# Contrast Data Mining: Methods and Applications

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### Contrast data mining - What is it ?

**Contrast** - ``To compare or appraise in respect to differences'' (Merriam Webster Dictionary)

**Contrast data mining** - The mining of patterns and models contrasting two or more classes/conditions.

# Contrast Data Mining - What is it ?

"Sometimes it's good to contrast what you like with something else. It makes you appreciate it even more" Darby Conley, Get Fuzzy, 2001

### What can be contrasted ?

- Objects at different time periods
  - ``Compare ICDM papers published in 2006-2007 versus those in 2004-2005''

#### Objects for different *spatial* locations

Find the distinguishing features of location x for human DNA, versus location x for mouse DNA"

#### Objects across different classes

Find the differences between people with brown hair, versus those with blonde hair"

# What can be contrasted ? Cont.

- Objects within a class
  - ``Within the academic profession, there are few people older than 80'' (*rarity*)
  - ``Within the academic profession, there are no rich people'' (*holes*)
  - ``Within computer science, most of the papers come from USA or Europe'' (*abundance*)
- Object positions in a *ranking*
  - Find the differences between high and low income earners"
- Combinations of the above

# Alternative names for contrast data mining

- Contrast={change, difference, discriminator, classification rule, ...}
- Contrast data mining is related to topics such as:

Change detection, class based association rules, contrast sets, concept drift, difference detection, discriminative patterns, (dis)similarity index, emerging patterns, high confidence patterns, (in)frequent patterns, top k patterns,.....

# Characteristics of contrast data mining

- Applied to multivariate data
- Objects may be relational, sequential, graphs, models, classifiers, combinations of these
- Users may want either
  - To find *multiple* contrasts (*all*, or top *k*)
  - A *single* measure for comparison
    - ``The degree of difference between the groups (or models) is 0.7"

## Contrast characteristics Cont.

- Representation of contrasts is important. Needs to be
  - Interpretable, non redundant, potentially actionable, expressive
  - Tractable to compute
- Quality of contrasts is also important. Need
  - Statistical significance, which can be measured in multiple ways
  - Ability to rank contrasts is desirable, especially for classification

# How is contrast data mining used ?

- Domain understanding
  - ``Young children with diabetes have a greater risk of hospital admission, compared to the rest of the population
- Used for building *classifiers* 
  - Many different techniques to be covered later
  - Also used for weighting and ranking instances
- Used in construction of synthetic instances
  - Good for rare classes
- Used for alerting, notification and monitoring
  - ``Tell me when the dissimilarity index falls below 0.3''

# Goals of this tutorial

- Provide an overview of contrast data mining
- Bring together results from a number of disparate areas.
  - Mining for different types of data
    - Relational, sequence, graph, models, ...
  - Classification using discriminating patterns

# By the end of this tutorial you will be able to ...

- Understand some principal techniques for representing contrasts and evaluating their quality
- Appreciate some mining techniques for contrast discovery
- Understand techniques for using contrasts in classification

# Don't have time to cover ...

String algorithms

. . .

- Connections to work in inductive logic programming
- Tree-based contrasts
- Changes in data streams
- Frequent pattern algorithms
- Connections to granular computing

# Outline of the tutorial

- Basic notions/univariate contrasts
- Pattern and rule based contrasts
- Contrast pattern based classification
- Contrasts for rare class datasets
- Data cube contrasts
- Sequence based contrasts
- Graph based contrasts
- Model based contrasts
- Common themes + open problems + summary

## Basic notions and univariate case

- Feature selection and feature significance tests can be thought of as a basic contrast data mining activity.
  - ``Tell me the discriminating features"
    - Would like a single quality measure
    - Useful for feature ranking
  - Emphasis is less on *finding* the contrast and more on *evaluating* its power

# Sample Feature-Class

ID	Height (cm)	Class
9004	150	Happy 🙂
1005	200	Sad 🙁
9006	137	Happy 🙂
4327	120	Happy 🙂
3325		••••

# Discriminative power

- Can assess discriminative power of *Height* feature by
  - Information measures (signal to noise, information gain ratio, ...)
  - Statistical tests (t-test, Kolmogorov-Smirnov, Chi squared, Wilcoxon rank sum, ...). Assessing whether
    - The mean of each class is the same
    - The samples for each class come from the same distribution
    - How well a dataset fits a hypothesis

#### No single test is best in all situations !

# Example Discriminative Power Test - Wilcoxon Rank Sum

- Suppose n<sub>1</sub> happy, and n<sub>2</sub> sad instances
- Sort the instances according to height value:

 $h_1 <= h_2 <= h_3 <= \dots h_{n_1+n_2}$ 

- Assign a rank to each instance, indicating how many values in the other class are less than it
- For each class
  - Compute the S=Sum(ranks of all its instances)
  - Null Hypothesis: The instances are from the same distribution
  - Consult statistical significance table to determine whether value of S is significant

# Rank Sum Calculation Example

ID	Height(cm)	Class	Rank
324	220	Happy 🙄	3
481	210	Sad 😕	2
660	190	Sad 😕	2
321	177	Happy 😊	1
415	150	Sad 😕	1
816	120	Happy 🙂	0

Happy: RankSum=3+1+0=4 Sad:RankSum=2+2+1=5

# Wilcoxon Rank Sum TestCont.

#### This test

- Non parametric (no normal distribution assumption)
- Requires an ordering on the attribute values
- Value of S is also equivalent to area under ROC curve for using the selected feature as a classifier

# Discriminating with attribute values

- Can alternatively focus on significance of attribute values, with either
  - 1) *Frequency/infrequency* (high/low counts)
    - Frequent in one class and infrequent in the other.
      - There are 50 happy people of height 200cm and only two sad people of height 200cm
  - 2) Ratio (high ratio of support)
    - Appears 25 times more in one class than the other assuming equal class sizes
      - There are 25 times more happy people of height 200cm than sad people

# Attribute/Feature Conversion

- Possible to form a new binary feature based on attribute value and then apply feature significance tests
  - Blur distinction between attribute and attribute value

150cm	200cm	•••	Class
Yes	No		Нарру 🙂
No	Yes	•••	Sad 😕

# Discriminating Attribute Values in a Data Stream

- Detecting changes in attribute values is an important focus in data streams
  - Often focus on univariate contrasts for efficiency reasons
  - Finding when change occurs (non stationary stream).
  - Finding the magnitude of the change. E.g. How big is the distance between two samples of the stream?
  - Useful for signaling necessity for model update or an impending fault or critical event

