Guiding Intuition with Saliency Analysis

Adam Zsolt Wagner

Hausdorff School: “Machine Learning and Theorem Proving”
Day 3

September 20, 2023
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?
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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?

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

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Generally more data $\implies$ better predictions.
Typical supervised learning applications

Predicting housing market prices

<table>
<thead>
<tr>
<th>Rooms</th>
<th>Size (m²)</th>
<th>Has Kitchen</th>
<th>Brick Type</th>
<th>Haunted</th>
<th>Price</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>130</td>
<td>Yes</td>
<td>Limestone</td>
<td>No</td>
<td>$1000000</td>
</tr>
<tr>
<td>2</td>
<td>50</td>
<td>Yes</td>
<td>Marble</td>
<td>No</td>
<td>$98000</td>
</tr>
<tr>
<td>2</td>
<td>25</td>
<td>No</td>
<td>Mud</td>
<td>No</td>
<td>$37500</td>
</tr>
<tr>
<td>3</td>
<td>80</td>
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- 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.
Supervised learning

There is a correct function, that maps grayscale pictures of cats and dogs to \{\text{cats, dogs}\}. This is a function

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F : [256]^{10000} \rightarrow \{\text{cat,dog}\}.
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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

Input 1

Hidden 1

Hidden 2

Hidden 3

Output

4.84615
10.6923
-61.05882

-3.84615
1.41176
-27.47058

1.41176
6.78946
2.05263
3.10526

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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
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Interpreting Neural Networks

- **Learning Patterns**: Neural networks excel at learning complex patterns from data.

- **Challenges for Humans**: However, understanding what these learned patterns represent can be difficult for humans.

- **Parameter Space**: The network’s parameters capture the learned patterns, but they may not be interpretable by humans.

- **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?

- **Overcoming the curse of dimensionality:**
  - Deep learning excels at handling high-dimensional data.
  - Traditional methods struggle as the dimensionality increases.

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- **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!
Input: 0-1 sequence of length 1000.
Output: $\sum x_i \mod 2$. 

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.
Simple examples in maths – the parity bit

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

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

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

Symmetry: $R(x) = L(x-1)$ (Symmetrical concepts).
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How we input data really matters!
Data Representation Matters

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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!
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Fixing the dataset

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

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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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.
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Problem: in mathematics we would often like to understand what this function is!
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- Coordinates causing significant output changes are deemed important features.
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**The main idea:**
- We wiggle the input coordinates one by one.
- 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, Petar Veličković, Lars Buesing, Sam Blackwell, Daniel Zheng, Nenad Tomašev, Richard Tanburn, Peter Battaglia, Charles Blundell, András Juhász, Marc Lackenby, Geordie Williamson, Demis Hassabis & Pushmeet Kohli

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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.

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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
- $s, \tau, \epsilon, \Upsilon$

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
\[ v(K) = (\text{volume, cusp shape, length spectrum, trace field, ...}). \]

We also calculate the signature of $K$. The training set of the neural network will consist of lots and lots of
\[ v(K) : \text{signature}(K) \]
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We created a huge dataset. For many knots $K$, we calculate the vector $\nu(K) = (\text{volume, cusp shape, length spectrum, trace field, ...})$.

We also calculate the signature of $K$. The training set of the neural network will consist of lots and lots of $\nu(K) : \text{signature}(K)$ pairs.

We train a neural network to try to predict the signature based on $\nu(K)$. If there is no connection between hyperbolic parameters in $\nu(K)$ and the signature, then the neural network will struggle. If the neural network does unreasonably well however, then there must be a connection between $\nu(K)$ and the signature that we don’t know about!
Turns out, the neural network does a really good job at predicting the signature.
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Let’s wiggle the entries of $v(K)$ and do saliency analysis:
Saliency analysis on knots

(a) Im(Meridional translation)
Im(Short geodesic)
Re(Meridional translation)
Longitudinal translation
Re(Short geodesic)
Injectivity radius
Cusp volume
Symmetry group
Torsion degree
Volume
Chern–Simons
Adjoint torsion degree

X(z): Geometric invariants
Knot theory

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**

\[
\text{signature}(K) \approx \frac{1}{2} \text{slope}(K).
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\begin{center}
\textbf{Conjecture}

\[
signature(K) \approx \frac{1}{2} \text{slope}(K).
\]
\end{center}

This turns out to be false. However, after a bit more work they proved the following two statements:
**Theorem 1:** There is a constant $c_1$ such that

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

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

**Theorem 2:** $\sigma(K)$ and

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

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

\[\square\]
To any pair of permutations we can associate two objects: the Bruhat graph, and the Kazhdan-Lusztig polynomial.
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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!
Figure 3. Bruhat interval pre and post saliency analysis.
Representation theory

Bruhat interval of 021435 – 240513

First-order neighbours and diamonds

Hypercube decomposition