COMP5310: Principles of Data Science

W7: Association Rule Mining

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Based on slides by previous lecturers of this unit of study

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Last week: Hypothesis testing and evaluation

Objective

- Overview of experimental design and learn Python tools for hypothesis testing and classifier evaluation.

Lecture

- **Significance**
  - Pairwise t-tests.
  - Non-normal data.
- **Evaluation**
  - Classifier evaluation.
  - User evaluation.

Readings

- Data Science from Scratch: Ch 7.
- Model evaluation (sklearn doco).
  - http://scikit-learn.org/stable/modules/model_evaluation.html#model-evaluation
- Hypothesis testing (scipy lectures).
  - http://www.scipy-lectures.org/packages/statistics/index.html#hypothesis- testing-comparing-two-groups

Exercises

- Scipy: statistical tests.
- Sklearn: evaluation metrics.

Machine Learning

What is machine learning?

- Creating and using models that are learned from data
  - Predicting whether an email is spam or not
  - Discovering hidden rules in complex datasets
  - Predicting whether a credit card transaction is fraudulent
  - Predicting tumour cells as benign or malignant

Machine Learning Problems

- Prediction
  - Classification and Regression
- Clustering, segmentation and association rules
  - Find patterns in the data
- Outlier/anomaly detection
  - Find unusual patterns
- Reinforcement learning
  - Learn from rewards (like babies)

Supervised vs. Unsupervised Learning

- Supervised learning (e.g. classification and regression)
  - Supervision: The training data are accompanied by **labels** indicating the class of the observations
- Unsupervised learning (e.g. clustering and association rules)
  - The class labels of training data is **unknown**
  - Given a set of measurements, observations, etc. with the aim of
    - Establishing the existence of classes or clusters in the data
    - Discovering hidden patterns or rules

Unsupervised Learning

- We'll focus on unsupervised machine learning techniques
  - ***Association rule mining***
  - Clustering
  - Dimensionality reduction
  - Outlier detection
  - Etc.

Association Rule Mining

Association Analysis

TID	Items
1	Bread, Milk
2	Bread, Diaper, Beer, Eggs
3	Milk, Diaper, Beer, Coke
4	Bread, Milk, Diaper, Beer
5	Bread, Milk, Diaper, Coke

Market-basket transactions

TID: Transaction Identifier

Items: Transaction item set

How can businesses improve sales by analysing customer purchase data?

Slides adapted from Tan et al. Introduction to data mining.
http://www-users.cs.umn.edu/~kumar/dmbook/
http://www-users.cs.umn.edu/~kumar/dmbook/dmslides/chap6_basic_association_analysis.pdf

Association Rule Mining

TID	Items
1	Bread, Milk
2	Bread, Diaper, Beer, Eggs
3	Milk, Diaper, Beer, Coke
4	Bread, Milk, Diaper, Beer
5	Bread, Milk, Diaper, Coke

Market-basket transactions

TID: Transaction Identifier

Items: Transaction item set

– Predict occurrence of an item based on other items in the transaction, eg:

```
{Diaper} → {Beer}
{Milk,Bread} → {Eggs,Coke}
{Beer,Bread} → {Milk}
```

– Note that arrows indicate co-occurrence, not causality

Definition: Itemset

TID	Items
1	Bread, Milk
2	Bread, Diaper, Beer, Eggs
3	Milk, Diaper, Beer, Coke
4	Bread, Milk, Diaper, Beer
5	Bread, Milk, Diaper, Coke

Market-basket transactions

TID: Transaction Identifier

Items: Transaction item set

– An **itemset** is a collection of one or more items
  `{Milk,Bread,Diaper}`

– A **k-itemset** is an itemset containing k items

Definition: Frequent Itemset

TID	Items
1	Bread, Milk
2	Bread, Diaper, Beer, Eggs
3	Milk, Diaper, Beer, Coke
4	Bread, Milk, Diaper, Beer
5	Bread, Milk, Diaper, Coke

Market-basket transactions

TID: Transaction Identifier

Items: Transaction item set

- **Support count** (σ) is the itemset frequency

  $\sigma(\{\text{Milk}, \text{Diaper}, \text{Beer}\}) = 2$

- **Support** (s) is the normalised itemset frequency

  $$s = \frac{\sigma(\{\text{Milk}, \text{Diaper}, \text{Beer}\})}{|T|} = \frac{2}{5}$$