# Odds ratio and Risk ratio

- Can be used for comparing or measuring effect size
- Useful for binary data
- Well known in clinical contexts
- Can also be used for quality evaluation of multivariate contrasts (will see later)
- A simple example given next

# Odds and risk ratio Cont.

Gender (feature)	Exposed (event)
Male	Yes
Female	No
Male	No
	• • •

## Odds Ratio Example

- Suppose we have 100 men and 100 women and 70 men and 10 women have been exposed
  - Odds of exposure(male)=0.7/0.3=2.33
  - Odds of exposure(female)=0.1/0.9=0.11
  - Odds ratio=2.33/.11=21.2
- Males have 21.2 times the odds of exposure than females
- Indicates exposure is much more likely for males than for females

# **Relative Risk Example**

- Suppose we have 100 men and 100 women and 70 men and 10 women have been exposed
  - Relative risk of exposure (male)=70/100=0.7
  - Relative risk of exposure(female)=10/100=0.1
  - The relative risk=0.7/0.1=7
- Men 7 times more likely to be exposed than women

# Pattern/Rule Based Contrasts

- Overview of ``relational'' contrast pattern mining
- Emerging patterns and mining
  - Jumping emerging patterns
  - Computational complexity
  - Border differential algorithm
    - Gene club + border differential
    - Incremental mining
  - Tree based algorithm
  - Projection based algorithm
  - ZBDD based algorithm
- Bioinformatic application: cancer study on microarray gene expression data

# Overview

- Class based association rules (Cai et al 90, Liu et al 98, ...)
- Version spaces (Mitchell 77)
- Emerging patterns (Dong+Li 99) many algorithms (later)
- Contrast set mining (Bay+Pazzani 99, Webb et al 03)
- Odds ratio rules & delta discriminative EP (Li et al 05, Li et al 07)
- MDL based contrast (Siebes, KDD07)
- Using statistical measures to evaluate group differences (Hilderman+Peckman 05)
- Spatial contrast patterns (Arunasalam et al 05)
- ..... see references

# **Classification/Association Rules**

- Classification rules -- special association rules (with just one item – class -- on RHS):
  - $X \rightarrow C$  (s,c)
    - X is a pattern,
    - C is a class,
    - s is support,
    - c is confidence

# Version Space (Mitchell)

- Version space: the set of all patterns consistent with given (D+,D-) – patterns separating D+, D-.
  - The space is delimited by a *specific* & a *general boundary*.
  - Useful for searching the true hypothesis, which lies somewhere b/w the two boundaries.
  - Adding +ve examples to D+ makes the specific boundary more general; adding -ve examples to D- makes the general boundary more specific.
- Common pattern/hypothesis language operators: conjunction, disjunction
- Patterns/hypotheses are crisp; need to be generalized to deal with percentages; hard to deal with noise in data

# STUCCO, MAGNUM OPUS for contrast pattern mining

- STUCCO (Bay+Pazzani 99)
  - Mining contrast patterns X (called contrast sets) between k>=2 groups: |suppi(X) – suppj(X)| >= minDiff
  - Use Chi2 to measure statistical significance of contrast patterns
    - cut-off thresholds change, based on the level of the node and the local number of contrast patterns
  - Max-Miner like search strategy, plus some pruning techniques
- MAGNUM OPUS (Webb 01)
  - An association rule mining method, using Max-Miner like approach (proposed before, and independently of, Max-Miner)
  - Can mine contrast patterns (by limiting RHS to a class)

# Contrast patterns vs decision tree based rules

- It has been recognized by several authors (e.g. Bay+Pazzani 99) that
  - rules generation from decision trees can be good contrast patterns,
  - but may miss many good contrast patterns.
  - Random forests can address this problem
- Different contrast set mining algorithms have different thresholds
  - Some have min support threshold
  - Some have no min support threshold; low support patterns may be useful for classification, etc

# **Emerging Patterns**

Emerging Patterns (EPs) are contrast patterns between two classes of data whose support changes significantly between the two classes. Change significantly can be defined by:

similar to Relative Risk;

- big support ratio:
  supp2(X)/supp1(X) >= minRatio
- +: allowing patterns with small overall support

- big support difference:
  - |supp2(X) supp1(X)| >= minDiff (as defined by Bay+Pazzani 99)
- If supp2(X)/supp1(X) = infinity, then X is a *jumping EP*.
  - jumping EP occurs in some members of one class but never occur in the other class.
- Conjunctive language; extension to disjunctive EP later

### A typical EP in the Mushroom dataset

- The Mushroom dataset contains two classes: edible and poisonous.
- Each data tuple has several features such as: odor, ring-number, stalk-surface-bellow-ring, etc.
- Consider the pattern

{odor = none,

```
stalk-surface-below-ring = smooth,
```

ring-number = one}

Its support increases from 0.2% in the poisonous class to 57.6% in the edible class (a growth rate of 288).

#### Example EP in microarray data for cancer



Jumping EP: Patterns w/ high support ratio b/w data classes E.G. {g1=L,g2=H,g3=L}; suppN=50%, suppC=0

# Top support *minimal* jumping EPs for colon cancer

#### Colon Normal EPs

{12-21-35+40+137+254+} 100% Colon Cancer EPs {12-35+40+71-137+254+} 100% {1+ 4- 112+ 113+} 100% {20-21-35+137+254+}100% {1+ 4- 113+ 116+} 100% {20-35+71-137+254+} 100% {1+ 4- 113+ 221+} 100% {5-35+137+177+}95.5% {1+ 4- 113+ 696+} 100% {5-35+137+254+}95.5% {1+ 108- 112+ 113+} 100% 5- 35+ 137+ 419-} 95.5% {1+ 108- 113+ 116+} 100<sup>6</sup>/<sub>5</sub>- 137+ 177+ 309+} 95.5% {4- 108- 112+ 113+} 100%{5- 137+ 254+ 309+} 95.5% {4- 109+ 113+ 700+} 100%{7- 21- 33+ 35+ 69+} 95.5% {4-110+112+113+} 100%{7-21-33+69+309+} 95.5% {4- 112+ 113+ 700+} 100%{7- 21- 33+ 69+ 1261+} 95.5% {4- 113+ 117+ 700+} 100%

These EPs have 95%--100% support in one class but 0% support in the other class.

