## Probabilistic Approach to Association Rule Mining

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## Motivation

We life in the era of big data. Examples:

- Transaction data: Retailers (point-of-sale systems, loyalty card programs) and e-commerce
- Web navigation data: Web analytics, search engines, digital libraries, Wikis, etc.
- Gene expression data: DNA microarrays


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- Gene expression data: DNA microarrays

Typical size of data sets:

- Typical Retailer: 10-500 product groups and 500-10,000 products
- Amazon: 480+ million products in the US (2015)
- Wikipedia: almost 5 million articles (2015)
- Google: estimated 47+ billion pages in index (2015)
- Human Genome Project: approx. 20,000-25,000 genes in human DNA with 3 billion base pairs.
- Typically 10,000-10 million transactions (shopping baskets, user sessions, observations, patients, etc.)


## Motivation

The aim of association analysis is to find 'interesting' relationships between items (products, documents, etc.). Example: 'purchase relationship':
milk, flour and eggs are frequently bought together.
or
If someone purchases milk and flour then that person often also purchases eggs.

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Applications of found relationships:

- Retail: Product placement, promotion campaigns, product assortment decisions, etc.
$\rightarrow$ exploratory market basket analysis (Russell et al., 1997; Berry and Linoff, 1997; Schnedlitz et al., 2001; Reutterer et al., 2007).
- E-commerce, dig. libraries, search engines: Personalization, mass customization
$\rightarrow$ recommender systems, item-based collaborative filtering (Sarwar et al., 2001; Linden et al., 2003; Geyer-Schulz and Hahsler, 2003).


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## Transaction Data

Example of market basket data:

| transaction ID | items |
| :---: | :--- |
| 1 | milk, bread |
| 2 | bread, butter |
| 3 | beer |
| 4 | milk, bread, butter |
| 5 | bread, butter |



Formally, let $I=\left\{i_{1}, i_{2}, \ldots, i_{n}\right\}$ be a set of $n$ binary attributes called items. Let $\mathcal{D}=\left\{t_{1}, t_{2}, \ldots, t_{m}\right\}$ be a set of transactions called the database. Each transaction in $\mathcal{D}$ has an unique transaction ID and contains a subset of the items in $I$.

Note: Non-transaction data can be made into transaction data using binarization.

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## Association Rules

A rule takes the form $X \rightarrow Y$

- $X, Y \subseteq I$
- $X \cap Y=\emptyset$
- $X$ and $Y$ are called itemsets.
- $X$ is the rule's antecedent (left-hand side)
- $Y$ is the rule's consequent (right-hand side)


## Example

$$
\{\text { milk, flower, bread }\} \rightarrow\{\text { eggs }\}
$$

## Association Rules

To select 'interesting' association rules from the set of all possible rules, two measures are used (Agrawal et al., 1993):
(1) Support of an itemset $Z$ is defined as $\operatorname{supp}(Z)=n_{Z} / n$. $\rightarrow$ share of transactions in the database that contains $Z$.
(2) Confidence of a rule $X \rightarrow Y$ is defined as

$$
\operatorname{conf}(X \rightarrow Y)=\operatorname{supp}(X \cup Y) / \operatorname{supp}(X)
$$

$\rightarrow$ share of transactions containing $Y$ in all the transactions containing $X$.

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Each association rule $X \rightarrow Y$ has to satisfy the following restrictions:

$$
\begin{aligned}
& \operatorname{supp}(X \cup Y) \geq \sigma \\
& \operatorname{conf}(X \rightarrow Y) \geq \gamma
\end{aligned}
$$

$\rightarrow$ called the support-confidence framework.

## Minimum Support

Idea: Set a user-defined threshold for support since more frequent itemsets are typically more important. E.g., frequently purchased products generally generate more revenue.

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## Minimum Support

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Apriori property (Agrawal and Srikant, 1994): The support of an itemset cannot increase by adding an item. Example: $\sigma=.4$ (support count $\geq 2$ )

$\rightarrow$ Basis for efficient algorithms (Apriori, Eclat).

