

# Large Scale Hierarchical Classification: Foundations, Algorithms and Applications

**Huzefa Rangwala**



Department of Computer Science  
MLBio+ Laboratory  
Fairfax, Virginia, USA

**CS 584, Fall 2016**

**11/14/2016**

# Roadmap

## 1 Introduction and Background

- Motivation
- Hierarchical Classification (HC) problem description
- Challenges
- Methods for solving HC

## 2 State-of-the-Art HC Approaches

- Parent-child regularization
- Cost-sensitive learning

## 3 Learning from Multiple Hierarchies

## 4 Inconsistent Hierarchy

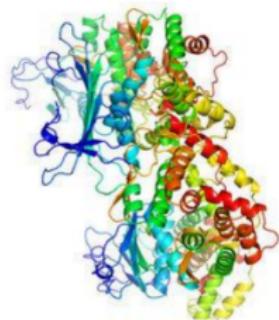
## 5 Conclusion

# Motivation

- Exponential growth in data (image, text, video) over time
  - Big data era - megabytes & gigabytes to terabytes & petabytes
  - growth in almost all fields - astronomical, biological, web content



Astronomy



Proteins

primates use their knowledge about the social world in which they live to form more complex alliances with each other than do other animals.

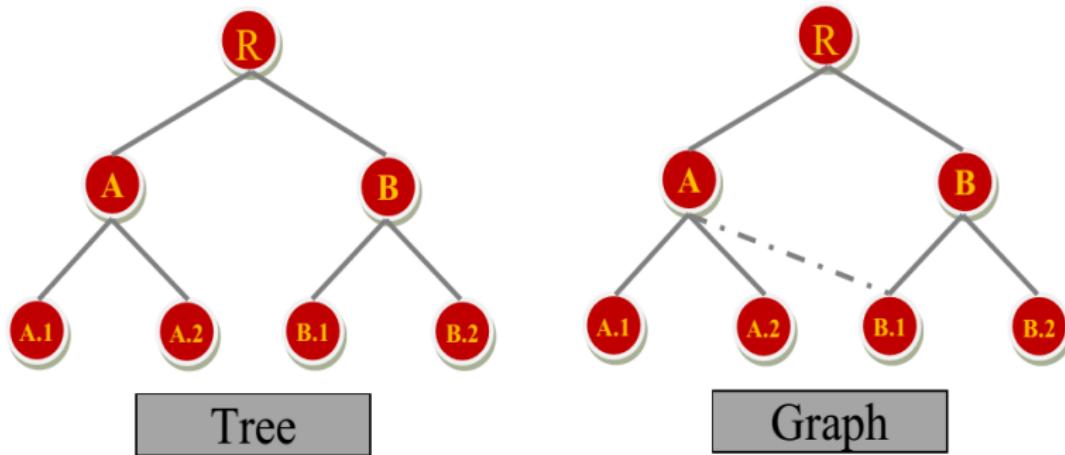
This social intelligence hypothesis is supported by a strong correlation between the size of the group, and hence complexity of the social world, and the relative size of the neocortex – the outer surface layer of the brain that is mainly responsible for conscious thinking – in various species of nonhuman primates. This result seems to reflect a limitation on the number (and/or quality) of relationships that an animal of a given species can keep track of simultaneously. Just as a computer's ability to handle complex tasks is limited by the size of its memory and processor, so the brain's ability to manipulate information about the constantly changing social domain may be limited by the size of its neocortex.

In evolutionary terms, the correlation between group size and neocortex size suggests that it was the need to live in larger groups that drove the evolution of large