Minimal: Each proper subset occurs in both classes.

EPs from Mao+Dong 2005 (gene club + border-diff).

{1+ 6+ 8- 700+} 97.5%

Very few 100% support EPs.

Colon cancer dataset (Alon et al, 1999 (PNAS)): 40 cancer tissues, 22 normal tissues. 2000 genes
## A potential use of minimal jumping EPs

- Minimal jumping EPs for <u>normal</u> tissues
  - ➔ Properly expressed gene groups important for normal cell functioning, but destroyed in all colon cancer tissues
  - → <u>Restore</u> these → ?cure colon cancer?
- Minimal jumping EPs for <u>cancer</u> tissues
  - ➔ Bad gene groups that occur in some cancer tissues but never occur in normal tissues
  - → <u>Disrupt</u> these → ?cure colon cancer?
- Possible targets for drug design ?

Li+Wong 2002 proposed "gene therapy using EP" idea: therapy aims to destroy bad JEP & restore good JEP

## Usefulness of Emerging Patterns

- EPs are useful
  - for building highly accurate and robust classifiers, and for improving other types of classifiers
  - for discovering powerful distinguishing features between datasets.
- Like other patterns composed of conjunctive combination of elements, EPs are easy for people to understand and use directly.
- EPs can also capture patterns about change over time.
- Papers using EP techniques in Cancer Cell (cover, 3/02).
- Emerging Patterns have been applied in medical applications for diagnosing acute Lymphoblastic Leukemia.

## The landscape of EPs on the support plane, and challenges for mining



## Challenges for EP mining

- EP minRatio constraint is neither monotonic nor antimonotonic (but exceptions exist for special cases)
- Requires smaller support thresholds than those used for frequent pattern mining

## Odds Ratio and Relative Risk Patterns [Li and Wong PODS06]

- May use odds ratio/relative risk to evaluate compound factors as well
  - May be no single factor with high relative risk or odds ratio, but a combination of factors
    - Relative risk patterns Similar to emerging patterns
    - Risk difference patterns Similar to contrast sets
    - Odds ratio patterns

## Mining Patterns with High Odds Ratio or Relative Risk

- Space of odds ratio patterns and relative risk patterns are not convex in general
- Can become convex, if stratified into plateaus, based on support levels

## **EP** Mining Algorithms

- Complexity result (Wang et al 05)
- Border-differential algorithm (Dong+Li 99)
- Gene club + border differential (Mao+Dong 05)
- Constraint-based approach (Zhang et al 00)
- Tree-based approach (Bailey et al 02, Fan+Ramamohanarao 02)
- Projection based algorithm (Bailey el al 03)
- ZBDD based method (Loekito+Bailey 06).

## Complexity result

- The complexity of finding emerging patterns (even those with the highest frequency) is MAX SNP-hard.
  - This implies that polynomial time approximation schemes do not exist for the problem unless P=NP.

## Borders are concise representations of convex collections of itemsets

< minB={12,13}, maxB={12345,12456}>

123, 1234

12	124, 1235	12345
	125, 1245	12456
	126, 1246	
13	134. 1256	

134, 1256 135, 1345 A collection S is convex: If for all X,Y,Z (X in S, Y in S, X subset Z subset Y)  $\rightarrow$  Z in S.

## **Border-Differential Algorithm**

<{{}},{1234}> - <{{}},{23,24,34}> = <{1,234},{1234}> {} <u>1</u>, 2, 3, 4 12, 13, 14, 23, 24, 34 123, 124, 134, <u>234</u> 1234

Algorithm:

- Use iterations of expansion & minimization of "products" of differences
- Use tree to speed up minimization

• Find minimal subsets of 1234 that are not subsets of 23, 24, 34.

• {1,234} = min ({1,4} X {1,3} X {1,2})

Good for: Jumping EPs; EPs in "rectangle regions," ...

Iterative expansion & minimization can be viewed as optimized Berge hypergraph transversal algorithm

## Gene club + Border Differential

- Border-differential can handle up to 75 attributes (using 2003 PC)
- For microarray gene expression data, there are thousands of genes.
- (Mao+Dong 05) used border-differential after finding many gene clubs -- one gene club per gene.
- A gene club is a set of k genes strongly correlated with a given gene and the classes.
- Some EPs discovered using this method were shown earlier. Discovered more EPs with near 100% support in cancer or normal, involving many different genes. Much better than earlier results.

### Tree-based algorithm for JEP mining

- Use tree to compress data and patterns.
- Tree is similar to FP tree, but it stores two counts per node (one per class) and uses different item ordering
- Nodes with non-zero support for positive class and zero support for negative class are called base nodes.
- For every base node, the path's itemset is a potential JEP. Gather negative data containing root item and item for based nodes on the path. Call border differential.
- Item ordering is important. Hybrid (support ratio ordering first for a percentage of items, frequency ordering for other items) is best.

## Projection based algorithm

- Form dataset H to contain the differences {p-ni | i=1...k}.
  - p is a positive transaction, n1, ..., nk are negative transactions.
- Let x1<...<xm be increasing item frequency (in H) ordering.
- For i=1 to m
  - let Hxi be H with all items y > xi projected out & with all transactions containing xi removed (data projection).
  - remove non minimal transactions in Hxi.
  - if Hxi is small, do iterative expansion and minimization.
  - Otherwise, apply the algorithm on Hxi.

Let H be: a b c d b e d b c e c d e

Item ordering: a < b < c < d < e

Ha is H with all items > a (red

items)

projected out and also edge with a removed, so Ha={}.

## ZBDD based algorithm

to mine disjunctive emerging patterns

- Disjunctive Emerging Patterns: allowing disjunction as well as conjunction of simple attribute conditions.
  - e.g. Precipitation = ( gt-norm OR lt-norm ) AND Internal discoloration = ( brown OR black )

Generalization of EPs

 ZBDD based algorithm uses Zero Surpressed Binary Decision Diagram for efficiently mining disjunctive EPs.

### Binary Decision Diagrams (BDDs)

- Popular in Boolean SAT solvers and reliability eng.
- Canonical DAG representations of Boolean formulae



 Caching principle: past computation results are automatically stored and can be retrieved

Efficient BDD implementations available, e.g. CUDD (U of Colorado)

## ZBDD Representation of Itemsets

James: what's the use of 0 edges? How do we reconstruct data?

