Spectral Clustering for Axiom Selection

Zishi Wu

Department of Computer Science
University of Miami

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Introduction

Definitions

- What is Automated Theorem Proving (ATP)?
- Show that the *conjecture* is a *logical consequence* of the axioms.
- Axioms are also known as *premises*.
- Together, the conjecture and the axioms of a logic problem are called the *formulae*.
- Applications:
  - Formal verification of software - Compilers (e.g. gcc, llvm)
  - Formal verification of hardware - CPU (e.g. 1994 Intel Pentium floating-point division bug)
  - Interactive proof assistants for mathematics (e.g. Isabelle, Mizar)

Introduction

Example

- Axiom 1: *All men are mortal*.
- Axiom 2: *Socrates is a man*.
- Conjecture: *Socrates is mortal*.

Logical Consequence

Logical Consequence

- Every model of the axioms is a model of the conjecture.
- A set of axioms has a *model* if there is an *interpretation* (assignment of boolean values) to the axioms such that the conjunction of the axioms evaluate to *True*.
- If we list all interpretations of N formulae on a truth table, we get 2^N rows. This search space grows exponentially.
- The faster way is to show that the union of the axioms and the negation of the conjecture is *unsatisfiable*. $Ax \cup \neg C = \emptyset$
- In other words, if no model of the axioms is a model of the negated conjecture, then all models of the axioms are models of the conjecture.

Problem Statement

Problem Statement

- A *large-theory* problem consists of a conjecture to be proven, and a large number of axioms to be considered.
- However, the solution set(s) usually consist of a few axioms.
- How do we select the necessary axioms? This is known as the problem of *premise selection*.

Benchmark Data

MPTP2078 Dataset

- Thousands of Problems for Theorem Provers (TPTP) [Sut17]
  - Standard set of test problems.
- Benchmark dataset of 2078 problems known as the Mizar Problems for Theorem Provers (MPTP2078) [AHK+14].
  - Encodes problems from the Mizar Mathematical Library (MML) of formalized mathematics into first-order logic form.
- There are two versions of each problem:
  - Bushy = smaller version (3 to 40 axioms, 1 to 15 needed)
  - Chainy = larger version (10 to 500 axioms, 2 to 119 needed)
- Premise selection performance compared to state-of-the-art Automated Theorem Provers:
  - E [Sch13]
  - Vampire [KV13]

Ranking Problem

Ranking Problem

- Formulate premise selection as a *ranking problem* [PB10, AHK+14]:
  - Rank the axioms by how likely they are to prove a conjecture, based on some kind of user-defined similarity metric.
  - Choose a threshold value.
  - Select all axioms whose score is above that threshold.
- Also a *classification problem*:
  - Given a feature matrix consisting of the similarity values between formulae in a problem, train different machine learning methods on the data to classify if an axiom is *likely* or *unlikely* to be in the proof.

Related Work

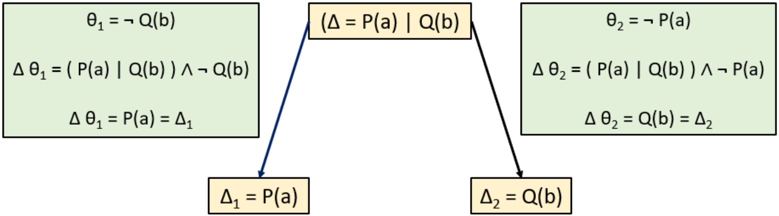
Extended Hutchinson Distance

- To construct an adjacency matrix, we require a measure of similarity or dissimilarity between each pair of nodes in a graph.
- Liu [LXH17] proposed a dissimilarity metric between two terms Δ_1 and Δ_2, that extends the Hutchinson distance [Hut97].
- Calculated by finding the Least Generalized Generalization (*lgg*) between two formulae. A term Δ is the *lgg* of Δ_1 and Δ_2 iff
  - There are substitutions θ_1 and θ_2 such that $\Delta\theta_1 = \Delta_1$ and $\Delta\theta_2 = \Delta_2$.
  - There exists no term Δ' and substitutions σ, σ_1 and σ_2 such that $\Delta\sigma_1 = \Delta'$ and $\Delta\sigma_2 = \Delta'$.

Related Work

Least Generalized Generalization Example

- Note that the substitutions θ_1 and θ_2 are not limited to a single substitution rule. They can also consist of multiple substitution rules occurring one after the other.



- P(a) could represent a predicate: **is_man(Socrates)**
- Q(b) could represent a predicate: **is_mortal (Man)**
- Here Δ is the least generalized generalization of Δ_1 and Δ_2

Related Work

Extended Hutchinson Distance

- If there is no Least Generalized Generalization Δ between two terms Δ_1 and Δ_2, then their extended Hutchinson distance is ∞. Formally, $\mathit{dissimilarity}(\Delta_1, \Delta_1) = \infty$ iff $\mathit{lgg}(\Delta_1, \Delta_2) = \emptyset$.
- If there exists a Least Generalized Generalization Δ between two terms Δ_1 and Δ_2, then the Extended Hutchinson Distance says:
  - More total substitutions required (from the *lgg* to both terms) equates to a higher dissimilarity score.
  - Fewer total substitutions required equates to a lower dissimilarity score.
- Note: this is an over-simplication of the actual metric.
- As expected, for any term Δ_1, $\mathit{dissimilarity}(\Delta_1, \Delta_1) = 0$