Text

# Data Organization

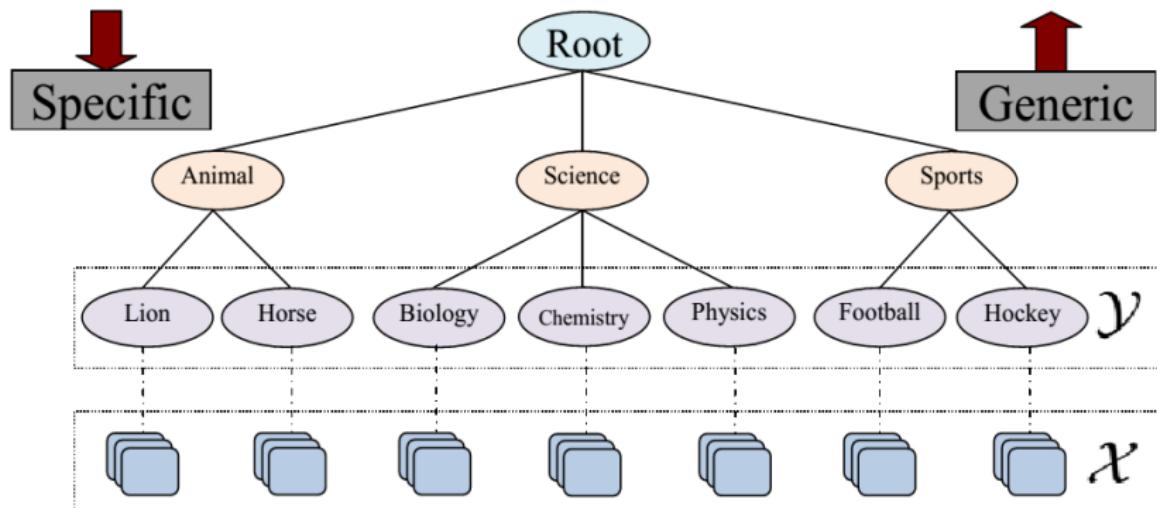
- Organize data into structure
  - tree, graph [LSHTC, BioASQ and ILSVRC challenge]



- Useful in various applications
  - query search, browsing and categorizing products

# Hierarchical Structure

- Classes organized into the hierarchical structure
- **Generic ( $\uparrow$ )** to **specific ( $\downarrow$ )** categories in top-down order



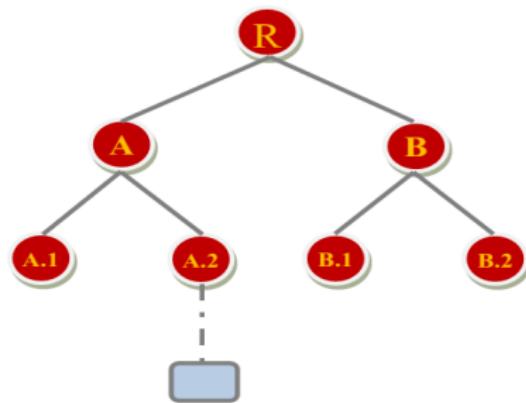
## Goal

Given hierarchy of classes **exploit the hierarchical structure** to learn models and classify unlabeled test examples (instances) to one or more nodes in the hierarchy

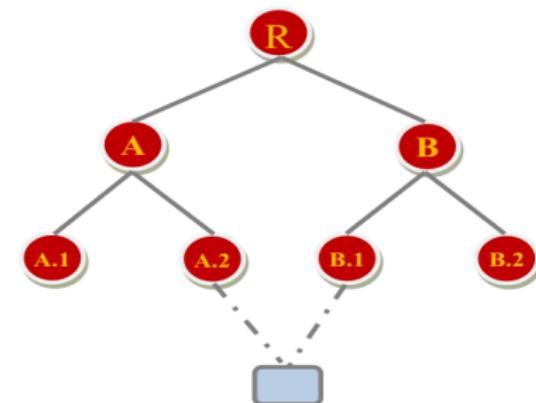
# Challenges - I

## Single label vs. multi-label

- **Single label classification** - each example belongs exclusively to one class only
- **Multi-label classification** - example may belong to more than one class



