Whither Data Mining?

Rakesh Agrawal
Ramakrishnan Srikant

Intelligent Information Systems Research
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Outline

- Association Rules & the Apriori Algorithm
  - A quick retrospection of VLDB 94 paper
- Developments since VLDB 94
  - Extensions to the Association Rules Formalism
  - Algorithmic Innovations
  - System Issues
  - Usability
- Interesting Applications
  - Beyond Market Basket Analysis
- Whither?
Association Rules
(Agrawal, Imielinski & Swami: SIGMOD ’93)

- \( I = \{ i_1, i_2 \ldots, i_m \} \): a set of literals, called items.
- Transaction \( T \): a set of items such that \( T \not\subseteq I \).
- Database \( D \): a set of transactions.
- A transaction \( T \) contains \( X \), a set of some items in \( I \), if \( X \not\subseteq T \).
- An association rule is an implication of the form \( X \epsilon Y \), where \( X, Y \not\subseteq I \).
  - Support: % of transactions in \( D \) that contain \( X \cdot Y \).
  - Confidence: Among transactions that contain \( X \), what % also contain \( Y \).
- Find all rules that have support and confidence greater than user-specified minimum support and minimum confidence.
What Was New About This Formalism?

- Emphasis on finding all rules (Completeness)
  - Strong rules tend to be already known.
- Discovery vs. Hypothesis Testing
Computing Association Rules: Problem Decomposition

- Find all sets of items that have minimum support (frequent itemsets).

- Use the frequent itemsets to generate the desired rules.
  - confidence (X \in Y) = support (X \cdot Y) / support (X)
Computing Association Rules: Problem Decomposition

Find all sets of items that have minimum support (frequent itemsets).

What itemsets should you count?
How do you count them efficiently?

Use the frequent itemsets to generate the desired rules.

- confidence \((X \in Y) = \text{support}(X \cdot Y) / \text{support}(X)\)
What itemsets do you count?

- Search space is exponential.
  - With $n$ items, $\binom{n}{k}$ potential candidates of size $k$.
- Anti-monotonicity: Any superset of an infrequent itemset is also infrequent (SIGMOD ’93).
  - If an itemset is infrequent, don’t count any of its extensions.
- Flip the property: All subsets of a frequent itemset are frequent.
- Need not count any candidate that has an infrequent subset (VLDB ’94)
  - Simultaneously observed by Mannila et al., KDD ’94
- Broadly applicable to extensions and restrictions.
Apriori Algorithm: Breadth First Search

{ }

a  b  c  d
Apriori Algorithm: Breadth First Search
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APRIORI Candidate Generation (VLDB 94)

- $L_k$: Frequent itemsets of size $k$, $C_k$: Candidate itemsets of size $k$
- Given $L_k$, generate $C_{k+1}$ in two steps:
  
  - Join Step: Join $L_k$ with $L_k$, with the join condition that the first $k-1$ items should be the same and $l^1[k] < l^2[k]$.

<table>
<thead>
<tr>
<th>$L_3$</th>
<th>$C_4$</th>
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<tbody>
<tr>
<td>{a b c}</td>
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\[
\begin{array}{c|c}
L_3 & C_4 \\
--- & --- \\
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\{a\ b\ d\} & \\
\{a\ c\ d\} & \\
\{a\ c\ e\} & \\
\{b\ c\ d\} & \{a\ c\ d\ e\}
\end{array}
\]
How do you count?

- Given a set of candidates $C_k$, for each transaction $T$:
  - Find all members of $C_k$ which are contained in $T$.

