BDD/ZDDを基盤とする種々の離散構造の演算処理と代数系について

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BDD/ZDD を基盤とする種々の離散構造の演算処理と代数系 (algebra) について

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2010/10/22

概要
本 ERATO プロジェクトでは、離散構造を統合的に扱う基本処理系としてBDD/ZDD を位置づけ、分野横断的な応用を持つ技術体系として再構築することを目指して研究活動を開始している。本講演では、BDD/ZDD を基盤とする離散構造とその演算処理の代数系 (algebra) の例として、BDD による論理関数処理系、ZDD による組合せ集合の処理系、ZDD ベクトル表現による組合せ頻度表の演算処理系、および Sequence BDD による系列集合の演算処理系を取り上げ、それらの代数系を比較するとともに、今後の展望について述べる。
Recent Topics on Decision Diagrams and Discrete Structure Manipulation

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Hokkaido University, Japan.

Background

- BDD-based algorithms have been developed mainly in VLSI logic design area. (since early 1990's.)
  - Equivalence checking for combinational circuits.
  - Symbolic model checking for logic / behavioral designs.
  - Logic synthesis / optimization.
  - Test pattern generation.
- Recently, BDDs are applied for not only VLSI design but also for more general purposes.
  - Data mining (Fast frequent itemset mining) [Minato2005,2008][Loekito,Bailey2006]
  - Computation of Bayesian networks for probabilistic system analysis.[Minato2007]

Contents of this talk

- BDD and ZDD for discrete structure manipulation
  - BDD and Boolean function algebra
  - ZDD and “Family algebra”
- Database analysis based on ZDD manipulation
  - Frequent itemset mining
  - ZDD vector and “Itemset-histogram algebra”
- Sequence BDD for set of sequences
  - Set of sequences and ZDD
  - Sequence BDD and “sequence family algebra”
- Our project for discrete structure manipulation system
  - JST “ERATO” project and current status

BDD (Binary Decision Diagram) [Bryant86]

- Graphical representation of Boolean function data.
  - Canonical form obtained by applying reduction rules to a binary tree with a fixed variable ordering.

BDD reduction rules

- Eliminate all redundant nodes.
- Share all equivalent nodes.

Gives a unique and compressed representation for a given Boolean function under a fixed variable ordering.
Effect of BDD reduction rules

- Exponential advantage can be seen in extreme cases.
- Depends on instances, but effective for many practical ones.

BDD-based logic operation algorithm

- If we generate BDDs from the binary tree: always requires exponential time & space. (→ impracticable for large number of variables)
- Innovative BDD synthesis algorithm
  - Proposed by R. Bryant in 1986.
  - Best cited paper for many years in EE&CS areas.

Boolean function and combinatorial itemsets

<table>
<thead>
<tr>
<th>a</th>
<th>b</th>
<th>c</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
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<td>1</td>
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<td>1</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

Boolean function: \( F = (a \land \lnot c) \lor (\lnot b \land c) \)

Combinatorial itemset: \( F = \{ab, ac, c\} \)

- Operations of combinatorial itemsets can be done by BDD-based logic operations.
  - Union of sets \( \to \) logical OR
  - Intersection of sets \( \to \) logical AND
  - Complement set \( \to \) logical NOT

Zero-suppressed BDD (ZDD) [Minato93]

- A variant of BDDs for combinatorial itemsets.
- Uses a new reduction rule different from ordinary BDDs.
  - Eliminate all nodes whose “1-edge” directly points to 0-terminal.
  - Share equivalent nodes as well as ordinary BDDs.
- If an item \( x \) does not appear in any itemset, the ZDD node of \( x \) is automatically eliminated.
  - When average appearance ratio of each item is 1%, ZDDs are more compact than ordinary BDDs, up to 100 times.

Algebraic operations for ZDDs

- Knuth evaluated not only the data structure of ZDDs, but more interested in the algebra on ZDDs.
- Formerly I called this “unate cube set algebra,” but Knuth reorganized as “Family algebra.”

\[\Phi, \{1\}, \text{Empty and singleton set}, (0/1-terminal)\]
\[P:\text{top}, \text{Returns the item-ID at the top node of } P.\]
\[P:\text{onset}(v), \text{Selects the subset of itemsets including or excluding } v.\]
\[P:\text{offset}(v), \text{Selects the subset of itemsets excluding or including } v.\]
\[P:\text{change}(v), \text{Switching } (\text{add }/\text{delete}) \text{ on each itemset.}\]
\[U, \cap, \cup, \wedge, \vee \text{ Returns union, intersection, and difference set.}\]
\[P:\text{count}, \text{Counts number of combinations in } P.\]
\[P \times Q, \text{Cartesian product set of } P \text{ and } Q.\]
\[P : Q, \text{Quotient set of } P \text{ divided by } Q.\]
\[P % Q, \text{Reminder set of } P \text{ divided by } Q.\]
Principles for performance improvement

- General principles: Data compression & Pruning search space.
- Two basic techniques for data compression:
  - Dictionary-based coding (= BDD/ZDD sub-graph sharing)
  - Run-length coding (= BDD/ZDD redundant node deletion)

General principles:

- Computability without decompression.