## Minimum Confidence

From the set of frequent itemsets all rules which satisfy the threshold for confidence $\operatorname{conf}(X \rightarrow Y)=\frac{\operatorname{supp}(X \cup Y)}{\operatorname{supp}(X)} \geq \gamma$ are generated.

Confidence


## Minimum Confidence

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Confidence

\{eggs $\}$
\{flour $\}$
\{eggs $\}$
\{milk $\}$
\{flour $\}$
\{milk $\}$
\{eggs, flour
\{eggs, milk $\}$
\{flour, milk $\}$
\{eggs $\}$
\{flour $\}$
\{milk $\}$
$\rightarrow \quad\{$ flour $\}$
$3 / 4=0.75$
$\rightarrow \quad$ \{eggs $\}$
$3 / 3=1$
$\rightarrow$ \{milk\}
$2 / 4=0.5$
$\rightarrow \quad$ eeggs $\}$
$2 / 4=0.5$
$\rightarrow \quad\{$ milk $\}$
$2 / 3=0.67$
$\rightarrow \quad\{$ flour $\}$
$2 / 4=0.5$
$\rightarrow \quad\{$ milk $\}$
$2 / 3=0.67$
$2 / 2=1$
\{flour, milk\} $\rightarrow \quad$ \{eggs\}
$2 / 2=1$
$\rightarrow \quad$ \{flour, milk
$2 / 4=0.5$
\{flour\} $\rightarrow \quad$ \{eggs, milk\}
$2 / 3=0.67$
$\rightarrow \quad$ \{eggs, flour $\}$
$2 / 4=0.5$
At $\gamma=0.7$ the following set of rules is generated:

|  |  |  | Support | Confidence |
| :---: | :---: | :---: | :---: | :---: |
| \{eggs $\}$ | $\rightarrow$ | \{flour\} | $3 / 5=0.6$ | $3 / 4=0.75$ |
| \{flour\} | $\rightarrow$ | \{eggs\} | $3 / 5=0.6$ | $3 / 3=1$ |
| \{eggs, milk | $\rightarrow$ | \{flour\} | $2 / 5=0.4$ | $2 / 2=1$ |
| \{flour, milk | $\rightarrow$ | \{eggs\} | $2 / 5=0.4$ | $2 / 2=1$ |

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## Probabilistic interpretation of Support and Confidence

Support

$$
\operatorname{supp}(Z)=n_{Z} / n
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corresponds to an estimate for $\hat{P}\left(E_{Z}\right)=n_{Z} / n$, the probability for the event that itemset $Z$ is contained in a transaction.

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Confidence can be interpreted as an estimate for the conditional probability

$$
P\left(E_{Y} \mid E_{X}\right)=\frac{P\left(E_{X} \cap E_{Y}\right)}{P\left(E_{X}\right)}
$$

This directly follows the definition of confidence:

$$
\operatorname{conf}(X \rightarrow Y)=\frac{\operatorname{supp}(X \cup Y)}{\operatorname{supp}(X)}=\frac{\hat{P}\left(E_{X} \cap E_{Y}\right)}{\hat{P}\left(E_{X}\right)}
$$

## Weaknesses of Support and Confidence

- Support suffers from the 'rare item problem' (Liu et al., 1999a): Infrequent items not meeting minimum support are ignored which is problematic if rare items are important.
E.g. rarely sold products which account for a large part of revenue or profit. Typical support distribution (retail point-of-sale data with 169 items):

- Support falls rapidly with itemset size. A threshold on support favors short itemsets (Seno and Karypis, 2005).


