Classification

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Talk Outline

- Introduction
 - Classification Problem
 - Applications
 - Metrics
 - Combining classifiers
- Classification Techniques

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The Classification Problem

Outlook	Temp	Humidity	Windy?	Class
	(°F)	(%)		
sunny	75	70	true	play
sunny	80	90	true	don't play
sunny	85	85	false	don't play
sunny	72	95	false	don't play
sunny	69	70	false	play
overcast	72	90	true	play
overcast	83	78	false	play
overcast	64	65	true	play
overcast	81	75	false	play
rain	71	80	true	don't play
rain	65	70	true	don't play
rain	75	80	false	play
rain	68	80	false	play
rain	70	96	false	play
sunny	77	69	true	?
rain	73	76	false	?

Play Outside?

Model relationship between class labels and attributes

⇒ Assign class labels to new data with unknown labels

Applications

- - Text classification

 Classify emails into spam / non-spam
 - Classify web-pages into yahoo-type hierarchyNLP Problems
- Tagging: Classify words into verbs, nouns, etc.
 Risk management, Fraud detection, Computer intrusion detection
 - Given the properties of a transaction (items purchased, amount, location, customer profile, etc.)
- Determine if it is a fraud

 Machine learning / pattern recognition applications

 - VisionSpeech recognition
- All of science & knowledge is about predicting future in terms of past
- So classification is a very fundamental problem with ultra-wide scope of applications

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Metrics

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- accuracy
- classification time per new record
- training time
- main memory usage (during classification)
- model size

Accuracy Measure

- Prediction is just like tossing a coin (random variable X)
 - "Head" is "success" in classification; X = 1
 - "tail" is "error"; X = 0
 - X is actually a mapping: {"success": 1, "error": 0}
- In statistics, a succession of independent events like this is called a bernoulli process
 - Accuracy = P(X = 1) = p
 - mean value = $\mu = E[X] = p \times 1 + (1-p) \times 0 = p$
 - variance = $\sigma^2 = E[(X-\mu)^2] = p (1-p)$
- Confidence intervals: Instead of saying accuracy = 85%, we want to say: accuracy ∈ [83, 87] with a confidence of 95%

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Binomial Distribution

- Treat each classified record as a bernoulli trial
- If there are n records, there are n independent and identically distributed (iid) bernoulli trials, X_i , i = 1,...,n
- Then, the random variable $X = \sum_{i=1,...,n} X_i$ is said to follow a binomial distribution
 - $P(X = k) = {}^{n}C_{k} p^{k} (1-p)^{n-k}$
- Problem: Difficult to compute for large n

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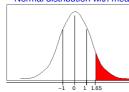
Normal Distribution

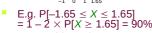
- Continuous distribution with parameters μ (mean), σ^2 (variance)
- Probability density: $f(x) = (1/\sqrt{(2\pi\sigma^2)}) \exp(-(x-\mu)^2/(2\sigma^2))$
- Central limit theorem:
 - Under certain conditions, the distribution of the sum of a large number of iid random variables is approximately normal
 - A binomial distribution with parameters n and p is approximately normal for large n and p not too close to 1 or 0
 - The approximating normal distribution has mean μ = np and standard deviation $\sigma^2 = (n p (1 - p))$

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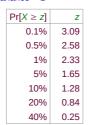
Confidence Intervals

Normal distribution with mean = 0 and variance = 1





- To use this we have to transform our random variable to have mean = 0 and variance
- Subtract mean from X and divide by standard deviation



Estimating Accuracy Holdout method

- - Randomly partition data: training set + test set
 - accuracy = |correctly classified points| / |test data points|
- Stratification
 - Ensure each class has approximately equal proportions in both partitions
- Random subsampling
 - Repeat holdout k times. Output average accuracy.
- k-fold cross-validation
 - Randomly partition data: S₁,S₂,...,S_k
 - lacksquare First, keep S_1 as test set, remaining as training set
 - Next, keep S₂ as test set, remaining as training set, etc.
- accuracy = |total correctly classified points| / |total data points|
- **Recommendation:**
- Stratified 10-fold cross-validation. If possible, repeat 10 times and average results. (reduces variance)

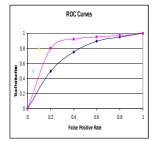
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Is Accuracy Enough?