Two basic techniques for data compression:

- Dictionary-based coding (= BDD/ZDD sub-graph sharing)
- Run-length coding (= BDD/ZDD redundant node deletion)

Comparison of BDDs and ZDDs

- Many of real-life problems are likely asymmetric.
- VLSI Logic Design
- Formal Verification
- etc.

- Data mining & Knowledge discovery
- Market data analysis
- Web data analysis
- Formal concept analysis
- Risk analysis
- Calculation with Bayesian networks
- Machine learning & clustering
- etc.

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Existing itemset mining algorithms

- Frequent itemset mining is one of the fundamental data mining problems.
- Previous work:
  - Apriori [Agrawal1993]
    First efficient method of enumerating all frequent patterns. Broad-first search with dynamic programming.
  - Eclat [Zaki1997]
    Depth-first search algorithm. Less memory consuming. In some cases, faster than Apriori.
  - FP-growth [Han2000]
    Depth-first search using “FP-tree,” graph-based data structure.
  - LCM (Linear time Closed itemset Miner) [Uno2003]
    - with a theoretical bound as output linear time.
    - known as one of the fastest implementation.

Frequent itemset mining

- Basic and well-known problem in database analysis.

<table>
<thead>
<tr>
<th>Record ID</th>
<th>Tuple</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>a b c</td>
</tr>
<tr>
<td>2</td>
<td>a b</td>
</tr>
<tr>
<td>3</td>
<td>a b c</td>
</tr>
<tr>
<td>4</td>
<td>b c</td>
</tr>
<tr>
<td>5</td>
<td>a b</td>
</tr>
<tr>
<td>6</td>
<td>a b c</td>
</tr>
<tr>
<td>7</td>
<td>c</td>
</tr>
<tr>
<td>8</td>
<td>a b c</td>
</tr>
<tr>
<td>9</td>
<td>a b c</td>
</tr>
<tr>
<td>10</td>
<td>a b</td>
</tr>
<tr>
<td>11</td>
<td>b c</td>
</tr>
</tbody>
</table>

Frequency threshold = 10 \{ b \}
Frequency threshold = 8 \{ ab, a, b, c \}
Frequency threshold = 7 \{ ab, bc, a, b, c \}
Frequency threshold = 5 \{ abc, ab, bc, ac, a, b, c \}
Frequency threshold = 1 \{ abc, ab, bc, ac, a, b, c \}

“LCM over ZDDs” [Minato et al. 2008]

- LCM: [Uno2003]
  Output-linear time algorithm of frequent itemset mining.
- ZDD: [Minato93]
  A compact graph-based representation for large-scale sets of combinations.

Combination of the two techniques

Generates large-scale frequent itemsets on the main memory, with a very small overhead from the original LCM.

(⇒ Sub-linear time and space to the number of solutions when ZDD compression works well.)
LCM over ZDDs: An example

The results of frequent itemsets are obtained as ZDDs on the main memory. (not generating a file.)

Freq. thres. \( \alpha = 7 \)

\( \{ab, bc, a, b, c\} \)

---

**Performance of LCM over ZDDs**

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Original LCM</th>
<th>LCM over ZDDs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Data</td>
<td># solutions</td>
<td>LCM over ZDDs</td>
</tr>
<tr>
<td>min. support</td>
<td>LCM over ZDDs</td>
<td>Time(s)</td>
</tr>
<tr>
<td></td>
<td>Time(s)</td>
<td>Time(s)</td>
</tr>
<tr>
<td>mushroom</td>
<td>100</td>
<td>560</td>
</tr>
<tr>
<td>T10ED</td>
<td>90</td>
<td>600</td>
</tr>
<tr>
<td>T10ED</td>
<td>100</td>
<td>700</td>
</tr>
<tr>
<td>BMS-WebView</td>
<td>5</td>
<td>200</td>
</tr>
<tr>
<td>connect</td>
<td>505</td>
<td>2000</td>
</tr>
<tr>
<td>BMS-WebView</td>
<td>50</td>
<td>2000</td>
</tr>
<tr>
<td>measured by a Linux PC, Core2Duo E6600, 2.4GHz, 2GB memory.</td>
<td>measured by a Linux PC, Core2Duo E6600, 2.4GHz, 2GB memory.</td>
<td></td>
</tr>
</tbody>
</table>

---

**Post Processing after LCM over ZDDs**

We can extract distinctive itemsets by comparing frequent itemsets for multiple sets of databases. Various ZDD algebraic operations can be used for the comparison of the huge number of frequent itemsets.