- Hash-tree data structure [VLDB '94]
  - $C2 : \{ \{a, b\}, \{e, f\}, \{e, g\}\}$
  - $T : \{c, e, f\}, g\}$

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Recursively construct hash tables if number of itemsets is above a threshold.
Synthetic Datasets

- Transactions designed to mimic transactions in the retailing environment.
- Model: People tend to buy certain sets of items together.
  - Each such set is potentially a maximal frequent itemset.
  - Some people may only buy some of the items from such a set.
  - Frequent itemsets often have common items.
- Used in many studies for comparing the performance of association rule discovery algorithms.
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  - Extensions to the Association Rules Formalism
    - Generalizations
    - Restrictions
  - Algorithmic Innovations
  - System Issues
  - Usability
- Interesting Applications
- Whither?
Can we just replace each item with its generalization?
  - “Navy Squall Jacket Med” ⊇ “Jackets”

J. Han and Y. Fu, “Discovery of Multiple-Level Association Rules from Large Databases”, VLDB ’95.
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Quantitative Associations

- How do we deal with categorical & quantitative attributes?
  - Example: “30% of married people between age 45 and 60 have at least 2 cars; 5% of records have these properties”
- Can we just map this problem to boolean associations?
- Can discretize intervals & map each attribute into a set of boolean attributes.
- But …

R. Srikant and R. Agrawal, "Mining Quantitative Association Rules in Large Relational Tables", SIGMOD ‘96
Quantitative Association: The Discretization Dilemma

Color denotes confidence of rule $\text{Age}[] \in \text{Income}[]$

Support too low

Confidence too low

R. Srikant and R. Agrawal, "Mining Quantitative Association Rules in Large Relational Tables", SIGMOD '96
Quantitative Association: The Discretization Dilemma

- Can we give completeness guarantee?

Color denotes confidence of rule Age[ ] \& Income[ ]

Just right!

Support too low

Confidence too low

R. Srikant and R. Agrawal, "Mining Quantitative Association Rules in Large Relational Tables", SIGMOD '96
Quantitative Associations: Optimized Rectilinear Rules

- Find the rectilinear region that maximizes support \times confidence (or other criteria) for a fixed RHS.
- Example: Color denotes confidence.
- Optimize tradeoff between including more regions (higher support) vs. focusing only on high confidence regions.

Sequential Patterns

- Example: 10% of customers bought “shirts” and “jackets” in one transaction, followed by “shoes” in another transaction.
  - Inter-transaction patterns.
  - Can extend to sequential pattern rules.

- Constraints, e.g., max/min time gap between successive elements of the pattern.

- Not all subsequences of a frequent sequence are frequent.
  - Sequence not supported if it doesn’t meet the constraint.

Graphs, Trees, ...

- **Graphs:**
  - M. Kuramochi and G. Karypis, “Discovering frequent geometric subgraphs”, ICDM ‘01
  - X. Yan and J. Han, “gSpan: Graph-Based Substructure Pattern Mining”, ICDM ’02.

- **Trees:**
  - M. Zaki, “Efficiently mining frequent trees in a forest”, KDD ‘02
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Closed Itemsets

{a c} not closed since {a b c} has same support

9: support

Can generate missing itemsets with support.

R.J. Bayardo et al., “Brute-force mining of high-confidence classification rules”, KDD ’97
Maximal Itemsets

Can generate missing itemsets, but not their support.

R.J. Bayardo, “Efficiently Mining Long Patterns from Databases”, SIGMOD ’98.

Constraints over Items

- Boolean expressions over (the presence of) items.
  - (Shirts AND Shoes) OR (Outerwear AND NOT Hiking Boots)
- Anti-monotonicity property no longer holds.
  - \{Shirt, Shoes\} satisfies the constraint but not \{Shirt\} or \{Shoes\}.

R. Srikant, Q. Vu and R. Agrawal, “Mining Association Rules with Item Constraints”, KDD '97
Constraints over Properties of Items

- Example: Avg. price of items in rule should be > $10.
- Can classify constraints into groups:
  - Anti-monotone, e.g., minimum support, min(S) \( \mu \nu \)
  - Monotone, e.g., min(S) \( \nu \)
  - Succint, e.g., min(S) \( \nu \), min(S) \( \mu \nu \)
  -Convertible, e.g., avg(S) \( \nu \), avg(S) \( \mu \nu \)
- These four groups can be pushed (to varying degrees).
- Not all important constraints fall into these groups, e.g., min confidence, sum(S) \( \mu \nu \)

R. Ng et al., “Exploratory Mining and Pruning Optimizations of Constrained Association Rules”, SIGMOD ’98.
J. Pei and J. Han, “Can We Push More Constraints into Frequent Pattern Mining?”, KDD 2000.
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Algorithmic Innovations

- Reducing the cost of checking whether a candidate itemset is contained in a transaction:
  - TID intersection.
  - Database projection.
- Reducing the number of passes over the data:
  - Sampling & Dynamic Counting
- Reducing the number of candidates counted:
  - For maximal patterns & constraints.
- Many other innovative ideas ... unfortunately, not covered in this talk – Apologies in advance!
Algorithmic Innovations

- Reducing the cost of checking whether a candidate itemset is contained in a transaction:
  - TID intersection.
  - Database projection.