- If only 1% population has cancer, then a test for cancer that classifies all people as non-cancer will have 99% accuracy.
- Instead output a confusion matrix:

Actual/	Class 1	Class 2	Class 3
Estimate			
Class 1	90%	5%	5%
Class 2	2%	91%	7%
Class 3	8%	3%	89%

Receiver Operating Characteristic



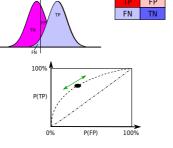
- Useful in visually comparing classifiers.
- Top-left is best.
- Bottom-right is worst.
- Area under curve is a measure of accuracy.

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ROC Interpretation Example

- Blood protein levels in healthy and diseased people are normally distributed with means of 1 g/dL and 2 g/dL.
- Experimenter can adjust threshold (to design a medical test; black vertical line in figure).
- Increasing threshold = fewer false positives

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Source: wikipedia. Image by Sharpr - Own work, CC BY-SA 3.0, https://commons.wikimedia.org/w/index.php?curid=44059691

Combining Classifiers

- Get k random samples with replacement as training sets (like in random subsampling).
- ⇒ We get k classifiers
- Bagging: Take a majority vote for the best class for each new record
- Boosting: Each classifier's vote has a weight proportional to its accuracy on training data
- Like a patient taking multiple opinions from several doctors

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Talk Outline

- Introduction
- Classification Techniques
 - Nearest Neighbour Methods
 - Decision Trees
 - ID3, CART, C4.5, C5.0, SLIQ, SPRINT
 - Bayesian Methods
 - Naïve Bayes, Bayesian Belief Networks
 - Maximum Entropy Based Approaches
 - 4. Association Rule Based Approaches
 - Soft-computing Methods:
 - Genetic Algorithms, Rough Sets, Fuzzy Sets, Neural Networks
 - Support Vector Machines

Nearest Neighbour Methods

k-NN, Reverse Nearest Neighbours

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k-Nearest Neighbours

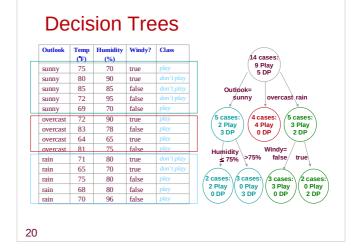
- Model = Training data
- Classify record R using the k nearest neighbours of R in the training data.
- Most frequent class among k NNs
- Distance function could be euclidean
- Use an index structure (e.g. R* tree) to find the k NNs efficiently

Reverse Nearest Neighbours

- Records which consider R as a k-NN
- Output most frequent class among RNNs.
- More resilient to outliers.

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Decision Trees



Basic Tree Building Algorithm

MakeTree (Training Data D):

Partition(D)

Partition (Data D):

if all points in D are in same class: return Evaluate splits for each attribute A Use best split found to partition D into D₁,D₂,..., D_n for each Di: Partition (D_i)

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ID3, CART

ID3

- Use information gain to determine best split
- $gain = H(D) \sum_{i=1...n}^{n} P(D_i) H(D_i)$
- $H(p_1, p_2, ..., p_m) = -\sum_{i=1...m} p_i \log p_i$
- like 20-question game
 - Which attribute is better to look for first: "Is it a living thing?" or "Is it a duster?"

CART

- Only create two children for each node
- Goodness of a split (Φ) $\Phi = 2 P(D_1) P(D_2) \sum_{i=1...m}^{\infty} |P(C_i / D_1) - P(C_i / D_2)|$

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Shannon's Entropy

- An expt has several possible outcomes
- In N (e.g. 12) expts, suppose each outcome occurs M (e.g. 3) times
- This means there are N/M (e.g. 4) possible outcomes
- To represent each outcome, we need log N/M (e.g. 2) bits.
 - This generalizes even when all outcomes are not equally frequent.
 - Reason: For an outcome j that occurs M times, there are N/M equi-probable events among which only one cp to j
- Since $p_i = M / N$ (e.g. 25%), information content of an outcome is -log p_i (e.g. 2)
- So, expected info content: $H = -\sum p_i \log p_i$ (e.g. 0.25*2*4 = 2)