---

**Itemset-histograms for DB analysis**

We sometimes need to represent not only yes/no but also the frequency (number of occurrence) for each itemset.

This is a histogram of itemsets if frequency of all itemsets are generated.

Integer-valued Sum-Of-Product form. (VSOP)

Function from Combination to Integer. (CtoI)

Multi-set of combinations

---

**ZDD Vectors and Multi-Terminal BDD**

The two representation can be considered. Just a variable ordering problem of a same BDD.

---
### ZDD vector for itemset-histogram
- A ZDD distinguishes only existence of each tuple in the transaction data. (cannot count frequency.)
- We use a binary encoded method with ZDD vectors:
  - Encode frequency numbers into \( m \)-bit binary code, and represent each bit of combination set using a ZDD.

\[
\begin{align*}
\text{itemset} & \quad \text{frequency} & \quad F_0 & \quad F_1 & \quad F_2 \\
abc & 5 (101) & 1 & 0 & 1 \\
ab & 3 (011) & 0 & 1 & 1 \\
bc & 2 (010) & 0 & 1 & 0 \\
c & 1 (001) & 0 & 0 & 1 \\
\end{align*}
\]
\[
F_0 = (abc, ab, c), \quad F_1 = (ab, bc), \quad F_2 = (abc)
\]

### Algebra for itemset-histograms
- Primitive operations:
  - Factoring into two parts by an item.
  - Attaching an item.
  - Sum of two histograms.
  - Counting lines in the table.

\[
\begin{align*}
H_1 \times d & \quad \text{Tuple} & \quad \text{Freq.} \\
abc & 5 & \quad a & 1 & b & 3 & c & 2 \\
ab & 3 & \quad a & 1 & b & 1 & c & 2 \\
bc & 2 & \quad a & 1 & b & 1 & c & 1 \\
c & 1 & \quad a & 1 & b & 1 & c & 1 \\
\end{align*}
\]

- Each table is compactly represented by ZDDs.
- ZDDs are shared each other in the memory.

### Sets of sequences (sets of strings)
- Sets of combinations:
  - Don’t consider order and duplication of items
    - “abcc” and “bca” are the same.
- Sets of sequences:
  - Distinguishes all finite sequences.
    - \( \{ \lambda \}, \{ \text{ab, aba, bbc} \}, \{ \text{a, aa, aaa, aaaa} \} \), etc.
  - Here we exclude infinite sequences such as \( \{ \text{a}^* \} \).
- So many real-life applications.
  - Text search and indexing
  - Web (html/xml) data mining
  - Bio informatics

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Encoded ZDDs for Sets of sequences

- Pair of (Item - position) is considered different symbol.
  - “aaa” → “a1 a2 a3”
  - “aba” → “a1 b2 a3”
- Alphabet size: |Σ|
- Maximum length of sequences: n
- Total encoded symbols: |Σ| × n
- Not very efficient.
  - Many symbols needed.
  - We need to put a fixed maximum length of sequences.

Sequence BDD (SeqBDD)

- Loekito, Bailey, and Pei (2009)
  - Same as ZDD reduction rule.
  - Only 0-edges keep variable ordering.
  - 1-edges have no restriction.
  - Still unique representation for a given set of sequences.
  - Each path from root to 1-terminal corresponds to a sequence.