- Zero-suppressed BDD, ZBDD : A BDD variant for manipulation of item combinations
- E.g. Building a ZBDD for  $\{\{a,b,c,e\},\{a,b,d,e\},\{b,c,d\}\}$

#### Ordering : *c* < *d* < *a* < *e* < *b*

 $\{\{a,b,c,e\}\} \cup_{z} \{\{a,b,d,e\}\} = \{\{a,b,c,e\},\{a,b,d,e\}\} \cup_{z} \{\{b,c,d\}\} = \{\{a,b,c,e\},\{a,b,d,e\},\{a,b,d,e\},\{a,b,d,e\}\} \cup_{z} \{\{a,b,c,e\},\{a,b,d,e\},\{a,$ 



U<sub>z</sub> = ZBDD set-union

## ZBDD based mining example

Use solid paths in ZBDD( $D_n$ ) to generate candidates, and use Bitmap of  $D_p$  to check frequency support in  $D_p$ .



# Contrast pattern based classification -- history

- Contrast pattern based classification: Methods to build or improve classifiers, using contrast patterns
  - CBA (Liu et al 98)
  - CAEP (Dong et al 99)
  - Instance based method: DeEPs (Li et al 00, 04)
  - Jumping EP based (Li et al 00), Information based (Zhang et al 00), Bayesian based (Fan+Kotagiri 03), improving scoring for >=3 classes (Bailey et al 03)
  - CMAR (Li et al 01)
  - Top-ranked EP based PCL (Li+Wong 02)
  - CPAR (Yin+Han 03)
  - Weighted decision tree (Alhammady+Kotagiri 06)
  - Rare class classification (Alhammady+Kotagiri 04)
  - Constructing supplementary training instances (Alhammady+Kotagiri 05)
  - Noise tolerant classification (Fan+Kotagiri 04)
  - EP length based 1-class classification of rare cases (Chen+Dong 06)

• ...

Most follow the aggregating approach of CAEP.

## **EP-based classifiers: rationale**

- Consider a typical EP in the Mushroom dataset, {odor = none, stalk-surface-below-ring = smooth, ring-number = one}; its support increases from 0.2% from "poisonous" to 57.6% in "edible" (growth rate = 288).
- Strong differentiating power: if a test T contains this EP, we can predict T as edible with high confidence 99.6% = 57.6/(57.6+0.2)
- A single EP is usually sharp in telling the class of a small fraction (e.g. 3%) of all instances. Need to aggregate the power of many EPs to make the classification.
- EP based classification methods often out perform state of the art classifiers, including C4.5 and SVM. They are also noise tolerant.

#### CAEP (Classification by Aggregating Emerging Patterns)

 Given a test case T, obtain T's scores for each class, by aggregating the discriminating power of EPs contained by T; assign the class with the maximal score as T's class.

 The discriminating power of EPs are expressed in terms of supports and growth rates. Prefer large supRatio, large support

The contribution of one EP X (support weighted confidence):

strength(X) = sup(X) \* supRatio(X) / (supRatio(X)+1)

Compare CMAR:

• Given a test T and a set E(Ci) of EPs for class Ci, the *Chi2 weighted Chi2* 

```
aggregate score of T for Ci is score(T, Ci) = Σ strength(X)
(over X of Ci
matching T)
```

For each class, using median (or 85%) aggregated value to normalize to avoid bias towards class with more EPs

### How CAEP works? An example

Given a test T={a,d,e}, how to classify T?

T contains EPs of class 1 : {a,e} (50%:25%) and {d,e} (50%:25%), so Score(T, class1) =

0.5\*[0.5/(0.5+0.25)] + 0.5\*[0.5/(0.5+0.25)] = 0.67

- T contains EPs of class 2: {a,d} (25%:50%), so
   Score(T, class 2) = 0.33;
- T will be classified as class 1 since Score1>Score2

Class 1 (D1)



Class 2 (D2)

а	b		
а	b	С	d
С	е		
а	b	d	е

#### DeEPs (Decision-making by Emerging Patterns)

- An instance based (lazy) learning method, like k-NN; but does not use normal distance measure.
- For a test instance T, DeEPs
  - First project each training instance to contain only items in T
  - Discover EPs from the projected data
  - Then use these EPs to select training data that match some discovered EPs
  - Finally, use the proportional size of matching data in a class C as T's score for C
- Advantage: disallow similar EPs to give duplicate votes!

#### DeEPs : Play-Golf example (data projection)

#### Test = {sunny, mild, high, true}

Original data

Projected data

					Outlook	Temperature	Humidity	Windy	Class
Outlook	Temperature	Humidity	Windy	Clas	ss <sub>:</sub> unny		high		N
sunny	hot	high	false	N	sunny		high	true	Ν
sunny	hot	high	true	N				true	N
rain	cool	normal	true	N	sunnv	mild	hiah		N
sunny	mild	high	false	N	Sunny	inite inite	high	<b>1</b>	
rain	mild	hiah	true	N		mild	nign	true	IN
overcast	hot	high	FALSE	P			high		P
rain	mild	high	FALSE	P		mild	high		P
rain	cool	normal	FALSE	P					
overcast	cool	normal	TRUE	P				TRUE	P
sunny	cool	normal	FALSE	P	sunny				Р
rain	mild	normal	FALSE	P		mild			Р
sunny	mild	normal	TRUE	P	sunnv	mild		TRUF	Р
overcast	mild	high	TRUE	P	Sanny	mild	biab		
overcast	hot	normal	FALSE	P		mila	nign	INUE	٢

Discover EPs and derive scores using the projected data

## PCL (Prediction by Collective Likelihood)

- Let X1,...,Xm be the m (e.g. 1000) most general EPs in descending support order.
- Given a test case T, consider the list of all EPs that match T. Divide this list by EP's class, and list them in descending support order:

P class: Xi1, ..., Xip N class: Xj1, ..., Xin

 Use k (e.g. 15) top ranked matching EPs to get score for T for the P class (similarly for N):

Score(T,P) =  $\sum_{t=1}^{k} \text{suppP}(Xit) / \text{supp}(Xt)$ 

normalizing factor

## **EP** selection factors

- There are many EPs, can't use them all. Should select and use a good subset.
- EP selection considerations include
  - Keep minimal (shortest, most general) ones
  - Remove syntactic similar ones
  - Use support/growth rate improvement (between superset/subset pairs) to prune
  - Use instance coverage/overlap to prune
  - Using only JEPs