C4.5, C5.0

- Handle missing data
 - During tree building, ignore missing data
 - During classification, predict value of missing data based on attribute values of other records
- Continuous data
 - Divide continuous data into ranges based on attribute values found in training data
- Pruning
 - Prepruning
 - Postpruning replace subtree with leaf if error-rate doesn't change much
- Goodness of split: Gain-ratio
 - gain favours attributes with many values (leads to over-fitting)
- gain-ratio = gain / $H(P(D_1), P(D_2), ..., P(D_n))$
- C5.0 Commercial version of C4.5
 - Incorporated boosting; other secret techniques

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SLIQ

- Motivations:
 - Previous algorithms consider only memoryresident data
 - In determining the entropy of a split on a noncategorical attribute, the attribute values have to

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SLIQ

Data structure: class list and attribute lists

Outlook	Temp (°F)	Humidity	Windy?	Class	Ш	Hitch	midity	(%) (las lass I	ist	Indefe
sunny	75	(%)	true	Play] [1	65		Play	8	N1
sunny	80	90	true	Don't Play		2	70	Do	t Play	1	N1
sunny	85	85	false	Don't Play		3	70	Do	t Play	5	N1
sunny	72	95	false	Don't Play		4	70	Do	t Play	11	N1
sunny	69	70	false	Play		5	75		Play	9	N1
overcast	72	90	true	Play	1 [6	78		Play	7	N1
overcast	83	78	false	Play	1 [7	80		Play	10	N1
overcast	64	65	true	Play	1 [8	80		Play	12	N1
overcast	81	75	false	Play	1 [9	80		Play	13	N1
rain	71	80	true	Don't Play		10	85	Do	t Play	3	N1
rain	65	70	true	Don't Play	1 [11	90	Do	t Play	2	N1
rain	75	80	false	Play		12	90		Play	6	N1
rain	68	80	false	Play	1	13	95		Play	4	N1
rain	70	96	false	Play	1 [14	96		Play	14	N1

The attribute that solisHumidity

Value Class Frequency

<=65 Play 1 <=70 Play 2

SLIQ

Data structure: class list and attribute lists



SLIQ

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Data structure: class list and attribute lists Node: N1

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Humidity (%)	Class List Index		Index	Class	Leaf
65	8	ابر [1	Play	N1
70	1		2	Don't Play	N1
70	5		3	Don't Play	N1
70	11] [4	Don't Play	N1
75	9		5	Play	N1
78	7] [6	Play	N1
80	10		7	Play	N1
80	12		8	Play	N1
80	13		9	Play	N1
85	3		10	Don't Play	N1
90	2		11	Don't Play	N1
90	6		12	Play	N1
95	4		13	Play	N1
96	14		14	Play	N1

The attribute list for Humidity

The class list

SLIQ

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Humidity (%)	Class List Index		Index	Class	Leaf	Node:	N1	
65	8		1	Play	N1	Value	Class	Frequence
70	1		2	Don't Play	N1	<=65	Plav	1
70	5		3	Don't Play	N1		- '4	
70	11		4	Don't Play	N1	<=70	Play	3
75	9	7	5	Play	N1			
78	7		6	Play	N1			
80	10		7	Play	N1			
80	12		8	Play	N1			
80	13		9	Play	N1			
85	3		10	Don't Play	N1			
90	2		11	Don't Play	N1			
90	6		12	Play	N1			
95	4		13	Play	N1			
96	14		14	Play	N1			

SLIQ

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Data structure: class list and attribute lists

Humidity (%)	Class List Index		Index	Class	Leaf
65	8		1	Play	N1
70	1		2	Don't Play	N1
70	5		3	Don't Play	N1
70	11		4	Don't Play	N1
75	9		5	Play	N1
78	7		6	Play	N1
80	10		7	Play	N1
80	12		8	Play	N1
80	13		9	Play	N1
85	3		10	Don't Play	N1
90	2		11	Don't Play	N1
90	6		12	Play	N1
95	4		13	Play	N1
96	14	\rightarrow	14	Play	N1

The class list The attribute list for Humidity

 Value
 Class
 Frequency

 <=65</td>
 Play
 1

 <=70</td>
 Play
 3

 <=70</td>
 DP
 1
 <=96 Play 9 <=96 DP 5

The entropies of various split points can be calculated from these figures. The next attribute list is then scanned