Basic operations of sequence family algebra

<table>
<thead>
<tr>
<th>Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>P</td>
<td>Returns empty set. (0-terminal node)</td>
</tr>
<tr>
<td>P^0</td>
<td>Returns the set of only null combination. (1-terminal node)</td>
</tr>
<tr>
<td>P(x)</td>
<td>Returns item x at root node of P</td>
</tr>
<tr>
<td>P^onset(x)</td>
<td>Selects the subset of sequences that begin with letter x, and then removes x from the head of each sequence.</td>
</tr>
<tr>
<td>P^offset(x)</td>
<td>Selects the subset of sequences that do not begin with letter x.</td>
</tr>
<tr>
<td>P^push(x)</td>
<td>Appends x to the head of every sequence in P.</td>
</tr>
<tr>
<td>P^UQ</td>
<td>Returns union set.</td>
</tr>
<tr>
<td>P^C</td>
<td>Returns intersection set.</td>
</tr>
<tr>
<td>P^D</td>
<td>Returns difference set. (in P but not in Q.)</td>
</tr>
<tr>
<td>P^count</td>
<td>Counts number of combinations.</td>
</tr>
<tr>
<td>P^xQ</td>
<td>Cartesian product of P and Q. (Concatenations of all pairs in P and in Q)</td>
</tr>
</tbody>
</table>

- ZDD-like algebraic operations.
  - onset, offset, and push operations are different.
  - Other operations are almost same.

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ERATO Projects

- Top projects for scientific research in Japan.
  - Executed by JST (Japan Science and Technology Agency).
  - 5 projects / Year are accepted from all scientific subjects. (Computer Science: 0 or 1 project / Year.)
  - 100 projects have been accepted in 30 years.
  - Each project has 5 years long, total 1 billion Yen. about 10 PD researchers and 3 admin staffs.

- This project is accepted on Oct. 2009.
  - Research activities started from April 2010, until March 2015.
Our main subject: Many problems solved by computers can be decomposed as a type of discrete structures using simple primitive operations. Often needs a huge amount of enumerative operations. Discrete structures and applications:

- Set theory
- Symbolic logic
- Inductive proof
- Combinatorics
- Graph theory
- Probabilistic theory
- Foundational materials for C.S. and math.

Technical stance of our project:

Application-specific technical areas:

- Discrete structure manipulation system
- Digital system optimization & verification
- Knowledge discovery & data mining
- Statistical Analysis & modeling

Our objective layer:

- Performance improvement (10–100x)
- Not only concept / theory, but also efficiency of implementation.
- Beauty of simplicity / universality.

Basis of CS & math. (conceptual, theoretical)

Direction of our research:

- Current ZDDs
  - Data mining, Machine learning
  - Advanced searching etc.

Further outputs:

- Applications in asymmetric world
  - Multisets
  - Sequences
  - Permutations
  - Partitions
  - Trees, DAGs
  - Networks
  - etc.

- Advanced ZDD-like structure
  - Numerical data processing
  - Processing of trees or semi-structured data

Location of laboratories:

- Main lab is located in Hokkaido Univ.
  - Center of attractive city: Sapporo.
  - 300m² space devoted for the project.
  - Convenient access from the airport and the station.
  - Good environment for the members to concentrate into research.

- Satellite labs located in Tokyo and Osaka.
  - Collaboration with many uni and companies.
  - Connecting by high-quality tele-conf. system.

Visit to Knuth’s home:

- May, 2010, during my trip to US for attending SIAM Data Mining Conference
- Visited Knuth’s home in Stanford Univ. campus.
  - Greetings and thanks for personal check giving for me and our students who found error of the Book.
  - Discussion on future work on BDD/ZDD and other discrete structures.

Outside of Knuth’s house:

- In the faculty’s house area of Stanford campus on an 80 years’ lease (1968～2048)
  - He has a room in Univ., but he mainly works in his home.
  - No educational work. Only attends annual special lecture. And weekly faculty’s lunch.
Knuth’s pipe-organ and his work room

Bookshelves

Material for his book

Kyoto-award medal and display frame

Discussion with Prof. Knuth

- Sequence BDD and applications.
  - He is very interested in the new data structure.
- I told him that I got too busy to manage the project since ZDD is written in Knuth book.
  - He recognizes his writing may have significant effect, and he said:
    “I’m partly responsible to make your life change. So, let’s discuss future work of your project.”
- Knuth’s proposals have same direction as our ERATO project: “Finding and organizing higher-level algebraic structures based on BDD/ZDD.”

Summary

- Focus on “discrete structure manipulation system.”
  - Fundamentals for various practical applications.
- Based on BDDs/ZDDs.
  - Representing “logic” and “set,” primitive models of discrete structures.
  - We will consider higher-level algebraic structures.
- Technical stance of the project.
  - Producing “Art” to connect Science and Engineering.
- Two objectives of the project.
  - Organizing new algebraic structures / operations.
  - Providing implementation with deep knowhow.
- Best use of ERATO framework
  - Organize an active research group with synergistic effect.
  - Contribution to the society to provide good research results as well as good researchers.