**....** 

#### Why EP-based classifiers are good

- Use discriminating power of **low** support EPs, together with high support ones
- Use **multi-feature** conditions, not just single-feature conditions
- Select from larger pools of discriminative conditions
  - Compare: Search space of patterns for decision trees is limited by early greedy choices.
- Aggregate/combine discriminating power of a diversified committee of "experts" (EPs)
- Decision is highly explainable

### Some other works

- CBA (Liu et al 98) uses one rule to make a classification prediction for a test
- CMAR (Li et al 01) uses aggregated (Ch2 weighted) Chi2 of matching rules
- CPAR (Yin+Han 03) uses aggregation by averaging: it uses the average accuracy of top k rules for each class matching a test case

**...** 

# Aggregating EPs/rules vs bagging (classifier ensembles)

- Bagging/ensembles: a committee of classifiers vote
  - Each classifier is fairly accurate for a large population (e.g. >51% accurate for 2 classes)
- Aggregating EPs/rules: matching patterns/rules vote
  - Each pattern/rule is accurate on a very small population, but inaccurate if used as a classifier on all data; e.g. 99% accurate on 2% of data, but 2% accurate on all data

## Using contrasts for rare class data

[Al Hammady and Ramamohanarao 04,05,06]

- Rare class data is important in many applications
  - Intrusion detection (1% of samples are attacks)
  - Fraud detection (1% of samples are fraud)
  - Customer click thrus (1% of customers make a purchase)

**...** 

## **Rare Class Datasets**

- Due to the class imbalance, can encounter some problems
  - Few instances in the rare class, difficult to train a classifier
  - Few contrasts for the rare class
  - Poor quality contrasts for the majority class
- Need to either increase the instances in the rare class or generate extra contrasts for it

## Synthesising new contrasts (new emerging patterns)

- Synthesising new emerging patterns by superposition of high growth rate items
  - Suppose that attribute A2=`a' has high growth rate and that {A1=`x', A2=`y'} is an emerging pattern. Then create a new emerging pattern {A1='x', A2='a'} and test its quality.
- A simple heuristic, but can give surprisingly good classification performance

## Synthesising new data instances

- Can also use previously found contrasts as the basis for constructing new rare class instances
  - Combine overlapping contrasts and high growth rate items
- Main idea intersect and `cross product' the emerging patterns and high growth rate (support ratio) items
  - Find emerging patterns
  - Cluster emerging patterns into groups that cover all the attributes
  - Combine patterns within each group to form instances

## Synthesising new instances

E1{A1=1, A2=X1}, E2{A5=Y1,A6=2,A7=3}, E3{A2=X2,A3=4,A5=Y2} - this is a group

V4 is a high growth item for A4

Combine E1+E2+E3+{A4=V4} to get four synthetic instances.

A1	A2	A3	A4	A5	A6	A7
1	X1	4	V4	Y1	2	3
1	X1	4	V4	Y2	2	3
1	X2	4	V4	Y1	2	3
1	X2	4	V4	Y2	2	3

# Measuring instance quality using emerging patterns

[Al Hammady and Ramamohanarao 07]

- Classifiers usually assume that data instances are related to only a single class (crisp assignments).
- However, real life datasets suffer from noise.
- Also, when experts assign an instance to a class, they first assign scores to each class and then assign the class with the highest score.
- Thus, an instance may in fact be related to several classes

## Measuring instance quality Cont.

- For each instance *i*, assign a weight that represents its strength of membership in each class. Can use emerging patterns to determine appropriate weights for instances
  - Use aggregation of EPs divided by mean value for instances in that class to give an instance weight
- Use these weights in a modified version of classifier, e.g. a decision tree
  - Modify information gain calculation to take weights into account

#### Using EPs to build Weighted Decision Trees

- Instead of crisp class membership,
  - let instances have weighted class membership,
  - then build weighted decision trees, where probabilities are computed from the weighted membership.
- DeEPs and other EP based classifiers can be used to assign weights.

An instance Xi's membership in k classes: (Wi1,...,Wik)

$$\hat{P}(T) = (\hat{p}_{1}(T) = \frac{\sum_{i \in T} Wi1}{|T|}, ..., \hat{p}_{k}(T) = \frac{\sum_{i \in T} Wik}{|T|})$$

$$Info_{WDT}(\hat{P}(T)) = -\sum_{j=1}^{k} \hat{p}_{j}(T) * \log_{2}(\hat{p}_{j}(T))$$

$$Info_{WDT}(A,T) = \sum_{l=1}^{m} \frac{|T_l|}{|T|} Info(\hat{P}(T_l))$$

Measuring instance quality by emerging patterns Cont.

- More effective than k-NN techniques for assigning weights
  - Less sensitive to noise
  - Not dependent on distance metric
  - Takes into account all instances, not just close neighbors
## Data cube based contrasts

- Gradient (Dong et al 01), cubegrade (Imielinski et al 02 – TR published in 2000):
  - Mining syntactically similar cube cells, having significantly different measure values
  - Syntactically similar: ancestor-descendant or sibling-sibling pair
  - Can be viewed as "conditional contrasts": two neighboring patterns with big difference in performance/measure
- Data cubes useful for analyzing multi-dimensional, multi-level, time-dependent data.
- Gradient mining useful for MDML analysis in marketing, business, medical/scientific studies

## Decision support in data cubes

- Used for discovering patterns captured in consolidated historical data for a company/organization:
  - rules, anomalies, unusual factor combinations
- Focus on modeling & analysis of data for decision makers, not daily operations.
- Data organized around major subjects or factors, such as customer, product, time, sales.
- Cube "contains" huge number of MDML "segment" or "sector" summaries at different levels of details
- Basic OLAP operations: Drill down, roll up, slice and dice, pivot

#### Data Cubes: Base Table & Hierarchies

 Base table stores sales volume (*measure*), a function of product, time, & location (dimensions)



#### Data Cubes: Derived Cells



#### Data Cubes: Cell Lattice

Compare: cuboid lattice



## Gradient mining in data cubes

- Users want: more powerful (OLAM) support: Find potentially interesting cells from the billions!
  - OLAP operations used to help users search in huge space of cells
  - Users do: *mousing*, *eye-balling*, *memoing*, *decisioning*, ...
- Gradient mining: Find syntactically similar cells with significantly different measure values
  - (teen clothing,California,2006), total-profit=100K
  - vs (teen clothing,Pensylvania,2006), total profit = 10K
  - A specific OLAM task