## Weaknesses of Support and Confidence

- Confidence ignores the frequency of $Y$ (Aggarwal and Yu, 1998; Silverstein et al., 1998).

|  | $\mathrm{X}=0$ | $\mathrm{X}=1$ | $\Sigma$ |
| :---: | :---: | :---: | :---: |
| $\mathrm{Y}=0$ | 5 | 5 | 10 |
| $\mathrm{Y}=1$ | 70 | 20 | 90 |
| $\Sigma$ | 75 | 25 | 100 |

$$
\operatorname{conf}(X \rightarrow Y)=\frac{n_{X \cup Y}}{n_{X}}=\frac{20}{25}=.8
$$

Weakness: Confidence of the rule is relatively high with $\hat{P}\left(E_{Y} \mid E_{X}\right)=.8$. But the unconditional probability $\hat{P}\left(E_{Y}\right)=n_{Y} / n=90 / 100=.9$ is higher!

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- The thresholds for support and confidence are user-defined. In practice, the values are chosen to produce a 'manageable' number of frequent itemsets or rules.
$\rightarrow$ What is the risk and cost attached to using spurious rules or missing important in an application?


## Lift

The measure lift (interest, Brin et al., 1997) is defined as

$$
\operatorname{lift}(X \rightarrow Y)=\frac{\operatorname{conf}(X \rightarrow Y)}{\operatorname{supp}(Y)}=\frac{\operatorname{supp}(X \cup Y)}{\operatorname{supp}(X) \cdot \operatorname{supp}(Y)}
$$

and can be interpreted as an estimate for $P\left(E_{X} \cap E_{Y}\right) /\left(P\left(E_{X}\right) \cdot P\left(E_{Y}\right)\right)$. $\rightarrow$ Measure for the deviation from stochastic independence:

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In marketing values of lift are interpreted as:

- $\operatorname{lift}(X \rightarrow Y)=1 \ldots X$ and $Y$ are independent
- $\operatorname{lift}(X \rightarrow Y)>1 \ldots$ complementary effects between $X$ and $Y$
- $\operatorname{lift}(X \rightarrow Y)<1 \ldots$ substitution effects between $X$ and $Y$


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## Example

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| $\mathrm{Y}=0$ | 5 | 5 | 10 |
| $\mathrm{Y}=1$ | 70 | 20 | 90 |
| $\Sigma$ | 75 | 25 | 100 |

$$
\operatorname{lift}(X \rightarrow Y)=\frac{.2}{.25 \cdot .9}=.89
$$

## Chi-Square Test for Independence

Tests for significant deviations from stochastic independence (Silverstein et al., 1998; Liu et al., 1999b).
Example: $2 \times 2$ contingency table ( $l=2$ dimensions) for rule $X \rightarrow Y$.

|  | $X=0$ | $X=1$ | $\Sigma$ |
| :---: | :---: | :---: | :---: |
| $\mathrm{Y}=0$ | 5 | 5 | 10 |
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Null hypothesis: $P\left(E_{X} \cap E_{Y}\right)=P\left(E_{X}\right) \cdot P\left(E_{Y}\right)$ with test statistic

$$
X^{2}=\sum_{i} \sum_{j} \frac{\left(n_{i j}-E\left(n_{i j}\right)\right)^{2}}{E\left(n_{i j}\right)} \quad \text { with } \quad E\left(n_{i j}\right)=\frac{n_{i} \cdot n_{\cdot j}}{n}
$$

asymptotically approaches a $\chi^{2}$ distribution with $2^{l}-l-1$ degrees of freedom. The result of the test for the contingency table above:
$X^{2}=3.7037, \mathrm{df}=1$, p -value $=0.05429$
$\rightarrow$ The null hypothesis (independence) can not be be rejected at $\alpha=0.05$.
Weakness: Bad approximation for $E\left(n_{i j}\right)<5$; multiple testing.

