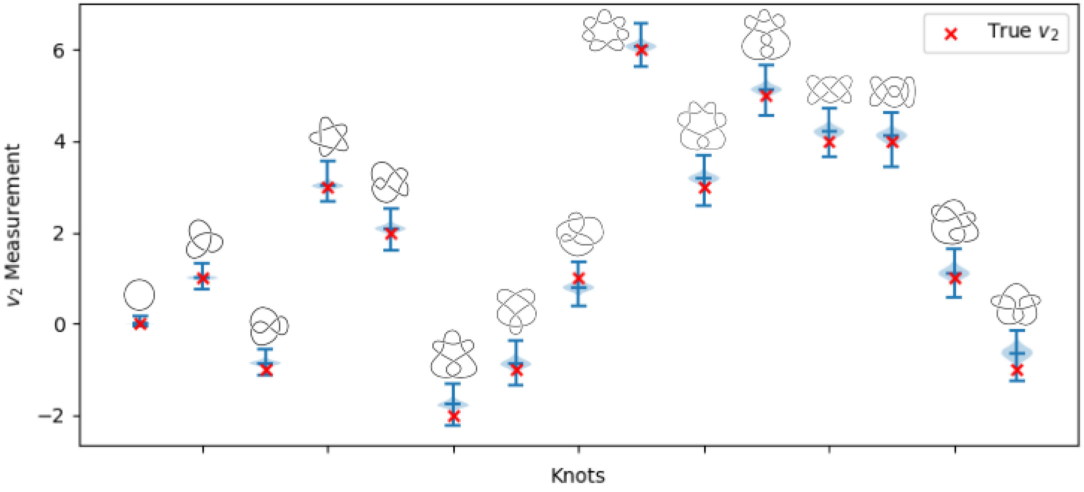
Understanding What's Being Learned: Vassiliev Invariants[4].

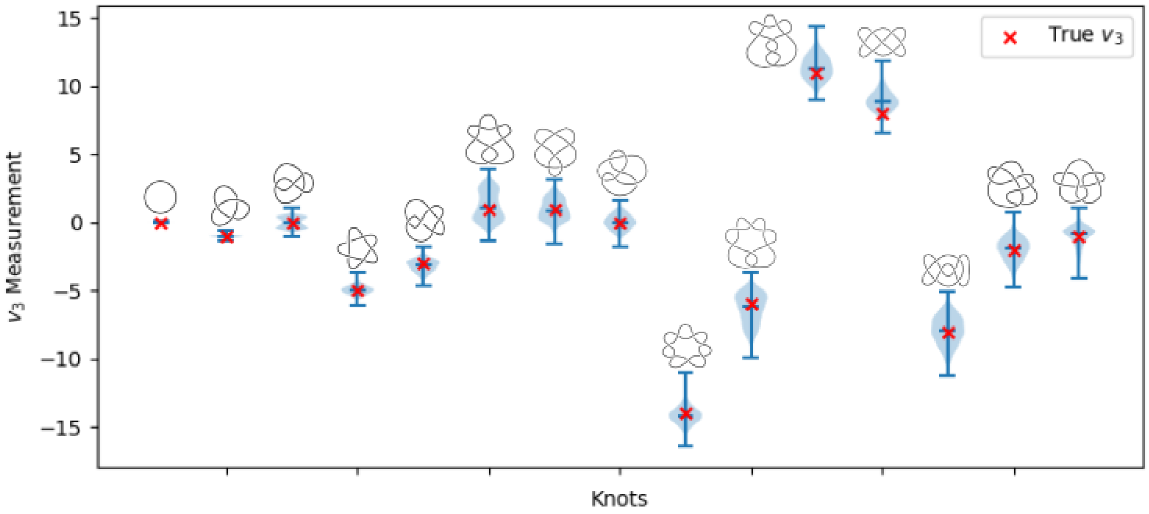
$$\int_{i<j<k<l} \omega(i,k) \cdot \omega(j,l)$$



[4] Panagiotou, E., & Kauffman, L. H. (2021). Vassiliev measures of complexity of open and closed curves in 3-space. *Proceedings of the Royal Society A*, *477*(2254), 20210440..