# LiveSet-Driven Algorithm for constrained gradient mining

- Set-oriented processing; traverse the cube while carrying the *live* set of cells having potential to match descendants of the current cell as gradient cells
  - A gradient compares two cells; one is the probe cell, & the other is a gradient cell. Probe cells are ancestor or sibling cells
- Traverse the cell space in a coarse-to-fine manner, looking for matchable gradient cells with potential to satisfy gradient constraint
- Dynamically prune the live set during traversal
- Compare: Naïve method checks each possible cell pair

# Pruning probe cells using dimension matching analysis

 Defn: Probe cell p=(a<sub>1</sub>,...,a<sub>n</sub>) is matchable with gradient cell g=(b<sub>1</sub>, ..., b<sub>n</sub>) iff

No solid-mismatch, or

- Only one solid-mismatch but no \*-mismatch
- A solid-mismatch: if  $a_i \neq b_i + none$  of  $a_i$  or  $b_i$  is \*
- A \*-mismatch: if  $a_i = *$  and  $b_i \neq *$

p=(00, Tor, \*, \*) : 1 solid g=(00, Chi, \*,PC) : 1 \*

 Thm: cell p is matchable with cell g iff p may make a probe-gradient pair with some descendant of g (using only dimension value info)

## Sequence based contrasts

- We want to compare sequence datasets:
  - bioinformatics (DNA, protein), web log, job/workflow history, books/documents
  - e.g. compare protein families; compare bible books/versions
- Sequence data are very different from relational data
  - order/position matters
  - unbounded number of "flexible dimensions"
- Sequence contrasts in terms of 2 types of comparison:
  - Dataset based: Positive vs Negative
    - Distinguishing sequence patterns with gap constraints (Ji et al 05, 07)
    - Emerging substrings (Chan et al 03)
  - Site based: Near marker vs away from marker
    - Motifs
    - May also involve data classes

Roughly: A site is a position in a sequence where a special marker/pattern occurs

### Example sequence contrasts

When comparing the two protein families zf-C2H2 and zf-CCHC, we discovered a protein MDS CLHH appearing as a subsequence in 141 of 196 protein sequences of zf-C2H2 but never appearing in the 208 sequences in zf-CCHC.

When comparing the first and last books from the Bible, we found the subsequences (with gaps) "having horns", "face worship", "stones price" and "ornaments price" appear multiple times in sentences in the Book of Revelation, but never in the Book of Genesis.

## Sequence and sequence pattern occurrence

- A <u>sequence</u>  $S = e_1 e_2 e_3 \cdots e_n$  is an ordered list of items over a given alphabet.
  - E.G. "AGCA" is a DNA sequence over the alphabet {A, C, G, T}.
  - *"AC"* is a subsequence of *"AGCA"* but not a substring;
  - "GCA" is a substring
- Given sequence S and a subsequence pattern S', an occurrence of S' in S consists of the positions of the items from S' in S.
- **EG: consider** *S* = *"ACACBCB"* 
  - <1,5>, <1,7>, <3,5>, <3,7> are occurrences of "AB"
  - <1,2,5>, <1,2,7>, <1,4,5>, ... are occurrences of "ACB"

#### Maximum-gap constraint satisfaction

- A (maximum) gap constraint: specified by a positive integer g.
- Given *S* & an occurrence  $o_s = \langle i_1, \dots, i_m \rangle$ , if  $i_{k+1} i_k \langle = g + 1 \rangle$ for all  $1 \leq k \leq m$ , then  $o_s$  fulfills the g-gap constraint.
- If a subsequence S' has one occurrence fulfilling a gap constraint, then S' satisfies the gap constraint.
  - The <3,5> occurrence of "AB" in S = "ACACBCB", satisfies the maximum gap constraint g=1.
  - The <3,4,5> occurrence of "ACB" in S = "ACACBCB" satisfies the maximum gap constraint g=1.
  - The <1,2,5>, <1,4,5>, <3,4,5> occurrences of "ACB" in S = "ACACBCB" satisfy the maximum gap constraint g=2.
- One sequence contribute to at most one to count.

## g-MDS Mining Problem

Given two sets *pos & neg* of sequences, two support thresholds *minp* & *maxn*, & a maximum gap *g*, a pattern *p* is a *Minimal Distinguishing Subsequence* with *g*-gap constraint (*g*-MDS), if these conditions are met:

**1.** Frequency condition:  $supp_{pos}(p, g) \ge minp;$ 

2. Infrequency condition:  $supp_{neg}(p, g) \ll maxn;$ 

3. Minimality condition: There is no subsequence of *p* satisfying 1 & 2.

Given *pos*, *neg*, *minp*, *minn* and *g*, the *g*-MDS mining problem is to find all the *g*-MDSs.

## Example g-MDS

- Given *minp*=1/3, *maxn*=0, *g*=1,
  - *pos* = {CBAB, AACCB, BBAAC},
  - neg = {BCAB,ABACB}
- 1-MDS are: BB, CC, BAA, CBA
  - "ACC" is frequent in pos & non-occurring in neg, but it is not minimal (its subsequence "CC" meets the first two conditions).

## g-MDS mining : Challenges

The support thresholds in mining distinguishing patterns need to be lower than those used for mining frequent patterns.

- Min supports offer very weak pruning power on the large search space.
- Maximum gap constraint is neither monotone nor anti-monotone.
- Gap checking requires clever handling.

## ConSGapMiner

- The *ConSGapMiner* algorithm works in three steps:
- 1 Candidate Generation:

Candidates are generated without duplication. Efficient pruning strategies are employed.

2.

Support Calculation and Gap Checking: For each generated candidate c,  $supp_{pos}(c, g)$  and  $supp_{neg}(c, g)$  are calculated using bitset operations.

3. Minimization:

Remove all the non-minimal patterns (using pattern trees).

#### ConSGapMiner : Candidate Generation



#### Use Bitset Operation for Gap Checking

- Storing projected suffixes and performing scans is expensive.
- e.g. Given a sequence
- to check whether **AG** is a subsequence for **g=1**:

We encode the occurrences' ending positions into a bitset and use a series of bitwise operations to generate a new candidate sequence's bitset.