Data structure: class list and attribute lists

Humidity (%)	Class List Index
65	8
70	1
70	5
70	11
75	9
78	7
80	10
80	12
80	13
85	3
90	2
90	6
95	4

Class	Leaf
1 Play	
Don't Play	N1
Don't Play	N1
Don't Play	N1
Play	N1
Play	N1
Play	N1
Play	N1
Play	N1
Don't Play	N1
Don't Play	N1
Play	N1
Play	N1
	Play Don't Play Don't Play Don't Play Play Play Play Play Play Play Play

The Humidity attribute list is scanned again to update the class list



The attribute list for Humidity

SLIQ

Data structure: class list and attribute lists







SLIQ

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Data structure: class list and attribute lists





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SLIQ

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Data structure: class list and attribute lists

Humidity (%)	Class List Index		Index	Class	Lea
65	8	1 [1	Play	N2
70	1		2	Don't Play	N3
70	5		3	Don't Play	N3
70	11		4	Don't Play	N3
75	9		5	Play	N2
78	7	1 [6	Play	N3
80	10		7	Play	N2
80	12		8	Play	N2
80	13	1 [9	Play	N2
85	3		10	Don't Play	N2
90	2		11	Don't Play	N2
90	6	1 [12	Play	N2
95	4		13	Play	N2
96	14		14	Play	N3



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SLIQ

Humidity (%)	Class List Index		Index	Class	Leaf	Node:	N2	
65	8		1	Play	N2	Value	Class	Frequenc
70	1		2	Don't Play	N3	<=65	Plav	1
70	5		3	Don't Play	N3	V=03	ricty	
70	11		4	Don't Play	N3	***		***
75	9		5	Play	N2	<=80	Play	7
78	7		6	Play	N3	<=80	DP	2
80	10		7	Play	N2			
80	12		8	Play	N2	Node:	N3	
80	13		9	Play	N2	Value	Class	Frequenc
85	3		10	Don't Play	N2	<=85	DP	1
90	2		11	Don't Play	N2		υ.	-
90	6		12	Play	N2	***	***	***
95	4	1	13	Play	N2	<=96	Play	2
96	14		14	Play	N3	<=96	DP	3

SLIQ

- Motivations (review):
 - Previous algorithms consider only memoryresident data
 - At any time, only the class list and 1 attribute list in memory
 - A new layer (vs. the child nodes of a single node) is created by at most 2 scans of each attribute list
 - In determining the entropy of a split on a noncategorical attribute, the attribute values have to be sorted
 - Presorting: each attribute list is sorted only once

SPRINT

- Motivations:
 - The class list in SLIQ has to reside in memory, which is still a bottleneck for scalability
 - Can the decision tree building process be carried out by multiple machines in parallel?
 - Frequent lookup of the central class list produces a lot of network communication in the parallel case

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SPRINT

- Proposed Solutions
 - Eliminate the class list
 - Class labels distributed to each attribute list
 - => Redundant data, but the memory-resident and network communication bottlenecks are removed
 - Each node keeps its own set of attribute lists => No need to lookup the node information
 - Each node is assigned a partition of each attribute list. The nodes are ordered so that the combined lists of non-categorical attributes remain sorted
 - Each node produces its local histograms in parallel, the combined histograms can be used to find the best splits

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Bayesian Methods

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Naïve Bayes

- New data point to classify: $X=(x_1,x_2,...x_m)$
- - Calculate P(C/X) for each class C_i.
 - Select C_i for which P(C_i/X) is maximum

$$\begin{array}{ll} P(C_i/X) &= P(X/C_i) \; P(C_i) \; / \; P(X) \\ &\propto \; P(X/C_i) \; P(C_i) \\ &\propto \; P(x_1/C_i) \; P(x_2/C_i) \ldots P(x_m/C_i) \; P(C_i) \end{array}$$

- Naïvely assumes that each x_i is independent
- We represent $P(X/C_i)$ by P(X), etc. when unambiguous

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Bayesian Belief Networks

- Naïve Bayes assumes independence between attributes - Not always correct!
- If we don't assume independence, the problem becomes exponential – every attribute can be dependent on every other attribute.
- Luckily, in real life most attributes don't depend (directly) on other attributes.
- A Bayesian network explicitly encodes dependencies between attributes.