Themes
- Focused on CPU cost.
- Dense data / longer rules.
- Transform the dataset.
- Cost of memory & disk.
TID Intersection

- Convert data from “horizontal” to “vertical” format.
- For each frequent item, list of TIDs of transactions that contain the item.

<table>
<thead>
<tr>
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<tbody>
<tr>
<td>10</td>
<td>a, c, e</td>
<td>a</td>
<td>10, 30</td>
</tr>
<tr>
<td>20</td>
<td>b, d</td>
<td>b</td>
<td>20, 40</td>
</tr>
<tr>
<td>30</td>
<td>a, e</td>
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Cost of intersection is low if lists are in memory.

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TID Intersection: Depth First Search

- Use depth-first search to keep TID lists in memory.

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Database Projection

- Example: To count all itemsets starting with \{a\}, with possible extensions \{b, e, f\}:

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R.C. Agarwal et al., “A Tree Projection Algorithm for Generation of Frequent Itemsets”, JPDC.
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FP Growth

- Transaction database converted to prefix-tree structure.
  - Items ordered in frequency descending order.

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J. Han, J. Pei and Y. Yin, “Mining Frequent Patterns without Candidate Generation”, SIGMOD 2000.
FP Growth

- Transaction database converted to prefix-tree structure.

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J. Han, J. Pei and Y. Yin, “Mining Frequent Patterns without Candidate Generation”, SIGMOD 2000.
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- Transaction database converted to prefix-tree structure.
  - Tree typically much smaller than database.

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- Transaction database converted to prefix-tree structure.

Can efficiently count support of candidates using prefix tree.

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Algorithmic Innovations

- Reducing the cost of checking whether a candidate itemset is contained in a transaction:
  - TID intersection.
  - Database projection.
- Reducing the number of passes over the data:
  - Sampling & Dynamic Counting

Themes:
Focused on IO cost.
Sparse data / shorter rules.
Reducing the number of passes

- Use independence assumption to estimate which itemsets will be frequent, and count all the expected frequent itemsets in a single pass (SIGMOD ’93).
  - Eagerly combine multiple passes to reduce cost of scanning the database (VLDB ’94).

- Use sampling instead of independence assumption to estimate which itemsets are frequent, and count all frequent itemsets + negative border in one pass (Toivonen, VLDB ’96)
  - Sample yields more accurate estimates than independence assumption.
  - Need mop-up pass(es) for those itemsets in negative border that turn out to be frequent.
Reducing the number of passes: Dynamic Counting

- Can combine “sampling” with pass over the database.
  - Assuming transactions are independent!

S. Brin et al, “Dynamic Itemset Counting and Implication Rules for Market Basket Data”, SIGMOD ‘97
Algorithmic Innovations

- Reducing the cost of checking whether a candidate itemset is contained in a transaction:
  - TID intersection.
  - Database projection.

- Reducing the number of passes over the data:
  - Sampling & Dynamic Counting

- Reducing the number of candidates counted:
  - For maximal patterns & constraints.
Maximal Itemsets

- MaxMiner: Uses pruning based on superset frequency in addition to pruning on subset infrequency.
- Set enumeration search.
- Lookahead: If \{a b c\} is frequent, don’t need to count \{a b\} or \{a c\}.
- Scales roughly linearly in number of maximal sets.

R.J. Bayardo, “Efficiently Mining Long Patterns from Databases”, SIGMOD ’98.
Outline

- Association Rules & the Apriori Algorithm
- Developments since VLDB 94
  - Extensions to the Association Rules Formalism
  - Algorithmic Innovations
  - System Issues
  - Usability
- Interesting Applications
- Whither?
Database Integration: Tight Coupling

- Motivation: Tighter integration for performance reasons.
  - Avoid copying of records from database address space to the application address space.
  - Avoid process context switching for each record retrieved.