Single Label

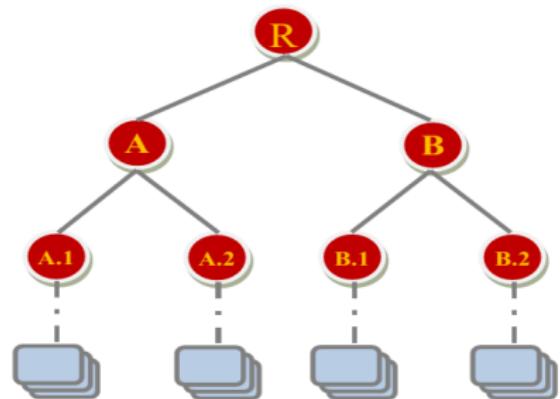


Multi Label

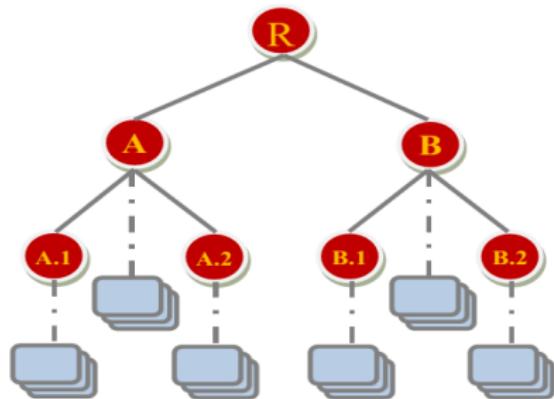
# Challenges - II

## Mandatory leaf node vs. internal node prediction

- Example may be assigned to internal nodes



Mandatory leaf node prediction

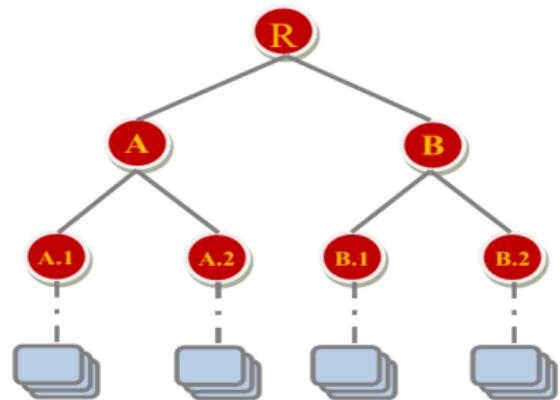


Internal/Orphan node prediction

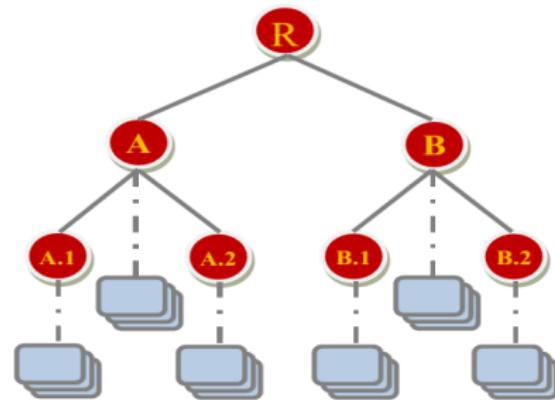
# Challenges - II

## Mandatory leaf node vs. internal node prediction

- Example may be assigned to internal nodes
- **Orphan node** detection problem



Mandatory leaf node prediction

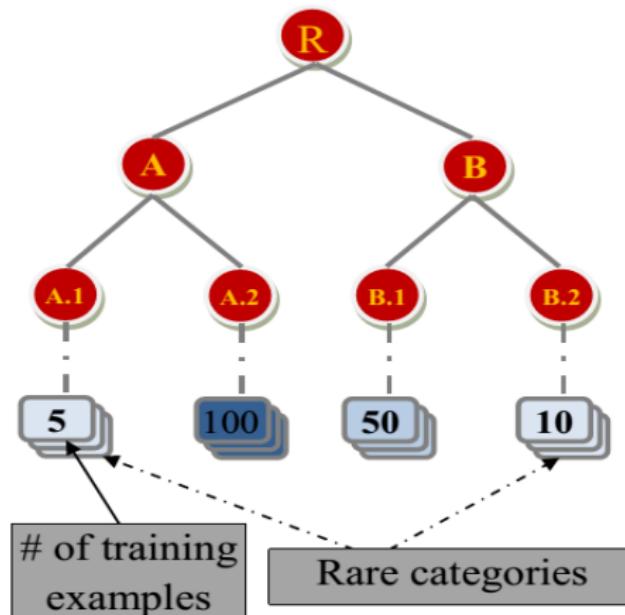


Internal/Orphan node prediction

# Challenges - III

## Rare categories

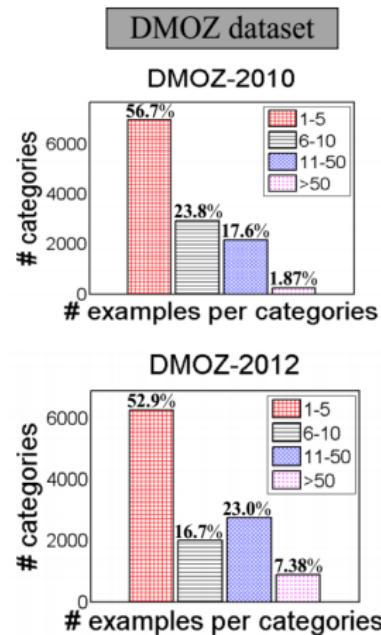
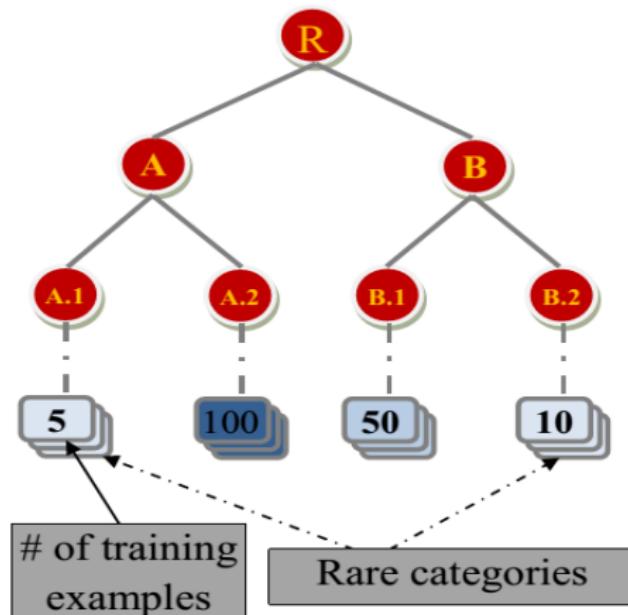
- Many classes with very few labeled examples



