Guiding Intuition with Saliency Analysis

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Hausdorff School: “Machine Learning and Theorem Proving”

Day 3

September 20, 2023

Day 2 overview

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We will use this method to come up with conjectures, and to guide our intuition.

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Generally more data $\implies$ better predictions.

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Rooms	Size	Has kitchen	Brick type	Haunted	...	Price
5	130m^2	Yes	Limestone	No	...	\$1000000
3	50m^2	Yes	Marble	No	...	\$98000
2	25m^2	No	Mud	No	...	\$37500
3	80m^2	No	Limestone	Yes	...	???

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Given an email, classify if it is spam or not. Given a handwritten characte classify it as one of the known characters. Facial emotion classi cation.

Supervised learning

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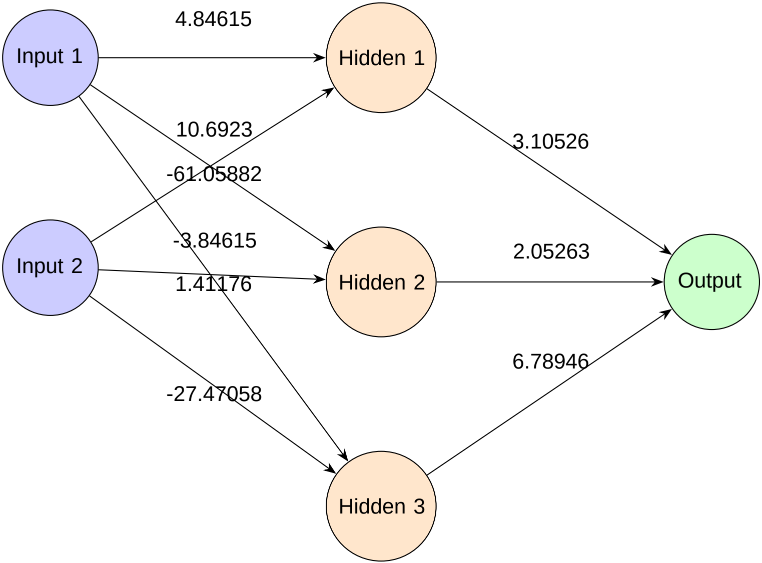
F is a very complicated function, we cannot completely learn it. Instead we will find a much simpler function f (given by the neural net), that is pretty close to F.

Neural networks



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We adjust the weights by using e.g. gradient descent, on the space of
weights of the network. We repeat this process many times, until we get
good at approximating F.

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Any* function can be approximated with a large enough neural network.

*: false in theory, and even more false in practice

TensorFlow Playground

Open TensorFlow Playground

Interpreting Neural Networks

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No Guarantee of Interpretability : There is no guarantee that we can extract meaningful human-understandable insights directly from the network's parameters.

When does supervised learning work best?

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- Working in the unit cube :
  - Normalize input data to the unit cube $[0,1]^d$.
  - Helps gradients flow consistently during training.
- Coordinates have low symbolic content :
  - Don't want noise sensitivity. Small changes in input shouldn't affect outcome much.
  - Abstract, high-level features are often more valuable.

Let's now see some simple examples
maths!

Simple examples in maths – the parity bit

Input: 0-1 sequence of length 1000.

Output: $\sum x_i \mod 2$.

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Noise Sensitivity:

This is the most noise sensitive problem you can come up with!
In this case, every single bit ip changes the outcome.
Very di cult to learn with a vanilla neural net.

Input: $x = (x_1; x_2; :::; x_n)$ a permutation of [n].

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We would like to predict the right and left descent sets:

$R(x) = \{i : x_i > x_{i+1}\}$ (Right Descent Set).
$L(x) = \{i : i$ occurs to the right of $i+1$ in $x\}$ (Left Descent Set).

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Symmetry:

- $R(x) = L(x^{-1})$ (Symmetrical concepts).

Data Representation Matters

Observation:

- Input permutation as a vector $x = (x_1, x_2, \ldots, x_n)$ - Neural network learns $R(x)$ quickly (for $n = 50$), but struggles on $L(x)$.
- Input permutation as a permutation matrix - Neural network easily learns both $R(x)$ and $L(x)$.

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How we input data really matters!

I really recommend Geordie Williamson's fantastic talk "What can the working mathematician expect from deep learning?"

The Importance of the Training Dataset

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The Unexpected Issue:

Every random matrix in the dataset is likely to be invertible!

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For half of the matrices in the dataset, we could pick a random row, and replace it with a random linear combination of all other rows. These matrices would now not be invertible.

Problem: these matrices will likely have entries less than 0 or bigger than 1, while the invertible ones in the dataset don't have such entries.

The network might just learn to predict "not invertible" if the matrix has an entry not in $[0, 1]$.

Issues with interpreting the result

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Problem: in mathematics we would often like to understand what this function is!

Saliency analysis to the rescue

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The main idea:

- We wiggle the input coordinates one by one.
- Observe how these perturbations a ect the network's output.
- Coordinates causing signi cant output changes are deemed importan features.
- If a coordinate's perturbation has little impact, the network likely doesn't rely on it for predictions.

A real application in maths

Knot theory

Knot theory

Type of questions knot theorists care about:

- Classifying all possible knots,
- deciding whether two knots are the same,
- how are various parameters of knots related, etc.

Knot Theory

Knot theory has three very distinct sub elds:

- Hyperbolic knot theory
- Gauge/Floer theory
- Quantum topology

Knot Invariants by eld:

Hyperbolic Invariants:

- Volume
- Cusp shape and volume
- Length spectrum
- Trace eld

Gauge Theory Invariants:

- signature
- Heegaard Floer homology
- Instanton Floer homology
- s, , ,

See Marc Lackenby's talk \Using machine learning to formulate mathematical conjectures" for more details about these invariants.