- Push part of the computation into UDFs.
  - Two-fold performance advantage.

R. Agrawal and K. Shim, “Developing Tightly-Coupled Data Mining Applications on a Relational Database System”, KDD ‘96
Database Integration: Using SQL

- Use SQL to perform computation.
- Motivation:
  - Composability: Combine selections and projections.
  - Use full power of database query optimization techniques.
- Need extensions to SQL ’92 and/or query optimization to get good performance.
  - Object-relational extension such as UDFs, Blobs, Table Functions allow for substantial performance improvement.

Database Integration: Pushing Apriori into Optimizers

- Flock: Parameterized query (e.g., pairs of items) and a filter condition (e.g., support > 20).
- Can generalize Apriori to apply to broader class of query flocks.
- Incorporating the generalized Apriori optimization into query optimizers can yield benefits for other data mining queries.

Standards: PMML

- Predictive Model Markup Language
  - Markup language for statistical and data mining models.
  - Includes association rules.
- Share models between PMML compliant applications.
- Allows users to mine association rules with one application, and use a different applications to visualize, analyze, evaluate or otherwise use the discovered rules.
PMML: Example

<AssociationModel functionName="associationRules"
    numberOfTransactions="4" numberOfItems="3" minimumSupport="0.6"
    minimumConfidence="0.5" numberOfItemsets="3" numberOfRules="2">
    ...
    <Item id="1" value="Cracker" />
    ...
    <Itemset id="3" support="1.0" numberOfItems="2">
        <ItemRef itemRef="1" />
        <ItemRef itemRef="3" />
    </Itemset>
    ...
    <AssociationRule support="1.0" confidence="1.0"
        antecedent="1" consequent="2" />
    ...

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    - Interesting Rules
    - Visualization
- Interesting Applications
- Whither?
Statistical Significance

- Statistical Significance, e.g., p-value of independence test between antecedent and consequent.
- Need to adjust the threshold to account for number of hypotheses tested.
- Number of hypotheses tested can be $>>$ number of rules.
  - Upper bound: number of candidates.
  - Upper bound too conservative since the hypotheses are not independent.
- Use resampling to determine appropriate threshold.
  - Generate synthetic dataset using item frequency information (assuming independence) and measure p-values of discovered associations.

Objective Interest Measures

- Objective Measures: Depend only on the structure of pattern and the underlying data.
- Lift: Ratio of support to expected support assuming independence.
  - For rule A \( \varepsilon B \), Lift = \( \frac{P(A \text{ and } B)}{P(A) \times P(B)} \)
- Other examples: chi-squared value, gini, conviction, etc.

Mining the Most Interesting Rules

- For fixed consequent, the best rule according to a broad class of interest metrics resides on a support/confidence border.
  - Example Metrics: support, confidence, gain, chi-squared, gini, entropy gain, laplace, lift, conviction.
- Can mine all rules that are best according to any of these criteria.

Subjective Interest Measures

- Subjective Measures: Depend on the class of users who examine the pattern.
- Actionability: User can use the pattern to take some action.
- Unexpectedness: Surprising to the user.
  - Can be defined via belief systems.


Interest Measures using Other Rules

- Jackets & Shoes [70% confidence]
- Jackets and Shirts & Shoes [71% confidence]
  - This rule not very surprising given the previous rule.
- Can take one step further & consider only the direction of the correlation (positive, negative or neutral).
  - Extension of a rule is interesting only if its direction is different.

Pruning based on confidence

- Fixed consequent
- Goal: Find all rules whose confidence is significantly higher than any of their simplifications.
- Can prune candidate itemsets based on confidence.
  - Although confidence does not map into any of the constraint classes, its constituent parts do.
  - Can be used prune search.

Interest Measures using Other Rules: Taxonomies

- Clothes & Shoes
  - 8% support, 70% confidence
- Quarter of sales of Clothes are Jackets
- Jackets & Shoes
  - expect 2% support, 70% confidence
- Interesting rule if support/confidence is significantly different than “expected” value.
- User-specified “interest level”
- Similar approach for quantitative associations.