# Challenges - III

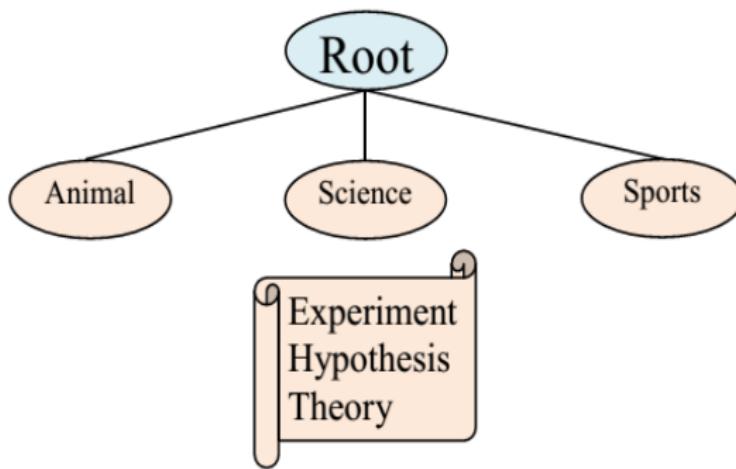
## Rare categories

- Many classes with very few labeled examples
- More prevalent in large scale datasets -  $\geq 70\%$  have  $\leq 10$  examples



## Feature selection

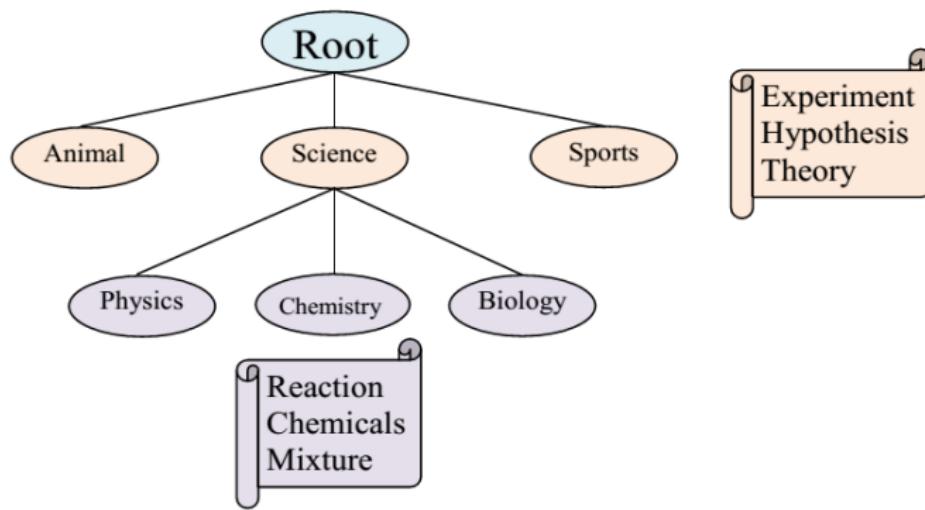
- All features are **not essential** to **discriminate** between classes
- Identify features to improve classification performance



# Challenges - IV

## Feature selection

- All features are **not essential** to **discriminate** between classes
- Identify features to improve classification performance



# Other Challenges

- **Parameter optimization**
  - incorporate relationships (**parent-child, siblings**) information

# Other Challenges

- **Parameter optimization**

- incorporate relationships (**parent-child, siblings**) information

- **Scalability**

- large # of classes, features and examples require **distributed computation**

Dataset	#Training examples	#Leaf node (classes)	#Features	#Parameters	Parameter size (approx)
DMOZ-2010	128,710	12,294	381,580	4,652,986,520	18.5 GB
DMOZ-2012	383,408	11,947	348,548	4,164,102,956	16.5 GB