We created a huge dataset. For many knots K, we calculate the vector

$v(K) =$ (volume, cusp shape, length spectrum, trace field, ...).

We also calculate the signature of K. The training set of the neural network will consist of lots and lots of

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We train a neural network to try to predict the signature based on $v(K)$. If there is no connection between hyperbolic parameters in $v(K)$ and the signature, then the neural network will struggle. If the neural network does unreasonably well however, then there must be a connection between $v(K)$ and the signature that we don't know about!

Knot theory

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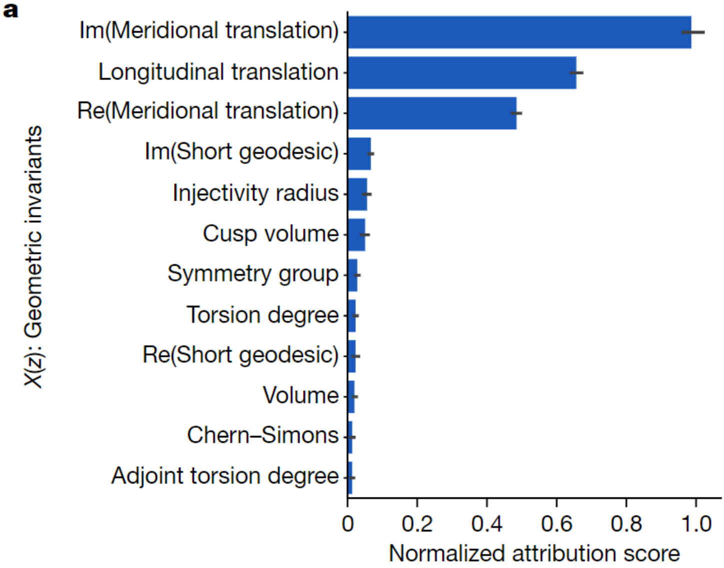
Let's wiggle the entries of $v(K)$ and do saliency analysis:

Saliency analysis on knots



We combine the first three parameters in something called the *slope*, and by plotting the signature versus the slope we come up with the following conjecture:

Conjecture

$$signature(K) \qquad \frac{1}{2} slope(K).$$

Knot theory

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$$signature(K) \quad \frac{1}{2} slope(K):$$

This turns out to be false. However, after a bit more work they proved the following two statements:

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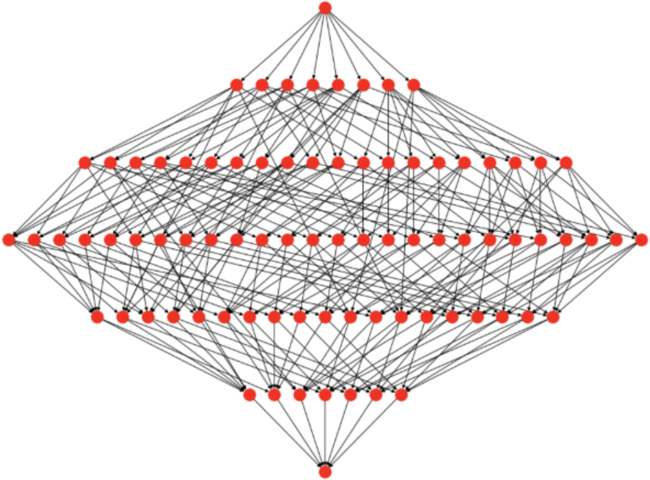
Combinatorial invariance conjecture: the KL polynomial can be compute from the Bruhat graph.

A neural network was trained on 20,000 Bruhat graphs, and achieved 98 accuracy. Reason for optimism!

Representation theory



$\leftrightarrow 1 + 3q + q^2$

Representation theory

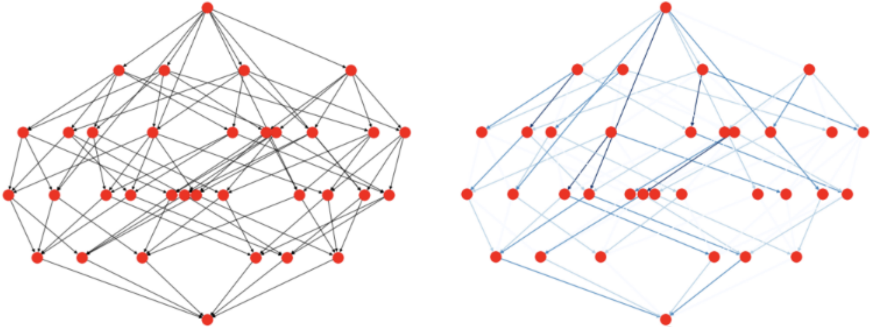
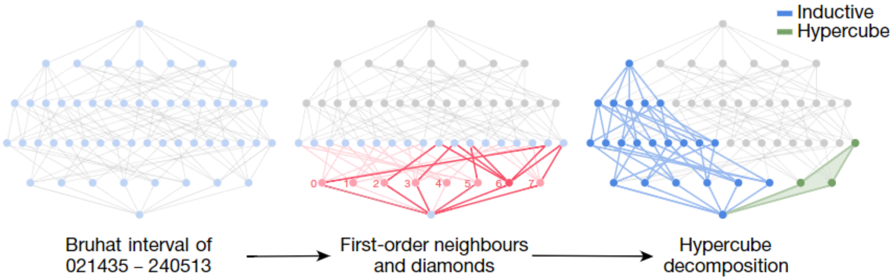


FIGURE 3. Bruhat interval pre and post saliency analysis.


Inductive
Hypercube
0
1
2
3
4
5
6
7
Bruhat interval of
021435 – 240513
First-order neighbours
and diamonds
Hypercube
decomposition