- A **frequent itemset** has $s \geq min\_support$

Definition: Association Rule

TID	Items
1	Bread, Milk
2	Bread, Diaper, Beer, Eggs
3	Milk, Diaper, Beer, Coke
4	Bread, Milk, Diaper, Beer
5	Bread, Milk, Diaper, Coke

Market-basket transactions

TID: Transaction Identifier

Items: Transaction item set

- An **association rule** is an implication of the form X→Y where X and Y are itemsets
  `{Milk,Diaper}→{Beer}`
- **Confidence** (c) measures how often Y occurs in transactions with X

$$c = \frac{\sigma(\{\text{Milk,Diaper,Beer}\})}{\sigma(\{\text{Milk,Diaper}\})} = \frac{2}{3}$$

- An **association rule** has c ≥ min_conf

Association Rule Mining Task

- Given a set of transactions T, the goal of association rule mining is to find all rules having
  - support ≥ *min_sup* threshold
  - confidence ≥ *min_conf* threshold

Finding Frequent Itemsets

TID	Items
1	Bread, Milk
2	Bread, Diaper, Beer, Eggs
3	Milk, Diaper, Beer, Coke
4	Bread, Milk, Diaper, Beer
5	Bread, Milk, Diaper, Coke

Market-basket transactions

TID: Transaction Identifier

Items: Transaction item set

Support {Bread → Milk}

- Let *min_support* = *50%*
- Freq. 1-itemsets:
  - Bread:4(80%); Milk:4(80%); Diaper:4(80%); Beer:3(60%);
- Freq. 2-itemsets:
  - {Bread, Milk}:3(60%)
    {Bread, Diaper}:3(60%)
    {Milk, Diaper}:3(60%)
    {Diaper, Beer}:3(60%)

Finding Association Rules

TID	Items
1	Bread, Milk
2	Bread, Diaper, Beer, Eggs
3	Milk, Diaper, Beer, Coke
4	Bread, Milk, Diaper, Beer
5	Bread, Milk, Diaper, Coke

Market-basket transactions

TID: Transaction Identifier

Items: Transaction item set

- Let *min_support* = 50%, min_conf = 50%
- Freq. Itemsets:
  - Bread:4; Milk:4; Diaper:4; Beer:3; {Bread, Milk}:3; {Bread, Diaper}:3; {Milk, Diaper}:3; {Diaper, Beer}:3;
- Association rules:
  - Beer → Diaper (100%)
  - Diaper → Beer (75%)
  - …

c(Beer → Diaper) = 3/3

3/4

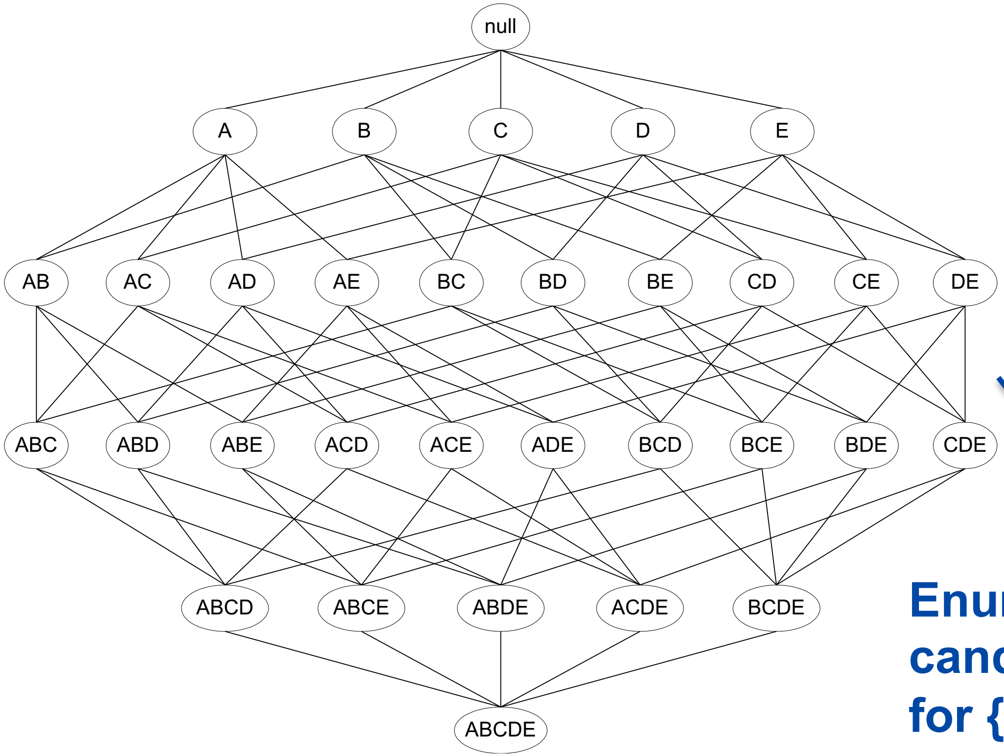
Association Rule Mining with Apriori Principle