# Other Challenges

- **Parameter optimization**

- incorporate relationships (**parent-child, siblings**) information

- **Scalability**

- large # of classes, features and examples require **distributed computation**

Dataset	#Training examples	#Leaf node (classes)	#Features	#Parameters	Parameter size (approx)
DMOZ-2010	128,710	12,294	381,580	4,652,986,520	18.5 GB
DMOZ-2012	383,408	11,947	348,548	4,164,102,956	16.5 GB

- **Inconsistent hierarchy**

- not suitable for classification (more details later)

# Notation

$n = \#$  of training examples (instances)

$\mathcal{N}$  = set of nodes in the hierarchy

$\mathcal{C}(t) =$  children of node  $t$

$D =$  dimension of each instance

$L =$  set of leaf node (classes)

$\pi(t) =$  parent of node  $t$

$$\mathbf{X} = \begin{bmatrix} x_1^1 & x_1^2 & \dots & x_1^D \\ x_2^1 & x_2^2 & \dots & x_2^D \\ \vdots & \vdots & \ddots & \vdots \\ x_n^1 & x_n^2 & \dots & x_n^D \end{bmatrix}_{\text{INSTANCES}} \quad \mathbf{Y} = \begin{bmatrix} 1 & 0 & \dots & 1 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 1 \\ 1 & 0 & \dots & 0 & 0 \end{bmatrix}_{\text{CLASSES}}$$

INSTANCE MATRIX

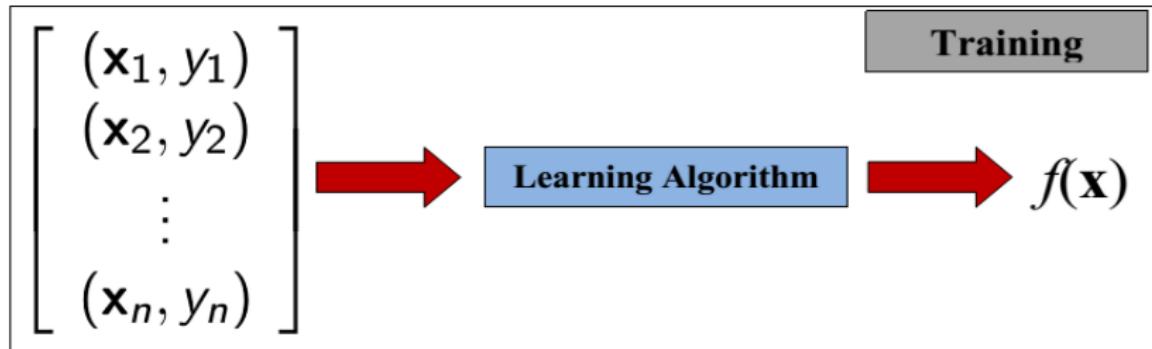
LABEL MATRIX

$$\mathbf{W} = \begin{bmatrix} w_1^1 & w_1^2 & \dots & w_1^D \\ w_2^1 & w_2^2 & \dots & w_2^D \\ \vdots & \vdots & \ddots & \vdots \\ w_L^1 & w_L^2 & \dots & w_L^D \end{bmatrix}_{\text{CLASSES}}$$

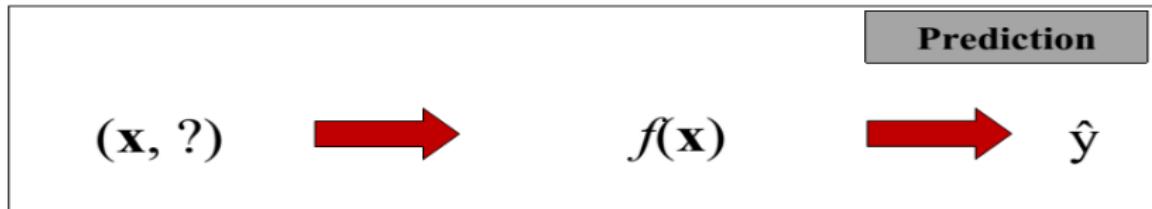
WEIGHT MATRIX

# Classification

**Training** - Learn mapping function using training data



**Testing** - Predict the label of test example



# Learning Algorithm: General Formulation

Combination of two terms:

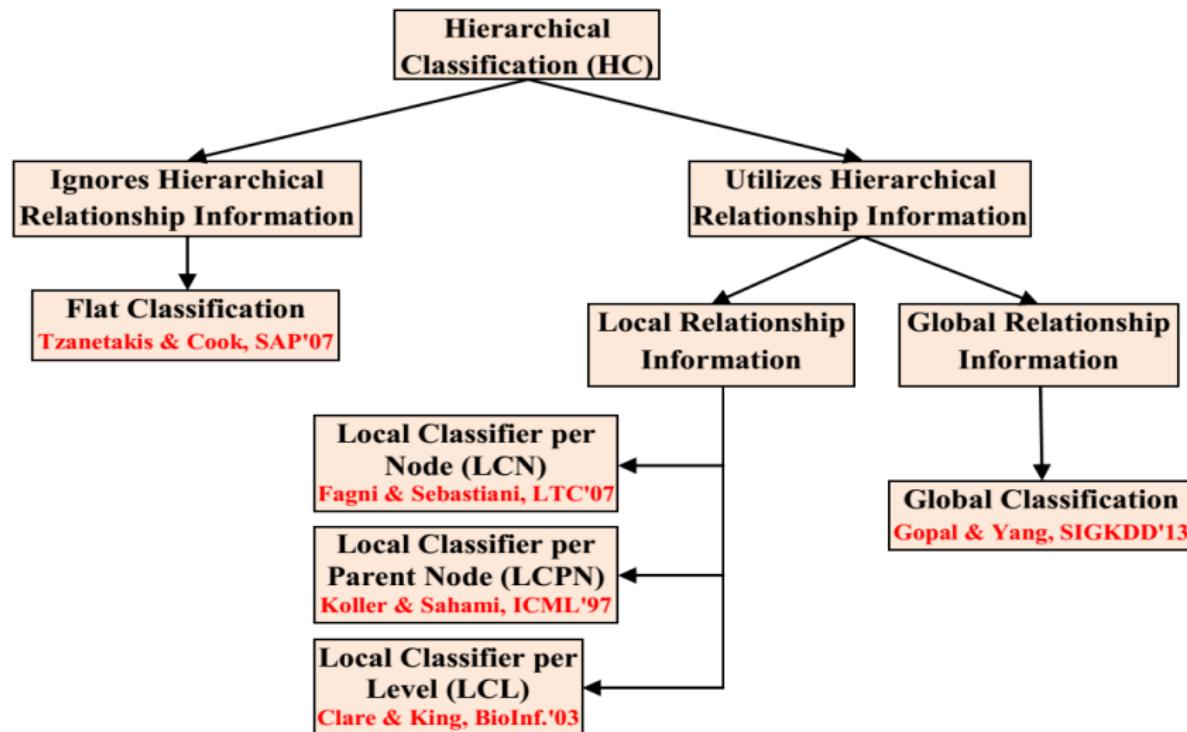
- 1 **Empirical loss** - controls how well the learnt models fits the training data
- 2 **Regularization** - prevent models from over-fitting and encodes additional information such as hierarchical relationships

$$\min_{\mathbf{W}} \mathcal{L}(f(\mathbf{X}, \mathbf{W}), \mathbf{Y}) + \lambda \Omega(\mathbf{W})$$

**Empirical Loss**

**Regularization**

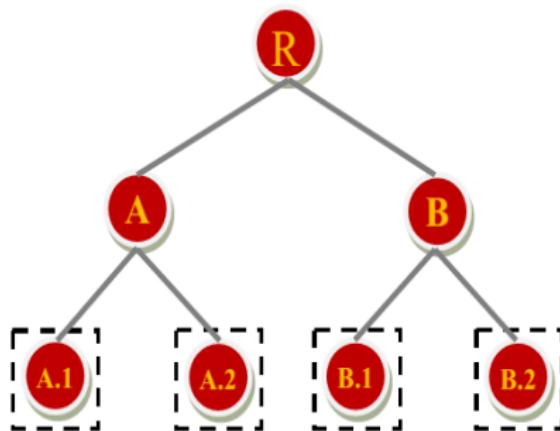
# Different Approaches for Solving HC Problem



# Flat Classification Approach

- Simplest method (ignores hierarchy)
- Learn discriminant classifiers for each leaf node in the hierarchy
- Unlabeled test example classified using the rule:

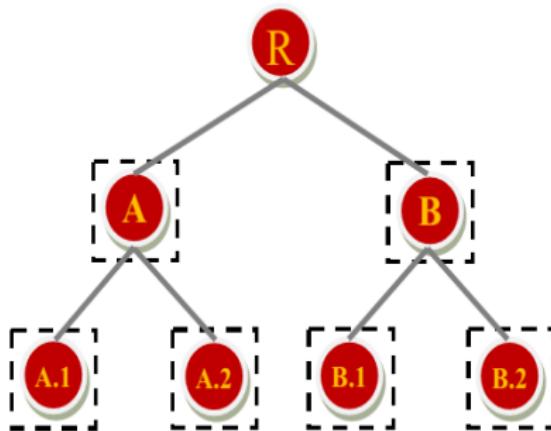
$$\hat{y} = \underset{y \in \mathcal{Y}}{\operatorname{arg\ max}} f(\mathbf{x}, y | \mathbf{w})$$