Graph Matrices

Graph Laplacian Matrix

- Von Luxburg [vL07] describes this technique to cluster vertices in an undirected graph according to some user-defined similarity metric.
- Adjacency matrix A consists of edge weights between pairs of vertices that represent their similarity.
- Degree matrix D is a diagonal matrix where the i^{th} element is the sum of the elements of the i^{th} column of A.
- Un-normalized Graph Laplacian matrix.
  - $L = D - A$
- Normalized Graph Laplacian matrix contains *features* of the graph
  - $L_{norm} = I - (D^{-1/2}\ L\ D^{-1/2})$

Example Graph

Calculate Normalized Laplacian Matrix

- Adjacency, Degree, and Un-normalized Graph Laplacian

$$A = \begin{bmatrix} 0 & 3 & 0 \\ 3 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \quad D = \begin{bmatrix} 3 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad L = \begin{bmatrix} 0 & 3 & 0 \\ 3 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

- Normalized Graph Laplacian

$$L_{norm} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 3 & 0 \\ 3 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Evaluation Metrics

Definitions

- The *N*umber of *A*xioms in a *P*roblem: *NAxP*.
- The *N*umber of axioms *Sel*ected: *NSel*.
- The *N*umber of axioms *N*eeded *f*or a *P*roof, i.e., the number of axioms in an adequate set *NNfP*.

Evaluation Metrics

Precision and Selectivity Metrics

- **Precision**
  If the axiom selection technique selects an adequate set of axioms (i.e. set that is known to lead to a proof), then **precision** is the minimum *NNfP*/*NSel* over the known adequate sets of axioms. Otherwise, if it selects an inadequate set, then **precision** is 0. Larger values are better because it means that fewer unnecessary axioms were selected.
- **Selectivity**: *NSel* / *NAxP*
  The fraction of axioms selected from the problem, regardless of whether an adequate set was selected or not. Smaller values are better.

Evaluation Metrics

Average and Adequacy Metrics

- **Average precision/selectivity/precision**
  For a set of problems, the average value of the metric over the problems.
- **Adequacy**
  For a set of problems, the fraction of problems for which the axiom selection technique selects an adequate set of axioms. Larger values are better.
- **Adequate precision/selectivity/precision**
  For a set of problems, the average over the problems for which the axiom selection technique selects an adequate set of axioms.

Methodology

Graph Representation

- Use Extended Hutchinson distance to get dissimilarity values of all pairs of vertices in a problem.
- Let Φ_1 and Φ_1 represent two formulae with dissimilarity of $dsim(\phi_i, \phi_j)$. We convert dissimilarity values into similarity values using the following formula:

$$maxdsim(\mathcal{F}) = max_{\phi_i, \phi_j \in \mathcal{F}}(dsim(\phi_i, \phi_j) \neq \infty) \tag{1}$$

$$sim(\Phi_1, \Phi_2, \mathcal{F}) = \max(0, maxdsim(\mathcal{F}) - dsim(\Phi_1, \Phi_2)) \tag{2}$$

- The logic problem becomes a fully-connected and undirected graph
  - Vertices $V = \{\text{Axioms} \cup \text{Conjecture}\}$
  - Edges E = weighted by similarity between vertices

Spectral Clustering Algorithm

Spectral Clustering [vL07]

1. Construct a weight matrix W (i.e. adjacency matrix A) containing similarity values of the edges of the graph.
2. Compute the normalized Laplacian matrix L_{norm} from W.
3. Compute the first k eigenvectors $v_1, \ldots, v_k$ of L_{norm} and construct a feature matrix U from those eigenvectors.
4. For $i = 1, \ldots, n$, let p_i be the feature vector for the i^{th} vertex, corresponding to the i^{th} row of U.
5. Cluster the vertices based on their feature vectors into k clusters: $C_1, C_2, \ldots, C_k$. Denote the cluster containing the conjecture as C_C.

K-Means Clustering

Problems with K-Means Clustering

5. Cluster the vertices based on their feature vectors into k clusters: $C_1, C_2, \dots, C_k$.
   - Each run of k-means chooses a different set of initial centroids for the k clusters.
   - Results in different clusterings each run.

- First, we need a deterministic way of initializing the centroids of the k clusters.
- Second, we need to figure out the optimal value for the parameter k, the number of clusters.

K-Means Clustering

Solution to Initial Centroids Problem

- The *degree centrality* of a vertex v is the sum of the weights of all the edges connected to v.
- Rank the vertices in descending order by their degree centrality.
- Select the top $(k-1)$ most central vertices and the conjecture. Use their feature vectors from the matrix U as the initial centroids for the k clusters.

K-Means Clustering

Solution to Number of Clusters Problem

- Let *NAxP* denote the number of axioms in a logic problem.
- Brute force: try all values of k from 2 to *NAxP*.
- For each problem, record the k number of clusters that gives us the best precision score.

Prediction of Optimal Number of Clusters

Median Regression

- Method description here.

Results

Predicted Number of Clusters

- Result description here.

Results

Evaluation on Bushy and Chainy Problems

- Result description here.

Conclusion

Conclusion

- Ranking and clustering methods for premise selection depend on how well the ranking metric (whether based on dissimilarity or similarity) manages to capture the relationship between the logical formulae.
- If the ranking metric is not good, then it affects everything downstream. Therefore, the next step is to validate different ranking metrics, including the Extended Hutchinson Distance.
- Recent work is being done with graph convolutional neural networks to rank the likelihood of axioms contributing towards a proof. However, these models also depend on a good ranking metric.

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