Two-step approach

1. **Frequent itemset generation**
   - Generate all itemsets with $s \geq min\_support$
2. **Rule generation**
   - Generate high-confidence rules from each frequent itemset
   - Each rule is a binary partitioning of a frequent itemset

Easy! But brute force enumeration is computationally prohibitive.

There are 2^d candidate itemsets!



Enumeration of 2^5-1 candidate itemsets for {A,B,C,D,E}

Reducing the number of candidates

- **Apriori Principle**
  If an itemset is frequent, then all of its subsets must also be frequent

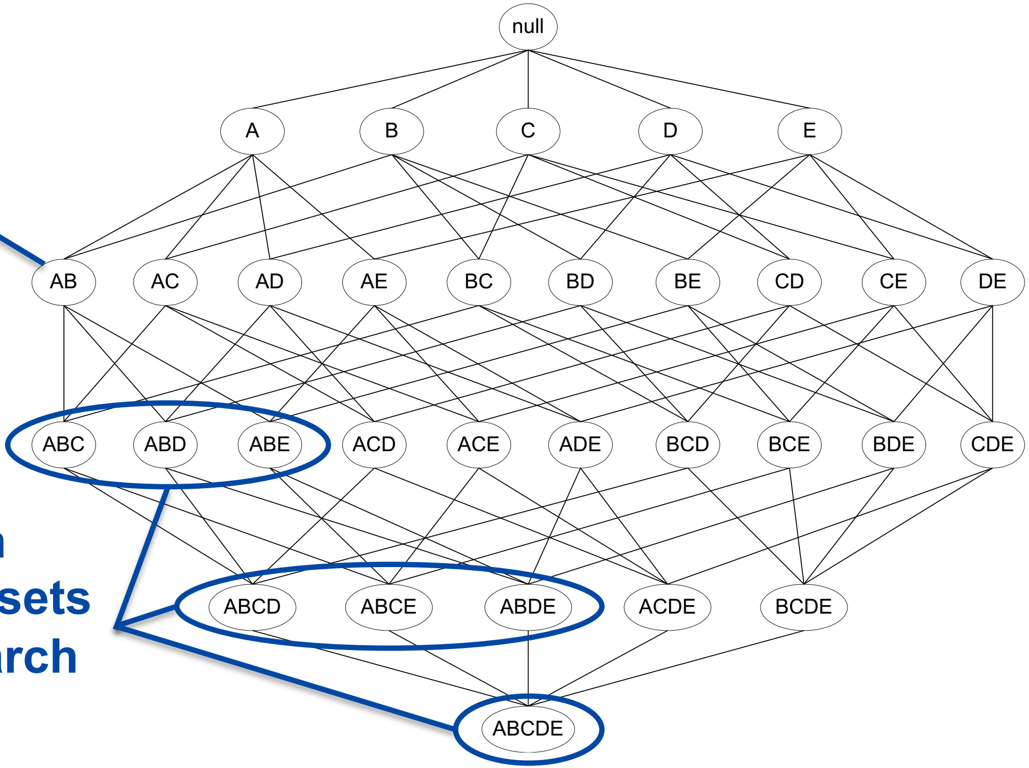
  ?

