Neural-Guided Learning of Integer Sequences

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November 30, 2022

Outline

This slide is just for reference. We will hide it on final presentation.

1. Introduction: Why does this problem matter? An example problem. (Jaden)
2. Previous works: See the report latex file. (Jaden)
3. Methods: show the results from each method following that method
   3.1 Experimental setup: Just explain all the code we have (Dennis)
   3.2 Human (To-Do, we'll include this if we actually do it)
   3.3 Brute force search (Dennis)
   3.4 Symbolic regression with genetic algorithm (Jaden)
   3.5 seq2seq (Jaden)
   3.6 GPT3 (Dennis)
   3.7 Our proposed method: MCTS (Tony)
4. Discussion and future directions (Tony)

0, 4, 1, 10, 2, 16, 3, 22, 4, __, __, __

What are the next few numbers?

0, 4, 1, 10, 2, 16, 3, 22, 4, __, __, __

The Collatz Map[1]

$$a_n = \begin{cases} n/2 & \text{if } n \text{ is even} \\ 3 * n + 1 & \text{if } n \text{ is odd} \end{cases}$$

Collatz Conjecture (unsolved)
Every integer eventually map to 1 through repeated application of this map.

[1] Animation from Veritasium on YouTube

Introduction

Problem setup

- $\{a_n\}_{n=1}^N$ is generated by a function $f(n) = a_n$, with $f : n, a_{n-s}, a_{n-s+1}, ..., a_{n-1} \to a_n$ and initial condition $a_1, ..., a_s \in \mathbb{Z}$
- **Goal**: given an observed sequence $\{a_n\}_{n=1}^N$, find f^* such that $f^*(n) = f(n)$ for all $1 \leq n \leq N$
- *In this project*, we restrict f to be a polynomial with integer coefficients. We also add restrictions on s and complexity of f to prevent overfitting

Introduction

Why do we want to solve integer sequences?

- Many integer sequences can have interesting structures behind them (e.g. Fibonacci sequence).
- Plus, quantitative trading firms like to ask about them on interviews...

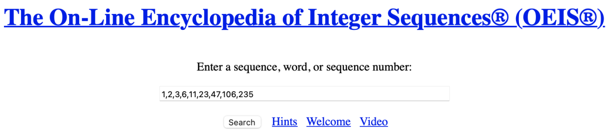
Difficulties

- The functional relation that generates the sequence is often hard to infer directly.
- Integer constraint is not guaranteed by standard seq2seq models.

Introduction

Neil Sloane and OEIS

Neil Sloane (1939 -)



How About Brute Force Search?

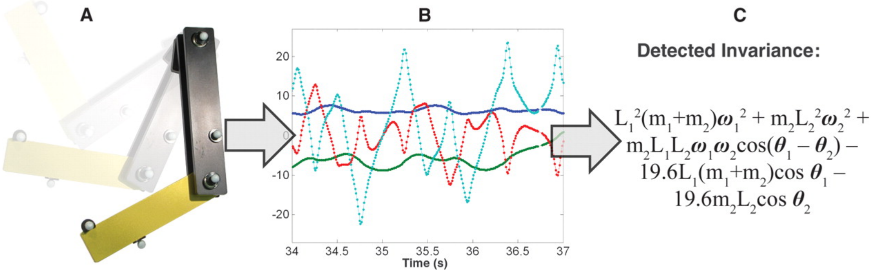
Given lists of allowed terms $\boldsymbol{t}$ ($|\boldsymbol{t}| = n$) and coefficients $\boldsymbol{c}$ ($|\boldsymbol{c}| = m$), some $1 < k \leq n$, and a target sequence $\boldsymbol{s}$ ($|\boldsymbol{s}| = h$),

1. Generate all possible k-combinations of the terms, $O({}_nC_k)$
2. For each combination, generate all possible functions by applying different coefficient permutations, $O(m^k)$
3. For each function, compute the respective sequence and compare with target, $O(h)$

In the worst case, the runtime is $O\left({}_nC_k \cdot m^k \cdot h\right) \approx O\left(\left(\frac{m \cdot n}{k}\right)^k \cdot h\right)$, which grows exponentially fast as we increase n and quickly becomes infeasible.

Previous Work

- **Schmidt and Lipson (2009)**: Symbolic regression with genetic algorithm to distil equations from experimental data



  - Led to the proprietary software Eureqa and startup Nutonian.

Symbolic Regression with Evolutionary Algorithm

- Algorithm used in Schmidt and Lipson (2009), reimplemented in package PySR (Cranmer, 2020)
- **Genetic algorithm**: Define a "fitness" for each function. "Mate" individuals with high fitness to produce better individuals. **Effectively searches non-convex space.**
- However, PySR does not support self-referencing terms[2] like $f(n) = 2f(n-1)$.

[2] Theoretically, we can implement it, but do we want to?