Application-Driven Visualization

Color shows support.

Can “walk” around and examine placement of frequent items.

Can have multiple colors to show profit & frequency.
Application-Driven Visualization

Select an item.

Associated items in red.

Flags to see associated items in other aisles.
Outline

- Association Rules & the Apriori Algorithm
- Developments since VLDB 94
- Interesting Applications (Beyond Market Basket Analysis)
  - Early Applications
  - Building Block for Other Data Mining Operations
  - Other Innovative Applications
- Whither?
Product Assortment Decisions in Automated Convenience Stores

- Context: Automated Convenience Stores that can hold about 200 products.
- Placement decisions traditionally based on profit per product.
  - Ignored cross-selling effects.
- Use frequent itemsets to identify cross-selling effects.
  - Feed into a microeconomic optimization model.
- Example: Cigarette paper is not justified by its profit margins, but drives sales of tobacco (which has high profit margins).

Health Insurance Claim Analysis

- Health Insurance Commission of Australia
  - Claim file over 550 GB
- Associations between medical payment codes
- Found that doctors were frequently claiming MCS2 with OCP, rather than claiming FCS with OCP.
  - $13.55 benefit for MCS2 versus OCP.
- However, this combination should be a rare event, not a common event.
- Potential savings of over $500,000 per year (in just one state).

M. Viveros, J.P. Nearhos and M.J. Rothman, “Applying Data Mining Techniques for Effective Health”, VLDB '96
Analyzing Automobile Warranty Claims

- Analyzed claims on DaimlerChrysler automobiles.
- Found associations “considered as very useful by domain experts”:
  - Dependency between problems with justification of headlights and the distance of the axes.
  - 20% of vehicles visiting a specific garage had problems with the cables.
    - Problems with cables not uniformly distributed over garages.
    - Further investigation may identify the root problem.

Reducing Telecommunications Failures

- Telecommunications service orders:
  - Around 3.5 sub-parts (USOCs).
    - Example: USOC for “call-waiting” in an order for new line.
  - Failure code (RMA) if automated processing failed.

- Classification problem: what combination USOCs predict an RMA?
  - But only 2.5% of orders fail, 25 different failure codes.

- Found frequent itemsets for each RMA,
  - Checked for statistically significant correlation between RMA & itemset.
  - Ranked itemsets by \( \Pr(\text{RMA} | \text{itemset}) / \Pr(\text{RMA} | \text{no itemset}) \).

- Results pointed to overhaul of certain mechanisms for ISDN orders.

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Classification

- Find all association rules where the consequent is a class label.
- Select a subset of rules and build a rule-based classifier.
- More accurate than C4.5

B. Liu, W. Hsu and Y. Ma, “Integrating Classification and Association Rule Mining”, KDD ’98.
W. Li, J. Han, and J. Pei, “Cmar: Accurate and efficient classification based on multiple class-association rules, ICDM ’01.
Subspace Clustering

- Problem: Find clusters embedded in subspaces of high dimensional data.
- Cluster: Maximal set of connected dense units in k-dimensions.
- Clusters are analogous to frequent itemsets.
- Anti-monotonicity: If a collection of points S is a cluster in a k-dimensional space, then S is also part of a cluster in any (k-1)-dimensional projection of this space.
- MDL used to identify interesting subspaces (and clusters).

Discovering Technology Trends from Patent Databases

- Input: i) patent database  ii) shape of interest.
- Find frequent patterns (e.g., sequence of phrases) in each time period.
- Use shape-based query language to identify trends over the change in support.

Outline

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■ Developments since VLDB 94

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■ Whither?
Intrusion Detection

- Mine frequent patterns from user command data.
  - Merge similar patterns to form the normal usage profile.
- Given a new session, mine its patterns.
  - Compare similarity of patterns against normal profile.
- Successful at detecting anomalies in DARPA dataset.

Identifying Social Links on the Web

- Input: Crawl of about 1 million pages.
- Find associations of what names occur together.