- **Conversely**
  ?
  If an itemset is infrequent, then its supersets are also infrequent
  - The support of an itemset never exceeds the support of its subsets
    - s({Bread}) $\geq$ s({Bread, Beer})
    - s({Milk}) $\geq$ s({Bread, Milk})
  - This is known as the anti-monotone property of support

Pruning the 2^d candidate itemsets

If *s({A,B})* < *min_support*

Then we can prune supersets from the search space



Apriori algorithm for generating frequent itemsets

While the list of (k-1)-itemsets is non-empty:

  Generate candidate k-itemsets

  Identify and keep frequent k-itemsets

The Apriori Algorithm—An Example

Min_sup = 2

Database TDB

Tid	Items
1	A, C, D
2	B, C, E
3	A, B, C, E
4	B, E

1st scan

C_1

Itemset	sup
{A}	2
{B}	3
{C}	3
{D}	1
{E}	3

L_1

Itemset	sup
{A}	2
{B}	3
{C}	3
{E}	3

C_2

Itemset
{A, B}
{A, C}
{A, E}
{B, C}
{B, E}
{C, E}

2nd scan

C_2

Itemset	sup
{A, B}	1
{A, C}	2
{A, E}	1
{B, C}	2
{B, E}	3
{C, E}	2

L_2

Itemset	sup
{A, C}	2
{B, C}	2
{B, E}	3
{C, E}	2

C_3

Itemset	sup
{B, C, E}	2

L_3

Itemset	sup
{B, C, E}	2

Create initial 1-itemsets

Add each item to the initial list of candidate itemsets

```
def createC1(dataset):
    "Create a list of candidate item sets of size one."
    c1 = []
    for transaction in dataset:
        for item in transaction:
            if not [item] in c1:
                c1.append([item])
    c1.sort()
    #frozenset because it will be a key of a dictionary.
    return list(map(frozenset, c1))
```

Sort and return as list of sets

Identify itemsets that meet the support threshold

```
def scanD(dataset, candidates, min_support):
    "Returns all candidates that meet a minimum support level"
    sscnt = {}
    for tid in dataset:
        for can in candidates:
            if can.issubset(tid):
                sscnt.setdefault(can, 0)
                sscnt[can] += 1

    num_items = float(len(dataset))
    retlist = []
    support_data = {}
    for key in sscnt:
        support = sscnt[key] / num_items
        if support >= min_support:
            retlist.append(key)
            support_data[key] = support
    return retlist, support_data
```

Calculate support counts for each candidate

Check whether candidates meet threshold

Generate the next list of candidates

(k-1)-itemsets

Iterate through all pairs of itemsets

Check whether pairs differ by a single item

A|B returns the union of A and B

```python
def aprioriGen(freq_sets, k):
    "Generate the joint transactions from candidate sets"
    retList = []
    lenLk = len(freq_sets)
    for i in range(lenLk):
        for j in range(i + 1, lenLk):
            L1 = list(freq_sets[i])[:k - 2]
            L2 = list(freq_sets[j])[:k - 2]
            L1.sort()
            L2.sort()
            if L1 == L2:
                retList.append(freq_sets[i] | freq_sets[j]) # | is set union
    return retList
```

Generate all Frequent Itemsets

```python
def apriori(dataset, min_support=0.5):
    "Generate a list of candidate item sets"
    C1 = createC1(dataset)
    D = list(map(set, dataset))
    L1, support_data = scanD(D, C1, min_support)
    L = [L1]
    k = 2
    while len(L[k - 2]) > 0:
        Ck = aprioriGen(L[k - 2], k)
        Lk, supK = scanD(D, Ck, min_support)
        support_data.update(supK)
        L.append(Lk)
        k += 1

    return L, support_data
```

Initialise L with frequent 1-itemsets

While the list of (k-1)-itemsets is non-empty:

Generate candidate k-itemsets

Identify frequent k-itemsets

Keep frequent k-itemsets

Rule Generation

- Given a frequent itemset **L**, find all non-empty subsets $\mathbf{x} \subset \mathbf{L}$ such that $\mathbf{x} \rightarrow \mathbf{L} - \mathbf{x}$ satisfies the minimum confidence requirement
  - If {A,B,C,D} is a frequent itemset, candidate rules are:

    A →BCD, B →ACD, C →ABD, D →ABC,

    AB →CD, AC → BD, AD → BC, BC →AD, BD →AC, CD →AB,

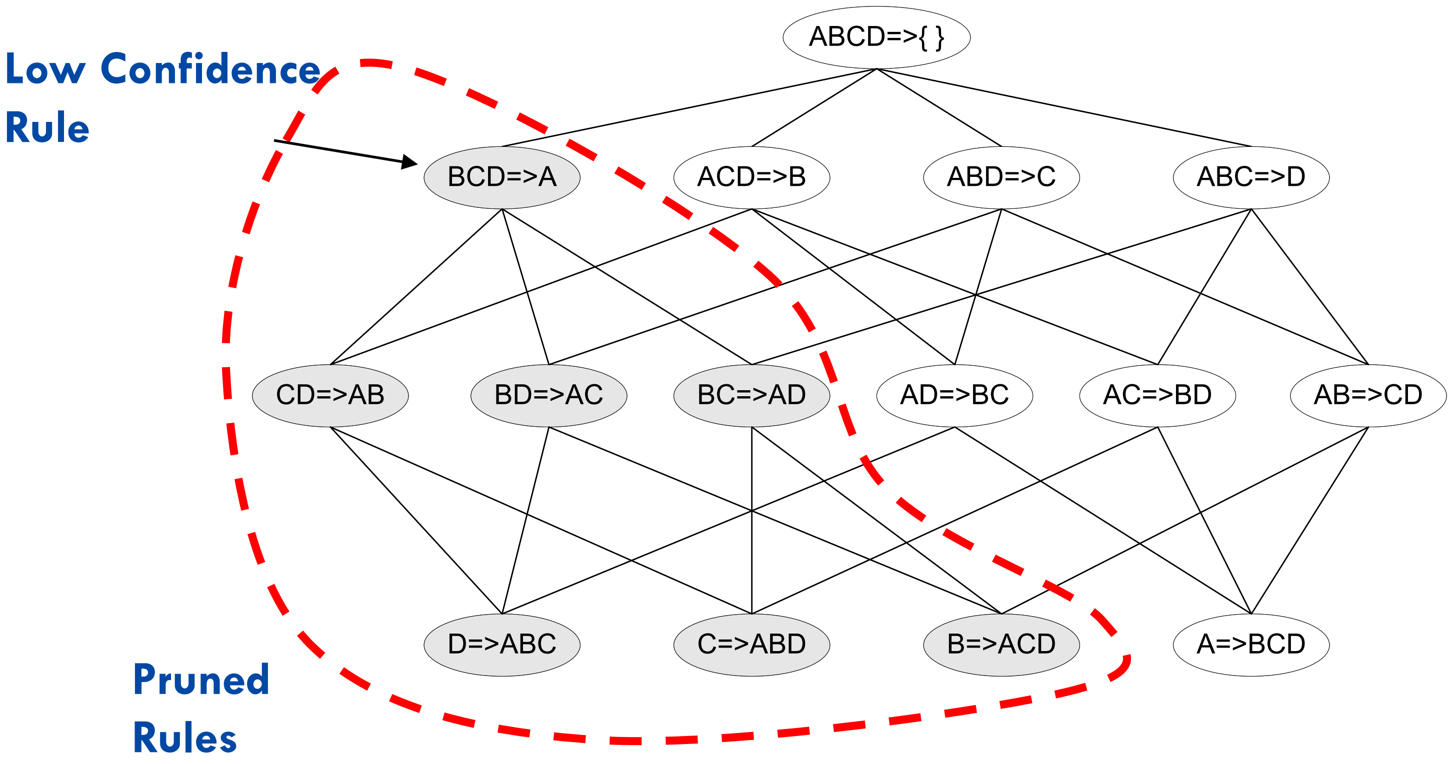
    ABC →D, ABD →C, ACD →B, BCD →A,

- If $|L| = k$, then there are $2^k - 2$ candidate association rules

Efficient Rule generation

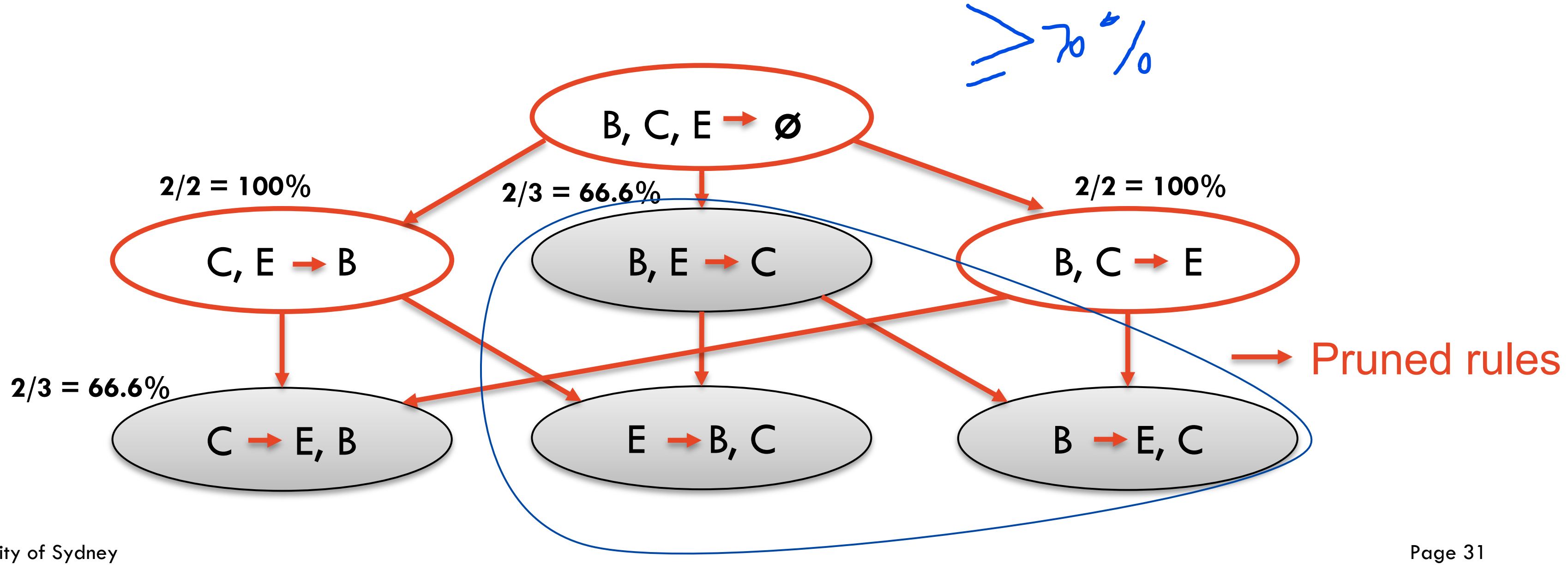
- How to efficiently generate rules from frequent an itemset?
- Similar to support, the confidence of rules generated from the same itemset has an anti-monotone property
- Example: $X = \{A,B,C,D\}$:
  - $c(ABC \rightarrow D) \geq c(AB \rightarrow CD) \geq c(A \rightarrow BCD)$
- Confidence is anti-monotone w.r.t. number of items on the RHS of the rule

Rule Generation for Apriori Algorithm



Association Rule

- From the example before, we had a frequent itemset: {B, C, E}
- From this frequent itemset {B, C, E}, we can have the following association rules



Identify rules that meet the confidence threshold

Frequent itemset (rule components)

Possible consequences (RHS of rule)

Rule accumulator

```
def calc_confidence(freqSet, H, support_data, rules, min_confidence=0.7):
    "Evaluate the rule generated"
    pruned_H = []
    for conseq in H:
        conf = support_data[freqSet] / support_data[freqSet - conseq]
        if conf >= min_confidence:
            #print(freqSet - conseq, '--->', conseq, 'conf:', conf)
            rules.append((freqSet - conseq, conseq, conf))
            pruned_H.append(conseq)
    return pruned_H
```

Calculate confidence

Add rule to accumulator if *conf* ≥ *min_confidence*

Return consequences that pass the confidence threshold

Recursively Evaluate Rules

Need at least 1 item for LHS

Generate candidate consequence itemsets

Update rules and return consequences that pass confidence threshold

```python
def rules_from_conseq(freqSet, H, support_data, rules, min_confidence=0.7):
    "Generate a set of candidate rules"
    m = len(H[0])
    pruned_H = calc_confidence(freqSet, H, support_data, rules, min_confidence)
    if len(freqSet) > (m + 1):
        Hmp = aprioriGen(pruned_H, m + 1)
        if len(Hmp) >= 1:
            rules_from_conseq(freqSet, Hmp, support_data, rules, min_confidence)
```

