Guiding Intuition with Saliency Analysis

Adam Zsolt Wagner

Hausdorff School: "Machine Learning and Theorem Proving"

Day 3

September 20, 2023

Adam Wagner

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Main idea: use supervised learning to train a neural net on a large dataset, and find patterns in it.

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The type of question we want to answer is: if we know a bunch of things about an object (such as a graph, a matrix, a knot), but not the object itself, can we predict other parameters of this object?

Main idea: use supervised learning to train a neural net on a large dataset, and find patterns in it.

The type of question we want to answer is: if we know a bunch of things about an object (such as a graph, a matrix, a knot), but not the object itself, can we predict other parameters of this object?

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.

Typical supervised learning applications

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| Rooms | Size | Has kitchen | Brick type | Haunted | Price |
|-------|---------------------------|-------------|------------|---------|---------------|
| 5 | 130 <i>m</i> ² | Yes | Limestone | No | \$1000000 |
| 3 | 50 <i>m</i> ² | Yes | Marble | No | \$98000 |
| 2 | 25 <i>m</i> ² | No | Mud | No | \$37500 |
| 3 | 80 <i>m</i> ² | No | Limestone | Yes | ??? |

Typical ML applications: Classification problems

- Given 1000 labeled images of cats and dogs. (Training set)
- Given a new image, guess whether it's a cat or dog.



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

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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 take a picture from the input dataset, let's say the label says "cat". Then we change the weights of the neural network a teeny-tiny bit in such a way that it outputs a bigger positive value next time we plug in this picture to the network. Let's say we want to train a neural network that output a positive value on pictures of cats, and a negative value on pictures of non-cats.

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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.

Supervised learning



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

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

Open TensorFlow Playground

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Image: A matched block

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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.

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When does supervised learning work best?

• Overcoming the curse of dimensionality:

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- Traditional methods struggle as the dimensionality increases.

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- 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 in maths!

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- **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 flip changes the outcome.
- Very difficult to learn with a vanilla neural net.

• Input:
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 a permutation of $[n]$.

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- Input: $x = (x_1, x_2, \dots, x_n)$ a permutation of [n].
- We would like to predict the right and left descent sets:
 - $R(x) = \{i : x_i > x_{i+1}\}$ (Right Descent Set).
 - $L(x) = \{i : i \text{ occurs to the right of } i + 1 \text{ in } x\}$ (Left Descent Set).

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• Symmetry:

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

Data Representation Matters

• Observation:

- Input permutation as a vector $\mathbf{x} = (x_1, x_2, \dots, x_n)$ 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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|-------|--------|---------|-----------|--------|------|-------|--------|-------|------|---------|-----------|----------|-------|-------|------|-------|------|------|-------|------|-------|--------|---------|-----------|
| Epoch | 299: | Train | loss 0.01 | , Test | loss | 0.01, | 4907 0 | ıt of | 5000 | correct | (98.14%). | Epoch 64 | I: T | rain | loss | 0.00, | Test | loss | 0.01, | 4975 | out o | f 5000 | correct | (99.50%). |
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How we input data really matters!

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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?"

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- Dataset: We start with a dataset of random matrices.

• The Unexpected Issue:

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

Imagine that our previous dataset consisted of 100 \times 100 matrices, with random real entries between 0 and 1.

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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].

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What we get is an approximation of a very complicated function F by another complicated function f, given by the neural network. We also get the ability to compute f at any point we want.

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

The main idea:

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- Observe how these perturbations affect the network's output.
- Coordinates causing significant output changes are deemed important features.
- If a coordinate's perturbation has little impact, the network likely doesn't rely on it for predictions.

Advancing mathematics by guiding human intuition with AI

Alex Davies ^{C2}, Petar Veličković, <u>Lars Buesing</u>, <u>Sam Blackwell</u>, <u>Daniel Zheng</u>, <u>Nenad Tomašev</u>, <u>Richard</u> <u>Tanburn</u>, <u>Peter Battaglia</u>, <u>Charles Blundell</u>, <u>András Juhász</u>, <u>Marc Lackenby</u>, <u>Geordie Williamson</u>, <u>Demis</u> <u>Hassabis</u> & <u>Pushmeet Kohli</u> ^{C2}

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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 subfields:

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

Knot Invariants by field:

Hyperbolic Invariants:

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

Gauge Theory Invariants:

- signature
- Heegaard Floer homology
- Instanton Floer homology

• s, τ, ε, Υ

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

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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

v(K) : signature(K)

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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!

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

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Conjecture

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

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

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

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

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

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

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



Representation theory



FIGURE 3. Bruhat interval pre and post saliency analysis.

Representation theory