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## The Independence Model

(1) Transactions occur following a homogeneous Poisson process with parameter $\theta$ (intensity).


$$
P(N=n)=\frac{e^{-\theta t}(\theta t)^{n}}{n!}
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$$
P(N=n)=\frac{e^{-\theta t}(\theta t)^{n}}{n!}
$$

(2) Each item has the occurrence probability $p_{i}$ and each transaction is the result of $k$ (number of items) independent Bernoulli trials.

$$
P\left(N_{i}=n_{i}\right)=\sum_{m=n_{i}}^{\infty} P\left(N_{i}=n_{i} \mid N=n\right) \cdot P(N=n)=\frac{e^{-\lambda_{i}} \lambda_{i}^{n_{i}}}{n_{i}!} \quad \text { with } \quad \lambda_{i}=p_{i} \theta t
$$

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## Application: Evaluate Quality Measures

Authors typically construct examples where support, confidence and lift have problems (see e.g., Brin et al., 1997; Aggarwal and Yu, 1998; Silverstein et al., 1998).

Idea: Compare the behavior of measures on real-world data and on data simulated using the independence model (Hahsler et al., 2006; Hahsler and Hornik, 2007).

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Idea: Compare the behavior of measures on real-world data and on data simulated using the independence model (Hahsler et al., 2006; Hahsler and Hornik, 2007).

Characteristics of used data set (typical retail data set).

- $t=30$ days
- $k=169$ product groups
- $n=9835$ transactions
- Estimated $\theta=n / t=327.2$ transactions per day.
- We estimate $p_{i}$ using the observed frequencies $n_{i} / n$.


## Comparison: Support



Only rules of the form: $\left\{i_{i}\right\} \rightarrow\left\{i_{j}\right\}$
X-axis: Items $i_{i}$ sorted by decreasing support.
$\mathbf{Y}$-axis: Items $i_{j}$ sorted by decreasing support.
Z-axis: Support of rule.

## Comparison: Confidence



$$
\operatorname{conf}\left(\left\{i_{i}\right\} \rightarrow\left\{i_{j}\right\}\right)=\frac{\operatorname{supp}\left(\left\{i_{i}, i_{j}\right\}\right)}{\operatorname{supp}\left(\left\{i_{i}\right\}\right)}
$$

Systematic influence of support

- Confidence decreases with support of the right-hand side $\left(i_{j}\right)$.
- Spikes with extremely low-support items in the left-hand side $\left(i_{i}\right)$.


## Comparison: Lift



Simulated data


Retail data

$$
\operatorname{lift}\left(\left\{i_{i}\right\} \rightarrow\left\{i_{j}\right\}\right)=\frac{\operatorname{supp}\left(\left\{i_{i}, i_{j}\right\}\right)}{\operatorname{supp}\left(\left\{i_{i}\right\}\right) \cdot \operatorname{supp}\left(\left\{i_{j}\right\}\right)}
$$

- Similar distribution with extreme values for items with low support.


## Comparison: Lift + Minimum Support



- Considerably higher lift values in retail data (indicate the existence of associations).
- Strong systematic influence of support.
- Highest lift values at the support-confidence border (Bayardo Jr. and Agrawal, 1999). If lift is used to sort found rules, small changes of minimum support/minimum confidence totally change the result.


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## Application: NB-Frequent Itemsets

Idea: Identification of interesting associations as deviations from the independence model (Hahsler, 2006).

1. Estimation of a global independence model using the frequencies of items in the database.
The independence model is a mixture of $k$ (number of items) independent homogeneous Poisson processes. Parameters $\lambda_{i}$ in the population are chosen from a $\Gamma$ distribution.

Global model


Number of items which occur in $r=\left\{0,1, \ldots, r_{\max }\right\}$ transactions
$\rightarrow$ Negative binomial distribution.

## NB-Frequent Itemsets

2. Select all transactions for itemset $Z$. We expect all items which are independent of $Z$ to occur in the selected transactions following the (rescaled) global independence model. Associated items co-occur too frequently with $Z$.

NB model for itemset $Z=\{89\}$


- Rescaling of the model for $Z$ by the number of incidences.
- Uses a user-defined threshold $1-\pi$ for the number of accepted 'spurious associations'.
- Restriction of the search space by recursive definition of parameter $\theta$.