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Bayesian Belief Network



Conditional Probability Table for LungCancer

FH,S FH,!S !FH,S !FH,!S LC 0.8 0.5 0.7 0.1 _{!LC} 0.2 0.5 0.3 0.9

 $P(X) = P(x_1 | Parents(x_1)) P(x_2 | Parents(x_2))...P(x_m | Parents(x_m))$ e.g. P(PositiveXRay, Dyspnea)

Maximum Entropy Approach

- Think emails, keywords, spam / non-spam
- Given a new data point X={x₁,x₂,...,x_m} to classify calculate P(C_i/X) for each class C_i.
- Select C_i for which P(C_i/X) is maximum

$$P(C_i/X) = P(X/C_i) P(C_i) / P(X)$$

$$\propto P(X/C_i) P(C_i)$$

- Naïve Bayes assumes that each x_i is independent
- Instead estimate P(X/C_i) directly from training data: support_{Ci}(X)
 - Problem: There may be no instance of X in training data.
- Training data is usually sparse
- Solution: Estimate P(X/C_i) from available features in training data: P(Y_i/C_i) might be known for several Y_i

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Background: Shannon's Entropy

- An expt has several possible outcomes
- In N expts, suppose each outcome occurs M times
- This means there are N/M possible outcomes
- To represent each outcome, we need log N/M bits.
 - This generalizes even when all outcomes are not equally frequent.
 - Reason: For an outcome j that occurs M times, there are N/M equi-probable events among which only one cp to j
- Since $p_i = M / N$, information content of an outcome is $-\log p_i$
- So, expected info content: $H = -\sum p_i \log p_i$

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Maximum Entropy Principle

- Entropy corresponds to the disorder in a system
 - Intuition: A highly ordered system will require less bits to represent it
- If we do not have evidence for any particular order in a system, we should assume that no such order exists
- The order that we know of can be represented in the form of constraints
- Hence, we should maximize the entropy of a system subject to the known constraints
- If the constraints are consistent, there is a unique solution that maximizes entropy.

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Max Ent in Classification

- Among the distributions P(X/C_i), choose the one that has maximum entropy.
- Use the selected distribution to classify according to bayesian approach.

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Distribution of a Dataset

- Let T_k be a bit-vector (0010110) representing the presence/absence of N items in a record; $k = (1...2^N)$
 - T_k's are the possible *outcomes* of each record
- Our first task is to find P(T_k) for each k
- Then, to estimate P(X), we can just add the P(T_k)'s for all T_k's that satisfy X

Constraints on the Distribution

- P(Y_i) = d_i (say) is known for several Y_i
- Let there be M such Yi's
- For each such Y_i, we have a constraint:

$$\sum_{(k: T_k \text{ satisfies } Y_j)} P(T_k) = d_j$$

We also have: $\sum_k P(T_k) = 1$

Maximum Entropy

Find P(Tk) that satisfies these constraints, while assuming nothing else about the distribution

- Maximize entropy $(-\Sigma_k P(T_k) \log P(T_k))$ subject to constraints
- Theorem: Resulting distribution can be written as a product:

```
P(T_k) = \mu_0 \prod_{\text{(constraint j satisfied by Tk)}} \mu_j
```

- where there is a μ_i for each constraint
- μ_0 is to ensure that $\Sigma_k P(T_k) = 1$
- If we can compute the μ_j values, we are done.

Generalized Iterative Scaling **Algorithm**

N items, M constraints

$$P(X_k) = 1 / 2^{N_{ij}}$$
 for $k = (1...2^{N})$; Uniform distribution

$$\mu_i$$
 = 1 # for j = (1...M)

while all constraints not satisfied:

for each constraint Ci:

$$S_j = \sum_{(k: T_k \text{ satisfies } Y_j)} P(X_k)$$

$$\mu_i$$
*= d_i / S_i

$$P(X_k) = \mu_0 \prod_{(j \text{ satisfied by } T_k)} \mu_j$$

μ_0 is to ensure that $\Sigma_k P(X_k) = 1$

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Example

- Imagine emails represented as sets of keywords and being classified as spam/non-spam
- Let us focus on 3 keywords A, B, C.
- From the training data, let us say we get 4 "constraints" for the
 - P(A) = 0.2 = d_1 (say)

 - P(B) = 0.3 = d_2
 P(C) = 0.1 = d_3
 - $P(AB) = 0.1 = d_4$
- Now, our task is to use the GIS algorithm to determine P(ABC).