Understanding What's Being Learned: Vassiliev Invariants[4].

$$\int_{i<j<k<l<m<n} \frac{1}{2}\omega(i,l)\cdot\omega(j,n)\cdot\omega(k,m)+\omega(i,l)\cdot\omega(j,m)\cdot\omega(k,n)$$



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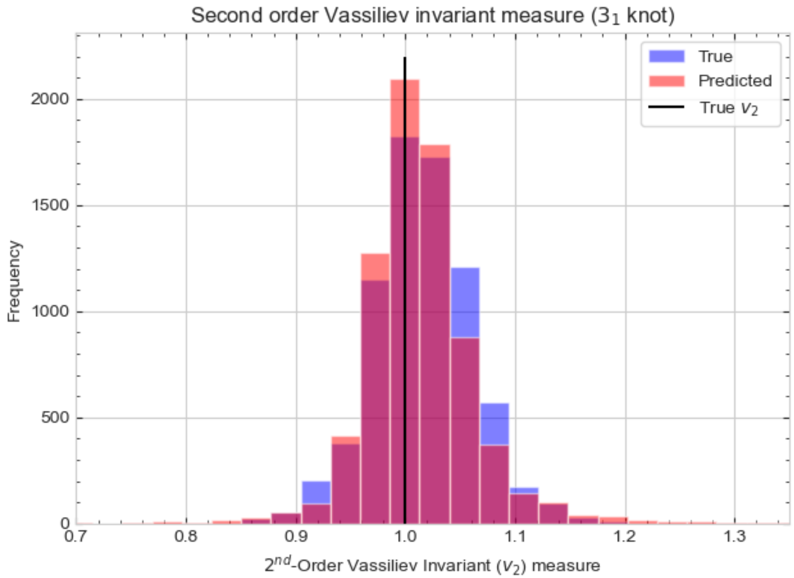
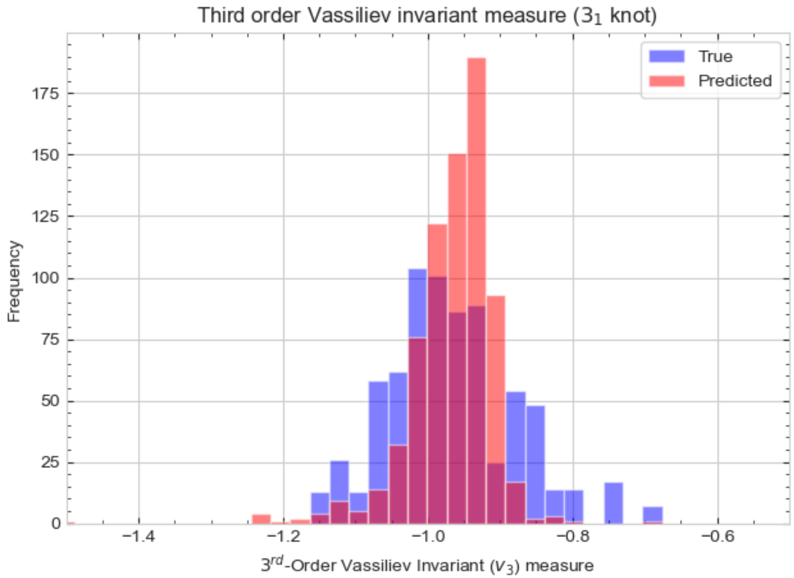
Machine Learning Capability to Learn Encoded Vassiliev Invariants.





Conclusion: Machine Learning architecture struggles to learn Vassiliev Invariants.
As ***order increases*** – ***accuracy decreases***.

Concluding Remarks

- Neural networks can use ‘writhe matrices’ to classify knots with very high accuracy up to 10 crossings.
- Vassiliev knot invariants are encoded within these writhe matrices.
- Neural networks struggle to learn high order vassiliev invariants from matrix data.

Concluding Remarks

- Open question: **what** is being learned by neural networks to classify knots with such high accuracy?