Details about the estimation procedure for the global model (EM), the mining algorithm and evaluation of effectiveness can be found in Hahsler (2006).

## NB-Frequent Itemsets

Mine NB-frequent itemsets from an artificial data set with know patterns.



- Performs better than support in filtering spurious itemsets.
- Automatically decreases the required support with itemset size.


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## Hyper-Confidence

Idea: Develop a confidence-like measure based on the probabilistic model (Hahsler and Hornik, 2007).

Informally: How confident, $0-100 \%$, are we that a rule is not just the result of random co-occurrences?

## Hyper-Confidence

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Informally: How confident, $0-100 \%$, are we that a rule is not just the result of random co-occurrences?

Model the number of transactions which contain rule $X \rightarrow Y(X \cup Y)$ as a random variable $N_{X Y}$. Give the frequencies $n_{X}$ and $n_{Y}$ and independence, $N_{X Y}$ has a hypergeometric distribution.

The hypergeometric distribution arises for the 'urn problem': An urn contains $w$ white and $b$ black balls. $k$ balls are randomly drawn from the urn without replacement. The number of white balls drawn is then a hypergeometric distributed random variable.

## Hyper-Confidence

The hypergeometric distribution arises for the 'urn problem': An urn contains $w$ white and $b$ black balls. $k$ balls are randomly drawn from the urn without replacement. The number of white balls drawn is then a hypergeometric distributed random variable.

Application: Under independence, the database can be seen as an urn with $n_{X}$ 'white' transactions (contain $X$ ) and $n-n_{X}$ 'black' transactions (do not contain $X$ ). We randomly assign $Y$ to $n_{Y}$ transactions in the database. The number of transactions that contain $Y$ and $X$ is a hypergeometric distributed random variable.
The probability that $X$ and $Y$ co-occur in exactly $r$ transactions given independence, $n, n_{X}$ and $n_{Y}$, is

$$
P\left(N_{X Y}=r\right)=\frac{\binom{n_{Y}}{r}\binom{n-n_{Y}}{n_{X}-r}}{\binom{n}{n_{X}}}
$$

## Hyper-Confidence

$$
\text { hyper-confidence }(X \rightarrow Y)=P\left(N_{X Y}<n_{X Y}\right)=\sum_{i=0}^{n_{X Y}-1} P\left(N_{X Y}=i\right)
$$

A hyper-confidence value close to 1 indicates that the observed frequency $n_{X Y}$ is too high for the assumption of independence and that between $X$ and $Y$ exists a complementary effect.
As for other measures of association, we can use a threshold:

$$
\text { hyper-confidence }(X \rightarrow Y) \geq \gamma
$$

Interpretation: At $\gamma=.99$ each accepted rule has a chance of less than $1 \%$ that the large value of $n_{X Y}$ is just a random deviation (given $n_{X}$ and $\left.n_{Y}\right)$.

## Hyper-Confidence

| $2 \times 2$ contingency table for rule $X \rightarrow Y$ |  |  |  |
| :---: | :---: | :---: | :---: |
|  | $X=0$ | $X=1$ |  |
| $Y=0$ | $n-n_{Y}-n_{X}-N_{X Y}$ | $n_{X}-N_{X Y}$ | $n-n_{Y}$ |
| $Y=1$ | $n_{Y}-N_{X Y}$ | $N_{X Y}$ | $n_{Y}$ |
|  | $n-n_{X}$ | $n_{X}$ | $n$ |

Using minimum hyper-confidence $(\gamma)$ is equivalent to Fisher's exact test.
Fisher's exact test is a permutation test that calculates the probability of observing an even more extreme value for given fixed marginal frequencies (one-tailed test). Fisher showed that the probability of a certain configuration follows a hypergeometric distribution.

The p-value of Fisher's exact test is

$$
\text { p-value }=1 \text { - hyper-confidence }(X \rightarrow Y)
$$

and the significance level is $\alpha=1-\gamma$.