# Local Classification Approach - I

## Local Classifier per Node (LCN)

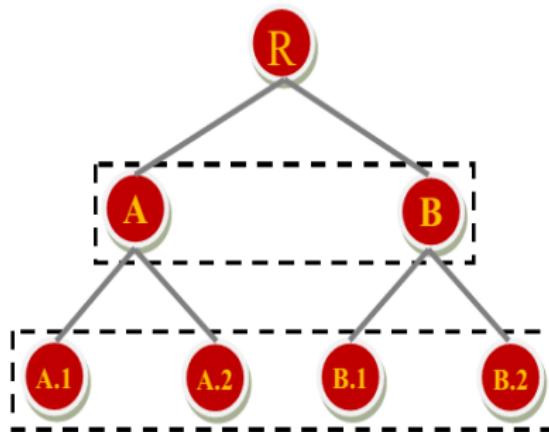
- Learn binary classifiers for all non-root nodes
- Goal is to effectively discriminate between the siblings
- Top-down approach is followed for classifying unlabeled test examples



# Local Classification Approach - II

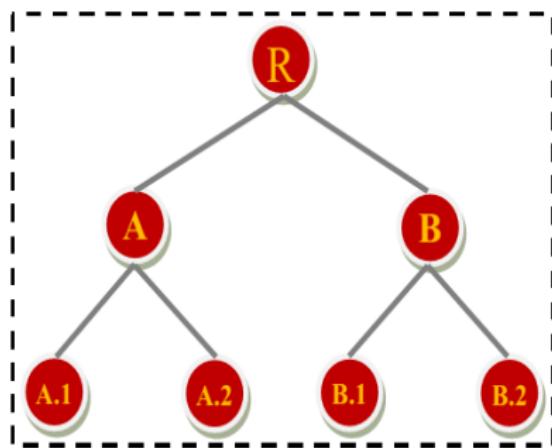
## Local Classifier per Level (LCL)

- Learn multi-class classifiers for all levels in the hierarchy
- Least popular among local approaches
- Prediction inconsistency may occur and hence post-processing step is required



# Global Classification Approach

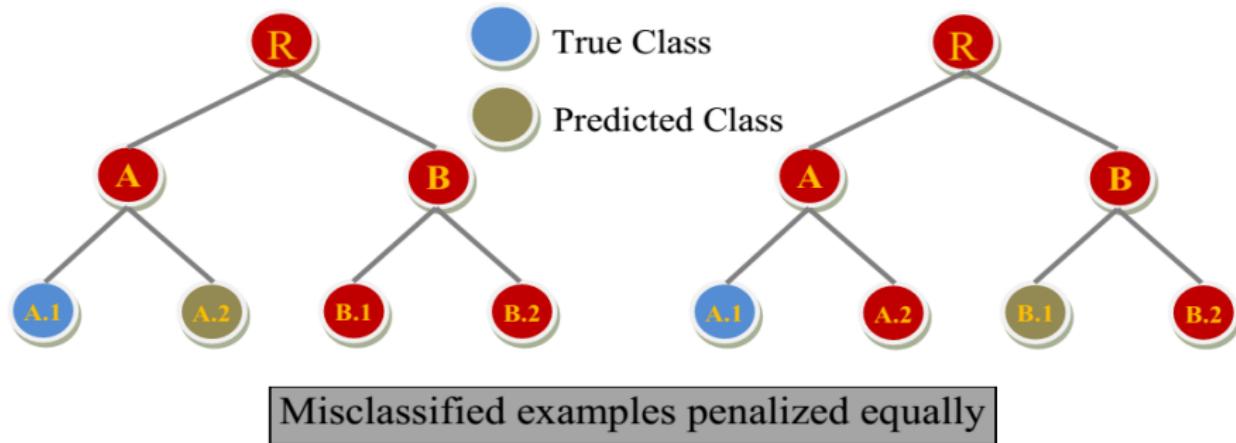
- Learn global function considering all hierarchical relationships
- Often referred as Big-Bang approach
- Unlabeled test instance is classified using an approach similar to flat or local methods