Recurse with new consequence candidates

Mine all Association Rules

For each k
For each k-itemset

```
def generateRules(L, support_data, min_confidence=0.7):
    """Create the association rules
    L: list of frequent itemsets
    support_data: support data for those itemsets
    min_confidence: minimum confidence threshold
    """
    rules = []
    for i in range(1, len(L)):
        for freqSet in L[i]:
            H1 = [frozenset([item]) for item in freqSet]
            rules_from_conseq(freqSet, H1, support_data, rules, min_confidence)
    return rules
```

Initial consequence candidates

Recursively evaluate rules

Association Rule Mining with FP-Growth

Performance Bottlenecks of Apriori

- Bottlenecks of *Apriori*:
  - Candidate generation:
    - Generate huge candidate sets
  - Multiple scans of database

Overview of FP-Growth:

- Compress a large database into a compact, *Frequent-Pattern tree* (FP-tree) structure
  - Highly compacted, but complete for frequent pattern mining
  - Avoid costly repeated database scans
- Develop an efficient, FP-tree-based frequent pattern mining method (FP-growth)
  - A divide-and-conquer methodology: decompose mining tasks into smaller ones
  - Avoid candidate generation

Construct FP-tree

Two Steps:

1. Scan the transaction DB for the first time, find frequent items (single item patterns) and order them into a list L in frequency descending order.

2. For each transaction, order its frequent items according to the order in L; Scan DB the second time, construct FP-tree by putting each frequency ordered transaction onto it.