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- Define T_i as a bit-vector representing the presence/absence of keywords.
- E.g. T_3 = 011 represents the presence of B,C and absence of A.
- Note that P(T_3) is "not" the same as P(BC) since the latter doesn't care about the presence/absence of A.

```
T_0 = 000
                The previous 4 constraints can be rewritten in
T_1 = 001
                 terms of the T_i's:
T_2 = 010
T_3 = 011
                 P(A) = P(T_4) + P(T_5) + P(T_6) + P(T_7) = 0.2
T_4 = 100
                 P(B) = ... = 0.3
T_5 = 101
T_{6} = 110
                P(C) = ... = 0.1
T_7 = 111
                P(AB) = P(T_6) + P(T_7) = 0.1
                        //AB is satisfied by T_6 and T_7
```

```
S_1 = P(T_4) + P(T_5) + P(T_6) + P(T_7) ----(1)
 S_2 = ... -----(2)
 S 3 = ... -----(3)
 S_4 = P(T_6) + P(T_7) -----(4)
 Start GIS with P(T_i) = 1/8 = 0.125 (for all i)
 Also, set mu_1 = mu_2 = mu_3 = mu_4 = 1 and mu_0 = 1
 There are 4 mu's because there are 4 constraints.
 Next, we calculate S_i for each constraint i, as per (1), (2),
   (3), (4) above.
 S_1 = 1/8 + 1/8 + 1/8 + 1/8 = 0.5
 _{\text{similarly}}, S_{2} = S_{3} = 0.5, S_{4} = 0.25
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```

```
S_1 is 0.5; but we want it to be 0.2 (since P(A) = 0.2). Since S_1 is the sum of some P(T_i)'s in equation (1), we want to reduce these P(T_i)'s. We want to scale them down by 0.2 / 0.5. So we set: mu_i *= d_i / S_i. Thus, we get:
       mu_1 = 1 * 0.2 / 0.5 = 0.4
       mu 2 = 1 * 0.3 / 0.5 = 0.6
       mu_3 = 1 * 0.1 / 0.5 = 0.8
mu_4 = 1 * 0.1 / 0.25 = 0.4
  Using these mu's, we recalculate P(T_i)'s as:
 P(T_i) = product of those mu_j's whose cp constraint is satisfied by T_i
  Thus:
 P(T_0) = 1
                        // T_0 (000) doesn't satisfy any constraint
 P(T_1) = mu_3 // T_1 (001) satisfies constraint 3 only
 P(T 2) = mu 2
 P(T_3) = mu_2 * mu_3 // T_3 (011) satisfies constraints 2 & 3
 P(T_4) = mu_1
 P(T_5) = mu_1 * mu_3
P(T_6) = mu_1 * mu_2 * mu_4 // T_6 (110) satisfies constraints 1, 2 & 4
 P(T_7) = mu_1 * mu_2 * mu_3 * mu_4 // T_7 (111) satisfies all 4 constraints
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```

But sum of above P(T_i)'s might not turn out to be 1. Infact, it turns out to be 2.5152 for this example. So we scale all of them down by 2.5152 to make the sum equal 1. Then, we get:

P(T_0) = 1 / 2.5152 = 0.4 (approx) P(T_1) = 0.08 P(T_2) = 0.24 P(T_3) = 0.048 P(T_4) = 0.16 P(T_5) = 0.032 P(T_6) = 0.04 P(T_7) = 0.008

That was the 1st iteration of GIS. These numbers are closer to the actual P(T_i) values. For example, we know that P(A)=0.2, P(B)=0.3, P(C)=0.1. If A,B,C are mutually exclusive, then P(A or B or C) = 0.6 (the sum). Notice that P(T_0) above is 0.4 which is 1 - 0.6. If we run the algorithm for more iterations we get better results.

Our task was to determine P(ABC). So we just output the value of P(T $_{-}$ 7) above.