Spectral Clustering for Axiom Selection

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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

- 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

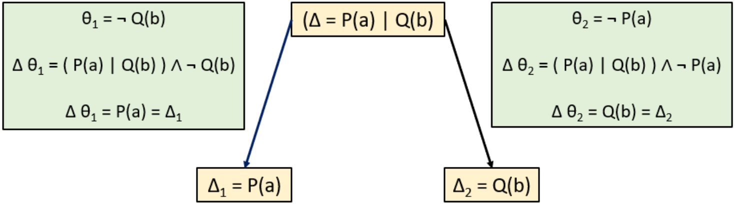
Extended Hutchinson Distance

- 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.



$(\Delta = P(a) \mid Q(b)$

$\theta_1 = \neg Q(b)$

$\Delta\,\theta_1 = (\,P(a) \mid Q(b)\,) \wedge \neg Q(b)$

$\Delta\,\theta_1 = P(a) = \Delta_1$

$\theta_2 = \neg P(a)$

$\Delta\,\theta_2 = (\,P(a) \mid Q(b)\,) \wedge \neg P(a)$

$\Delta\,\theta_2 = Q(b) = \Delta_2$

$\Delta_1 = P(a)$

$\Delta_2 = Q(b)$

- 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, *dissimilarity(*Δ_1, Δ_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 *Ax*ioms 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:

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

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

- 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 $v_1, ..., v_k$ of L_{norm} and construct a feature matrix U from those eigenvectors.
4. For $i = 1, ..., n$, 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: $C_1, C_2, ..., C_k$. Denote the cluster containing the conjecture as C_C.

K-Means Clustering

Problems with K-Means Clustering

- First, each run of k-means chooses a different set of initial centroids for the k clusters. This results in a different clustering each time.
- We need 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 Optimal 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** value. Call this the optimal k.
- Recall that **precision** is *the minimum number of axioms needed for a proof* divided by *the number of axioms selected by the axiom selection technique*.

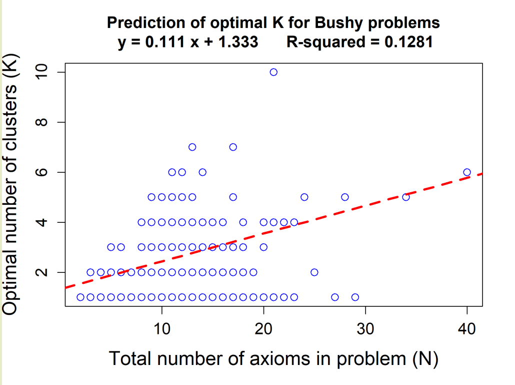
Predict Optimal Number of Clusters

Median Regression

- Use median regression to create a regression line where the y-axis is the optimal k and the x-axis is the number of axioms in the problem.
- For each problem, use the regression line to predict the optimal k based on the number of axioms in the problem. Denote the predicted value as k_{pred}.
- For each problem, run spectral clustering using k_{pred} and record the precision, selectivity, and adequacy.

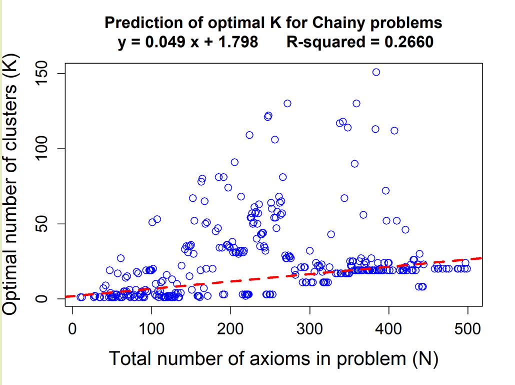
Results

Predicted Number of Clusters for Bushy



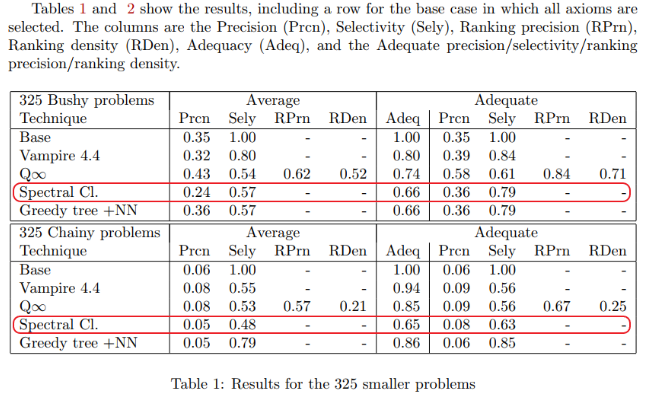
Results

Predicted Number of Clusters for Chainy



Results

Evaluation on 325 Bushy and Chainy Problems



Tables 1 and 2 show the results, including a row for the base case in which all axioms are selected. The columns are the Precision (Prcn), Selectivity (Sely), Ranking precision (RPrn), Ranking density (RDen), Adequacy (Adeq), and the Adequate precision/selectivity/ranking precision/ranking density.

325 Bushy problems	Average				Adequate				
Technique	Prcn	Sely	RPrn	RDen	Adeq	Prcn	Sely	RPrn	RDen
Base	0.35	1.00	-	-	1.00	0.35	1.00	-	-
Vampire 4.4	0.32	0.80	-	-	0.80	0.39	0.84	-	-
Q∞	0.43	0.54	0.62	0.52	0.74	0.58	0.61	0.84	0.71
Spectral Cl.	0.24	0.57	-	-	0.66	0.36	0.79	-	-
Greedy tree +NN	0.36	0.57	-	-	0.66	0.36	0.79	-	-

325 Chainy problems	Average				Adequate				
Technique	Prcn	Sely	RPrn	RDen	Adeq	Prcn	Sely	RPrn	RDen
Base	0.06	1.00	-	-	1.00	0.06	1.00	-	-
Vampire 4.4	0.08	0.55	-	-	0.94	0.09	0.56	-	-
Q∞	0.08	0.53	0.57	0.21	0.85	0.09	0.56	0.67	0.25
Spectral Cl.	0.05	0.48	-	-	0.65	0.08	0.63	-	-
Greedy tree +NN	0.05	0.79	-	-	0.86	0.06	0.85	-	-

Table 1: Results for the 325 smaller problems

Results

Evaluation on 325 Bushy and Chainy Problems

- Spectral Clustering is more selective than E and Vampire. However, this lead it to perform the worst in terms of selecting an adequate set of axioms, for both Bushy and Chainy problems.
- Spectral Clustering performs equally as well as E and Vampire in terms of precision for the problems on which it selects an adequate set of axioms, for both Bushy and Chainy problems. This means when Spectral Clustering does select an adequate set, it is good at removing unnecessary axioms.
- Q_∞ is Qinghua's method of removing all axioms with infinite dissimilarity to the conjecture. It's a simple method that performs very well, beating Vampire in terms of selectivity and on par with Vampire in terms of precision.

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.
- Sometimes the simple method (e.g. Q_∞) performs better than the complex method (e.g. Spectral Clustering).

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