FP-tree Example: step 1

Step 1: Scan DB for the first time to generate L

Min_sup = 2

TID	Items bought
1	*A, C, D*
2	*B, C, E*
3	*A, B, C, E*
4	*B, E*

Item	Frequency
A	2
B	3
C	3
D	1
E	3

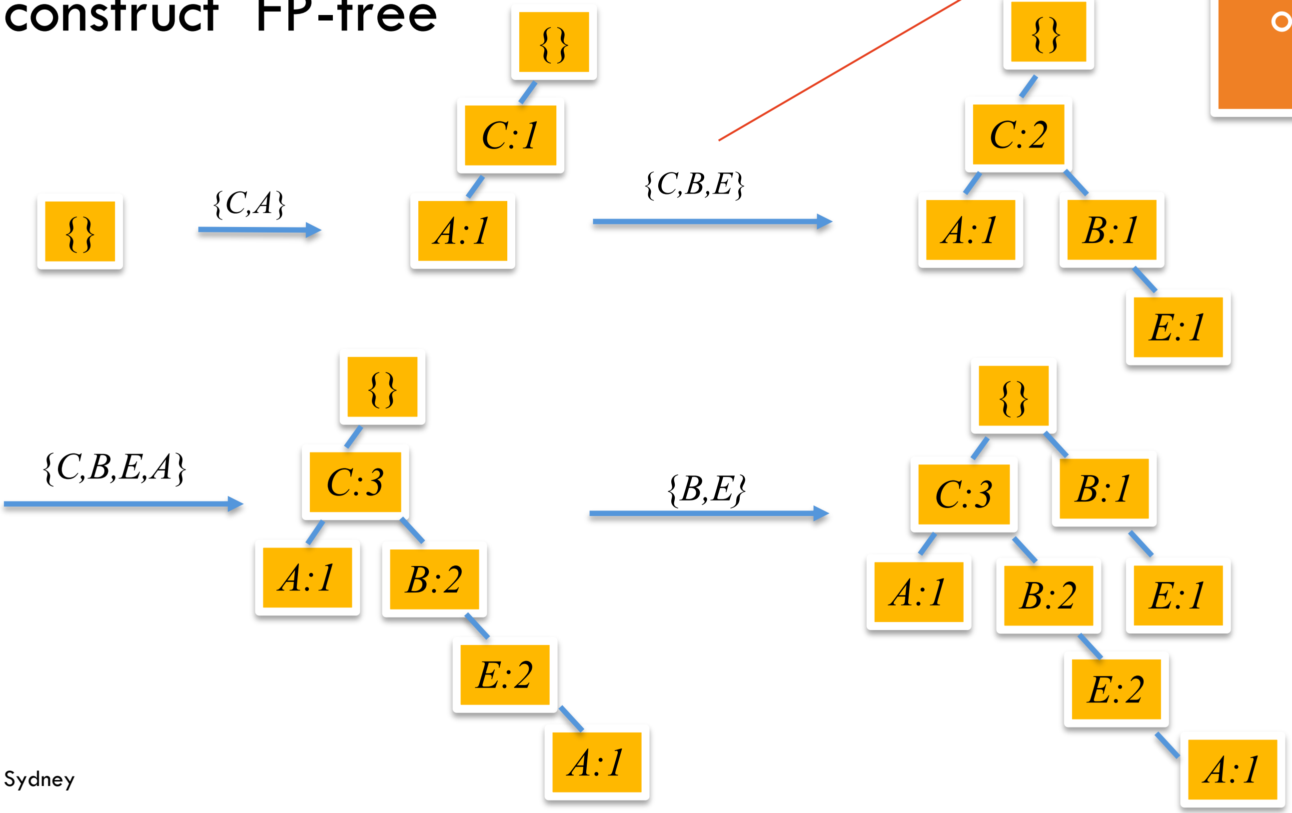
FP-tree Example: step 2

Step 2: scan the DB for the second time, order frequent items in each transaction

TID	Items bought	Ordered frequent items
1	A, C, D	C, A
2	B, C, E	C, B, E
3	A, B, C, E	C, B, E, A
4	B, E	B, E

FP-tree Example: step 2

Step 2: construct FP-tree



NOTE: Each transaction corresponds to one path in the FP-tree

Mining Frequent Patterns Using FP-tree

Starting the processing from the end of list L:

Step 1:

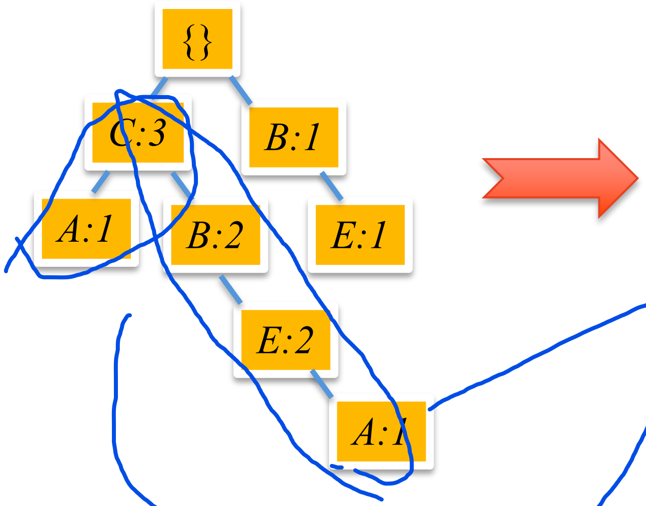
Construct **conditional pattern base** for each item in L

Step 2:

Construct **conditional FP-tree** from each conditional pattern base

Step 1: Construct Conditional Pattern Base

- Traverse the FP-tree by following the link of each frequent item
- Accumulate all of **transformed prefix paths** of that item to form a **conditional pattern base**



***Conditional* pattern bases**

item	cond. pattern base
A	EBC:1, C:1
E	BC:2, B:1
B	C:2
C	{}

Step 2: Construct Conditional FP-tree

- For each pattern base
  - Accumulate the count for each item in the base
  - Construct the conditional FP-tree for the frequent items of the pattern base

***A**-cond.* **pattern base:**		***A**-conditional* **FP-tree**	**Frequent patterns ending with *A*:**
EBC:1, C:1	→	**{ (C:2) } | A**	**CA:2**

Step 2: Construct Conditional FP-tree

E-*cond.* **pattern base:**

BC:2, B:1

→

E-*conditional* **FP-tree**

{ (B:3, C:2, BC:2) } | E

Frequent patterns ending with *E*:

BE:3, CE:2, BCE:2

B-*cond.* **pattern base:**

C:2

→

B-*conditional* **FP-tree**

{ (C:2) } | B

Frequent patterns ending with *B*:

CB:2

All Frequent Itemsets: { A:2, E:3, B:3, C:3, BC:2, EC:2, AC:2, EB:3, BCE:2 }

Review

W7 review: Association Rule Mining

Objective

Learn techniques for unsupervised learning, with tools in Python.

Lecture

- Association rule mining

Readings

- Intro to Data Mining, Ch. 5
  https://www-users.cse.umn.edu/~kumar001/dmbook/ch5_association_analysis.pdf
- Data Science from Scratch, Ch. 11

Exercises

- Associations from scratch
- Associations using mlxtend
- Associations using pyfpgrowth