Experiment Setup: Dataset Generation

- **Terms**: constant, index-based (n, n^2, n^3), self-referencing ($f[n-i]^j$, $1 \leq i \leq 3$, $1 \leq j \leq 2$)
- **Functions**: $f = \sum_{i=1}^{k} c_i \cdot \text{term}_i$, where $\{\text{term}_i\}_{i=1}^{k}$ is a random k-combination of the terms (represented as a boolean mask) and c_i is chosen randomly in $(-5, 5)$
- **Sequences**: generated based on f, with initial terms chosen from $(1, 3)$ as needed
- Given an absolute value bound b on the sequence and k, the dataset consists of tuples $(sequence, boolean\_mask)$ where $\max(|sequence|) < b$ and exactly k values in *boolean_mask* are True
- With $b = 1000$, we generated 1000 tuples for each of $k = 2, 3$ and randomly split them into size 800 and 200 sets for training and test

Experiment Setup: Evaluation

Note that we cannot simply check for equality of the boolean masks

- Consider the sequence 1,3,6,10,15,21 where both $f(n) = n + f(n-1)$ and $f(n) = n^2 - f(n-1)$ are valid

Hence, we primarily evaluate the models based on two metrics:

1. **Average RMSE** (based on element-wise loss)
   - Given the predicted boolean mask, grid search over all valid term coefficients and generate the corresponding sequences
   - Compute the minimum RMSE achieved between the target sequence and all generated sequences, and average over all test sequences
   - Recall for sequences $\{a_i\}_{i=1}^n$, $\{b_i\}_{i=1}^n$, RMSE $:= \sqrt{\frac{1}{n}\sum_{i=1}^n (a_i - b_i)^2}$
2. **% Correct**
   - Percentage of predictions for which the best sequence generated from grid search matches the target perfectly (RMSE $= 0$)

Simple seq2seq

- Takes sequence of integers, outputs boolean mask of terms
- A simple encoder-decoder network with attention[3]
- Training: 20 epochs, 1000 functions, evaluated every 500 steps. 200 functions not in the training set evaluated randomly at each time
- **Results:**
  - Taking the **best** result from each trial across evaluations

% terms	% correct
3	17%

  - Just taking the **last** results:

Trial number	% correct
3	9%

[3] Taken from a tutorial on PyTorch

GPT3

Training

- Further split the 800 training sequences into 640 for training and 160 for validation
- Fine-tuned four base models, listed in increasing number of parameters: `ada`, `babbage`, `curie`, `davinci`
- Default hyperparameters: n_epochs=4, batch_size=1, learning_rate_multiplier=0.05

Results

- % correctly solved test sequences

# terms in f	ada	babbage	curie	davinci
2	18.0%	22.5%	25.5%	30.5%
3	9.0%	11.5%	11.0%	9.0%

- Mean RMSE on test sequences

# terms in f	ada	babbage	curie	davinci
2	40.1	25.0	28.1	23.5
3	334.7	215.0	119.6	284.0

Neural Network with MCTS

MCTS Recap

- Selection: starting at current node, pick the most promising leaf node L (a node that has unexplored child) based on a "tree policy"
- Expansion: if L doesn't end the game, append a child node C of L to the tree
- Simulation (rollout): play the game randomly starting from C, until game ends
- Backpropagation: Update score of nodes from u to C based on simulation outcome
- Repeat these steps for many times, and choose the best move. Go to the best move node and repeat.

Neural Network with MCTS

Methodology (inspired by AlphaGo)

- Search tree
  - Each node is a list of terms in a function expression (coefficients excluded). Root is $f(n) = 0$
  - Child nodes can be obtained by appending a new term.
  - Each node has a reward and a policy.
  - Evaluate reward at terminal nodes: when the number of terms in node reaches a depth limit, or when MCTS chooses to append an <EOS> token.
  - Reward: $10 - depth$ if $\exists$ a solution using exactly the node's terms, otherwise $-RMSE$
- Neural network: (sequence, current node's terms) $\rightarrow$ (reward, policy).
- Idea: Neural network guides MCTS, generating reward and policy estimates; then, neural network is trained to learn the updated reward and policy (critic); repeat.

Neural Network with MCTS

Training

- Training schedule: for each training sequence, run 3 MCTS iterations. Reinitialize an empty search tree at the start of every iteration.
- At the end of every iteration, neural network is trained on training examples collected from the node reward and policy in the search tree.
- Loss function at node u is
  $L(u) = [reward_{NN}(u) - reward_{MCTS}(u)]^2 + \sum_{a \in A} -policy_{MCTS}(u)_a \log \left[policy_{NN}(u)_a\right]$
- Neural network architecture: GRU or MLP backbone, with two projection heads (for reward and policy).

Neural Network with MCTS

Results

- % correctly solved test sequences

# terms in f	GRU	MLP
2	5.5%	13.0%
3	0.0%	0.5%
3 (with hint)	4.5%	3.5%

- Mean RMSE on test sequence

# terms in f	GRU	MLP
2	25.0	33.4
3	107.8	48.6
3 (with hint)	96.0	72.6

Comments

Concerns/Difficulties

- For PySR, maybe just experiments on functions without self-referencing terms?
- MCTS-driven training is slower than other methods

Plans Going Forward

- Finish symbolic regression experiments
- Use more sophisticated neural network architecture for MCTS and tune hyperparameters to improve performance
- Test the generalization ability of our models (test sequence expression has more terms than training sequence)
- Add human baseline
- Use more terms (e.g. interaction term)

Thank you!