#### **Projections with prefix** *A* :

ACTGTATTACCAGTATCG

ATTACCAGTATCG

ACCAGTATCG

AGTATCG

ATCG

**Projections with** *AG obtained from the above*:

**AGTATCG** 

#### ConSGapMiner: Support & Gap Checking (1)

Initial Bitset Array Construction: For each item x, construct an array of bitsets to describe where x occurs in each sequence from *pos* and *neg*.

Dataset			
ID	Sequence	Class	
1	CBAB	pos	
2	AACCB	pos	
3	BBAAC	pos	
4	BCAB	neg	
5	ABACB	neg	

**Initial Bitset Array** 

single-item A
0010
11000
00110
0010
10100

#### ConSGapMiner: Support & Gap Checking (2)

Two steps: (1) g+1 right shifts; (2) OR them

EG: generate mask bitset for X = A'' in sequence 5 (with max gap g = 1):

ID	Sequence	Class			
1	CBAB	pos	10100	$\rangle \rangle$	01010
2	AACCB	pos	01010	> >	0 0 1 0 1
3	BBAAC	pos	01010	OR	00101
4	BCAB	neg			
5	ABACB	neg	Mask bitset f	or X :	0 1 1 1 1

Mask bitset: all the legal positions in the sequence at most (g+1)-positions away from tail of an occurrence of the (maximum prefix of the) pattern.

#### ConSGapMiner: Support & Gap Checking (3)

EG: Generate bitset array (ba) for X' = "BA" from X = 'B' (g = 1)

- Get ba for X='B' 1.
- 2. Shift ba(X) to get mask for X' = 'BA'
- AND ba('A') and mask(X') 3. to get ba(X')

ID	Sequence	Class
1	CBAB	pos
2	AACCB	pos
3	BBAAC	pos
4	BCAB	neg
5	ABACB	neg

ba(X):			mask(X'):	
0101			0011	Number
00001	2 shifts plus Ol	; 7	00000	of arrays
11000 -		→	01110	with
1001			0110	some 1 =
01001			00110	count /
mask(X'): 0011 00000 01110 0110 00110	&	ba('A'): 0010 11000 00110 0010 10100		ba(X'): 0010 00000 00110 0010

# Execution time performance on protein families



#### Pattern Length Distribution -- Protein Families

The length and frequency distribution of patterns: TaC vs TatD\_DNase, g = 5,  $\alpha = 13$ . 5%.



Length distribution

**Frequency distribution** 

#### **Bible Books Experiment**



runtime vs support, for g = 6.



runtime vs g, for  $\alpha = 0.0013$ .

New Testament (Matthew, Mark, Luke and John) vs Old Testament (Genesis, Exodus, Leviticus and Numbers):

#Pos	#Neg	Alphabet	Avg. Len.	Max. Len.
3768	4893	3344	7	25

Some interesting terms found from the Bible books (New Testament vs Old Testament):

Substrings (count)	Subsequences (count)
eternal life (24)	seated hand (10)
good news (23)	answer truly (10)
Forgiveness in (22)	Question saying (13)
Chief priests (53)	Truly kingdom (12)

## Extensions

- Allowing min gap constraint
- Allowing max window length constraint
- Considering different minimization strategies:
  - Subsequence-based minimization (described on previous slides)
  - Coverage (matching tidset containment) + subsequence based minimization
  - Prefix based minimization

## Motif mining

- Find sequence patterns frequent around a site marker, but infrequent elsewhere
- Can also consider two classes:
  - Find patterns frequent around site marker in +ve class, but in frequent at other positions, and infrequent around site marker in –ve class
  - Often, biological studies use background probabilities instead of a real -ve dataset
- Popular concept/tool in biological studies

## **Contrasts for Graph Data**

- Can capture structural differences
  - Subgraphs appearing in one class but not in the other class
    - Chemical compound analysis
    - Social network comparison

## Contrasts for graph data Cont.

- Standard frequent subgraph mining
  - Given a graph database, find connected subgraphs appearing frequently
- Contrast subgraphs particularly focus on discrimination and minimality

Minimal contrast subgraphs [Ting and Bailey 06]

- A contrast graph is a subgraph appearing in once class of graphs and never in another class of graphs
  - Minimal if none of its subgraphs are contrasts
  - May be disconnected
    - Allows succinct description of differences
    - But requires larger search space
- Will focus on one versus one case

### Contrast subgraph example



## Minimal contrast subgraphs

- From the example, we can see that for the 1-1 case, contrast graphs are of two types
  - Those with only vertices (a vertex set)
  - Those without isolated vertices (edge sets)
- Can prove that for 1-1 case, the *minimal* contrast subgraphs are the union of

Min. Vertex Sets + Minimal Edge Sets

## Mining contrast subgraphs

- Main idea
  - Find the maximal common edge sets
    - These may be disconnected
  - Apply a minimal hypergraph transversal operation to derive the minimal contrast edge sets from the maximal common edge sets
  - Must compute minimal contrast vertex sets separately and then minimal union with the minimal contrast edge sets

## Contrast graph mining workflow



### Using discriminative graphs for containment search and indexing [Chen et al 07]

 Given a graph database and a query q. Find all graphs in the database contained in q.



- Applications
  - Querying image databases represented as attributed relational graphs. Efficiently find all objects from the database contained in a given scene (query).

## Discriminative graphs for indexing

#### Main idea:

- Given a query graph q and a database graph g
  - If a feature *f* is not contained in *q* and *f* is contained in *g*, then *g* is not contained in *q*
- Also exploit similarity between graphs.
  - If f is a common substructure between g1 and g2, then if f is not contained in the query, both g1 and g2 are not contained in the query

## Graph Containment Example [From Chen et al 07]


### Discriminative graphs for indexing

- Aim to select the ``contrast features'' that have the most pruning power (save most isomorphism tests)
- These are features that are contained by many graphs in the database, but are unlikely to be contained by a query graph.
- Generate lots of candidates using a frequent subgraph mining and then filter output graphs for discriminative power

### Generating the Index

- After the contrast subgraphs have been found, select a subset of them
  - Use a set cover heuristic to select a set that ``covers'' all the graphs in the database, in the context of a given query q
  - For multiple queries, use a maximum coverage with cost approach

### Contrasts for trees

- Special case of graphs
  - Lower complexity
  - Lots of activity in the document/XML area, for change detection.
- Notions such as edit distance more typical for this context