WebFountain Project, IBM Almaden.
Template Detection for the Web

- Three important Hypertext IR principles:
  - Relevant Linkage: Google, Citeseer
  - Topical Unity: Co-cited documents are related.
  - Lexical Affinity: Proximity is correlated with relevance.

- Templates: Collection of pages that share the same look and feel, and are controlled by a single authority.
  - Templates violate these principles.
  - Detection instance of frequent itemset counting problem.

- Eliminating templates results in “surprising increases in precision at all levels of recall” in (pure) search algorithms.

Discovering Micro-communities

- Japanese elementary schools
- Turkish student associations
- Oil spills off the coast of Japan
- Australian fire brigades
- Aviation/aircraft vendors
- Guitar manufacturers

Frequently co-cited pages are related. Pages with large bibliographic overlap are related.

Developments since VLDB ’94: A Snapshot

- Extensions to Association Rules
- Algorithmic Innovations
- Database Integration
- Usability
- Published Applications
Speculation On Why Association Rules Got Attention Beyond Our Wildest Dreams

- Essence of formalism was small.
- Grounded in real, unfulfilled need.
  - Being used in the field and getting feedback, allowed us to identify the key generalizations.
- Emphasis on finding all rules rather than strong rules.
  - Could run against whole dataset.
  - Discovery vs. Hypothesis Testing (Completeness).
Speculation On Why Association Rules Got Attention Beyond Our Wildest Dreams

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- Emphasis on finding all rules rather than strong rules.
  - Could run against whole dataset.
  - Discovery vs. Hypothesis Testing (Completeness).
- Since the abstraction was simple, there was a lot of flexibility in extending the problem.
- While the formalism was simple, efficient solutions were not!
  - Scope for innovation.
Outline

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Whither Data Mining: The Dream (circa 1994)

- Data mining should aspire to become the technology that allows entities to derive maximal economic value from data.
Whither Data Mining: The Dream (circa 2004).

- Data mining should aspire to become the technology that allows entities to derive maximal economic value from data while respecting the sovereignty of data.
Sovereignty of Individual

- Goal: Build accurate data mining models while preserving the privacy of individual records.
- Initial Approach: Data Perturbation.
- Research Challenges:
  - How do you define privacy?
  - What is the tradeoff between privacy and accuracy?
  - Other approaches?

R. Agrawal and R. Srikant, SIGMOD 2000
A. Evfimievski et al., PODS 2003
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- Business Imperative:
  - Competitive Advantage
  - Compliance with legislation.
- Moral Imperative: “Privacy is … the most comprehensive of rights, and the right most valued by civilized man.” -- Louis D. Brandeis

R. Agrawal and R. Srikant, SIGMOD 2000
A. Evfimievski et al., PODS 2003
Organizational Sovereignty

- The network era is forcing organizations to share information and make decisions across organizational boundaries.
- Goal: Data mining that transcends organizational boundaries while preserving sovereignty.
- Initial Approach: Cryptographic Protocols
- Research Challenges:
  - New framework for thinking about ownership, privacy and security.
  - What is the tradeoff between Generality, Performance, Accuracy, and Potential disclosure?

Purdue Toolkit [Clifton et al 2003]
R. Agrawal, A. Evfimievski and R. Srikant, SIGMOD 2003
Organizational Sovereignty

Closing Thought
Tremendous opportunity for innovation and making fundamental contributions.

- Initial Approach: Cryptographic Protocols
- Research Challenges:
  - New framework for thinking about ownership, privacy and security.
  - What is the tradeoff between Generality, Performance, Accuracy, and Potential disclosure?
Acknowledgements

To all the researchers who worked on association rules and thus helped create the field:

Thank You!
Ack: The Quest Group (circa 1995)

Left to Right:
H. Miranda
K. Shim
R. Srikant
D. Lin
J. Shafer
R. Agrawal
M. Mehta
M. Zait
Acks: Our Colleagues in Germany

Left to Right:
L. Knoth-Weber
P. Vigants
U. Baumbach
C. Lingenfelder
N.P. Friedrich
B. Hartel
R. Keuler
W. Staub
A. Arning
T. Bollinger
H. Meiwes
S. Bayerl
P. Greissl
## Acknowledgments

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