## Hyper-Confidence: Complementary Effects




Simulated data
Retail data

$$
\gamma=.99
$$

Expected spurious rules: $\alpha\binom{k}{2}=141.98$

## Hyper-Confidence: Complementary Effects



Simulated data
Retail data

$$
\gamma=.9999993
$$

Bonferroni correction $\alpha=\frac{\alpha_{i}}{\binom{k}{2}}$

## Hyper-Confidence: Substitution Effects

Hyper-confidence uncovers complementary effects between items.
To find substitution effects we have to adapt hyper-confidence as follows:
hyper-confidence ${ }^{\mathrm{sub}}(X \rightarrow Y)=P\left(N_{X Y}>n_{X, Y}\right)=1-\sum_{i=0}^{n_{X Y}} P\left(N_{X Y}=i\right)$
with

$$
\text { hyper-confidence }^{\text {sub }}(X \rightarrow Y) \geq \gamma
$$

## Hyper-Confidence: Substitution Effects




Retail data

$$
\gamma=.99
$$

## Hyper-Confidence: Simulated Data

PN-Graph for the synthetic data set T10I4D100K with a corruption rate of .9 (Agrawal and Srikant, 1994).


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## Conclusion

The support-confidence framework cannot answer some important questions sufficiently:

- What are sensible thresholds for different applications?
- What is the risk of accepting spurious rules?


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- What are sensible thresholds for different applications?
- What is the risk of accepting spurious rules?

Probabilistic models can help to:

- Evaluate and compare measures of interestingness, data mining processes or complete data mining systems (with synthetic data from models with dependencies).
- Develop new mining strategies and measures (e.g., NB-frequent itemsets, hyper-confidence).
- Use statistical test theory as a solid basis to quantify risk and justify thresholds.


## Thank you for your attention!

- Contact information and full papers can be found at http://michael.hahsler.net
- The presented models and measures are implemented in arules (an extension package for $R$, a free software environment for statistical computing and graphics; see http://www.r-project.org/).


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## The arules Infrastructure



Simplified UML class diagram implemented in R (S4)

- Uses the sparse matrix representation (from package Matrix by Bates \& Maechler (2005)) for transactions and associations.
- Abstract associations class for extensibility.
- Interfaces for Apriori and Eclat (implemented by Borgelt (2003)) to mine association rules and frequent itemsets.
- Provides comprehensive analysis and manipulation capabilities for transactions and associations (subsetting, sampling, visual inspection, etc.).
- arulesViz provides visualizations.


## Simple Example

```
R> library("arules")
R> data("Groceries")
R> Groceries
transactions in sparse format with
    9835 transactions (rows) and
    169 items (columns)
R> rules <- apriori(Groceries, parameter = list(support = .001))
apriori - find association rules with the apriori algorithm
version 4.21 (2004.05.09) (c) 1996-2004 Christian Borgelt
set item appearances ...[0 item(s)] done [0.00s].
set transactions ...[169 item(s), 9835 transaction(s)] done [0.01s].
sorting and recoding items ... [157 item(s)] done [0.00s].
creating transaction tree ... done [0.01s].
checking subsets of size 1 2 3 4 5 6 done [0.05s].
writing ... [410 rule(s)] done [0.00s].
creating S4 object ... done [0.00s].
```


## Simple Example

```
R> rules
set of 410 rules
R> inspect(head(sort(rules, by = "lift"), 3))
    lhs rhs support confidence lift
1 {liquor,
    red/blush wine} => {bottled beer} 0.001931876 0.9047619 11.23527
2 {citrus fruit,
    other vegetables,
    soda,
    fruit} => {root vegetables} 0.001016777 0.9090909 8.34040
3 {tropical fruit,
    other vegetables,
    whole milk,
    yogurt,
    oil} => {root vegetables} 0.001016777 0.9090909 8.34040
```


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