### Contrasts of models

- Models can be clusterings, decision trees, ...
- Why is contrasting useful here ?
  - Contrast/compare a user generated model against a known reference model, to evaluate accuracy/degree of difference.
  - May wish to compare degree of difference between one algorithm using varying parameters
  - Eliminate redundancy among models by choosing dissimilar representatives

### Contrasts of models Cont.

- Isn't this just a dissimilarity measure ? Like Euclidean distance ?
  - Similar, but operating on more complex objects, not just vectors
- Difficulties are
  - For rule based classifiers, can't just report on number of different rules

### Clustering comparison

- Popular clustering comparison measures
  - Rand index and Jaccard index
    - Measure the proportion of point pairs on which the two clusterings agree
  - Mutual information
    - How much information one clustering gives about the other
  - Clustering error
    - Classification error metric

### **Clustering Comparison Measures**

Nearly all techniques use a 'Confusion Matrix' of two clusterings. Example : Let C = {c<sub>1</sub>, c<sub>2</sub>, c<sub>3</sub>) and C' = {c'<sub>1</sub>, c'<sub>2</sub>, c'<sub>3</sub>}

m	<b>c</b> <sub>1</sub>	<b>c</b> <sub>2</sub>	<b>c</b> <sub>3</sub>
<b>c'</b> <sub>1</sub>	5	14	1
<b>c'</b> <sub>2</sub>	10	2	8
c' <sub>3</sub>	8	7	5

$$m_{ij} = | c_i \cap c'_j |$$

### Pair counting

- Considers the number of points on which two clusterings agree or disagree. Each pair falls into one of four categories
  - N<sub>11</sub> contains the pairs of points which are in the same cluster both in C and C'
  - N<sub>00</sub> contains the pairs of points which are not in the same cluster in both C and C'
  - N<sub>10</sub> contains the pairs of points which are in the same cluster in C but not in C'
  - N<sub>01</sub> contains the pairs of points which are in the same cluster in C' but not in C
  - N total number of pairs of points

Pair Counting

Two popular indexes - Rand and Jaccard

• Rand(C,C')= 
$$\frac{N_{11} + N_{00}}{N}$$

Jaccard(C,C') = 
$$\frac{N_{11}}{N_{11} + N_{01} + N_{10}}$$

### Clustering Error Metric (Classification Error Metric)

Is an injective mapping of C={1,...,K} into C'={1,...,K'}. Need to find *maximum* intersection for all possible mappings.

m	$\mathbf{c}_1$	<b>c</b> <sub>2</sub>	<b>c</b> <sub>3</sub>
c' <sub>1</sub>	5	14	1
<b>c'</b> <sub>2</sub>	10	2	8
c' <sub>3</sub>	8	7	5

Best match is  $\{c_2, c'_1\}, \{c_1, c'_2\}, \{c_3, c'_{3}\}$ 

Clustering error= (14+10+5)/60=0.483

### **Clustering Comparison Difficulties**



# Comparing datasets via induced models

- Give two datasets, we may compare their difference, by considering the difference or deviation between the models that can be induced from them
- Models here can refer to decision trees, frequent itemsets, emerging patterns, etc
- May also compare an old model to a new dataset
  - How much does it misrepresent ?

### The FOCUS Framework [Ganti et al 99]

- Develops a single measure for quantifying the difference between the interesting characteristics in each dataset.
- Key Idea: ``A model has a structural component that identifies interesting regions of the attribute space ... each such region summarized by one (or several) measure(s)
- Difference between two classifiers is measured by amount of work needed to change them into some common specialization

### Focus Framework Cont.

- For comparing two models, divide the models each into regions and then compare the regions individually
  - For a decision tree, compare leaf nodes of each model
  - Aggregate the pairwise differences between each of the regions

## Decision tree example [Taken from Ganti et 99]



Difference(D1,D2)=|0.5-0.1|+|0.4-0.3|+|0.1-0.5|+|0.25-0.05|+|0.05-0.2|=1.125

### Correspondence Tracing of Changes [Wang et al 03]

Correspondence tracing aims to make change between the two models understandable by explicitly describing changes and then ranking them

### Correspondence Tracing Example

[Taken from Wang et al 03]

- Consider old and new rule based classifiers
- Old
  - O1: If A4=1 then C3 [0,2,7,9,13,15,17]
  - O2: If A3=1 and A4=2 then C2 [1,4,6,10,12,16]
  - O3: If A3=2 and A4=2 then C1 [3,5,8,11,14]
- New
  - N1: If A3=1 and A4=1 then C4 [0,9,15]
  - N2: If A3=1 and A4=2 then C2 [1,4,6,10,12,16]
  - N3: If A3=2 and A4=1 then C2 [2,7,13,17]
  - N4: If A3=2 and A4=2 then C1 [3,5,8,11,14]

### Correspondence Example cont.

Rules N1 and N3 classify the examples that were classified by rule O1. So the changes for the sub population covered by O1 can be described as

<01,N1> and <01,N3>

Changes <O2,N2> and <O3,N4> are trivial because the old and new rules are identical.

### Rule Accuracy Increase.

- The quantitative change Q of <O,N> is the estimated accuracy increase (+ or -) due to the change from O to N.
- Changes are ranked according to quantitative change Q and then presented to the user

# Common themes for contrast mining

- Different representations
  - Minimality is the most common
  - Support/ratio constraints most popular, though not necessarily the best
  - Conjunctions most popular for relational case
- Large output size

### **Recommendations to Practitioners**

- Some important points are
  - Contrast patterns can capture distinguishing patterns between classes
  - Contrast patterns can be used to build high quality classifiers
  - Contrast patterns can capture useful patterns for detecting/treating diseases

### Open Problems in Contrast Data Mining

- How to meaningfully assess quality of contrasts, especially for nonrelational data.
  - Little work on contrasts for mixed forms of data
- How to explain the semantics of contrasts
- Highly expressive contrasts (first order ..)
- Develop new ways to build contrast based classifiers
- Discovery of contrasts in massive datasets.
  - Efficiently mine contrasts when there are thousand of attributes
  - Efficient mining of top-k contrast patterns
  - Are there meaningful approximations (e.g. sampling) ?

### Summary

- We have given a wide survey of contrast mining. It should now be clearer
  - Why contrast data mining is important and when it can be used
  - How it can be used for very powerful classifiers
  - What algorithms can be used for contrast data mining

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