# Evaluation Metrics - I

## Flat evaluation measures

- Misclassifications treated equally

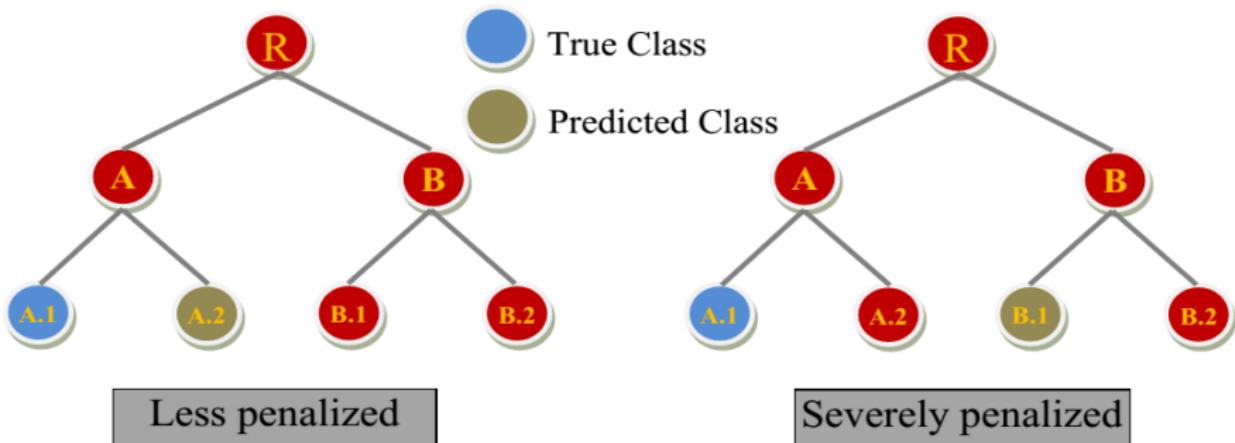


- Common evaluation metrics:
  - **Micro-F1** - gives equal weightage to all examples, dominated by common class
  - **Macro-F1** - gives equal weightage to each class

# Evaluation Metrics - II

## Hierarchical evaluation measures

- Hierarchical distance between the true and predicted class taken into consideration for performance evaluation



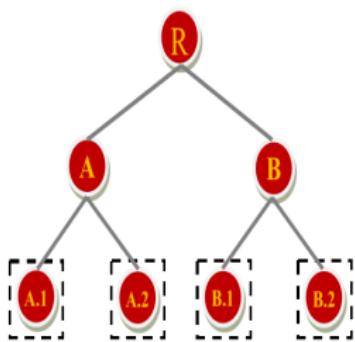
- Common evaluation metrics:
  - **Hierarchical-F1** - common ancestors between true and predicted class
  - **Tree Error** - average hierarchical distance b/w true and predicted class

# Multi-Task Learning (MTL)

- Involves **joint training** of multiple related tasks to improve generalization performance
- Independent learning problems can utilize the **shared knowledge**
- Exploits **inductive biases** that are helpful to all the related tasks
  - similar set of parameters
  - common feature space

## Motivation

- Traditional approach learn classifiers for each leaf node (task) to discriminate one class from other



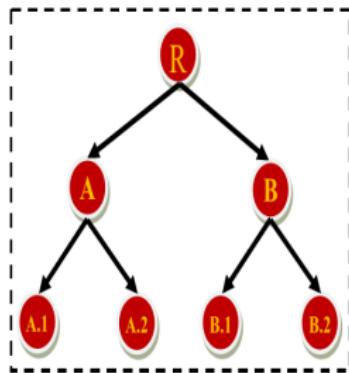
$$\min_{\mathbf{w}_t} \frac{1}{2} \|\mathbf{w}_t\|_2^2 + C \sum_{i=1}^n \left[ 1 - \mathbf{Y}_{it} \mathbf{w}_t^T \mathbf{x}_i \right]_+$$

- Works well if:
  - Dataset is small
  - Balanced
  - Sufficient positive examples per class to learn generalized discriminant function

## Drawbacks

- Real world datasets suffers from rare categories issue  
Remember: **70% classes have less than 10 examples per class**
- Large number of classes (**scalability issue**)

## Motivation - II



- Can we improve the performance of **data sparse** leaf nodes by taking advantage of **data rich** nodes at higher levels?
- Incorporate **inter-class dependencies** to improve classification
  - examples belonging to Soccer category is less likely to belong to Software category

$$\min_{\mathbf{w}_t} \frac{1}{2} \|\mathbf{w}_t - \mathbf{w}_{\pi(t)}\|_2^2 + C \sum_{k \in \mathcal{C}(t)} \sum_{i=1}^n [1 - \mathbf{Y}_{ik} \mathbf{w}_t^T \mathbf{x}_i]_+$$

## Objective

- How to effectively incorporate the hierarchical relationships into the objective function to improve generalization performance
- Make it scalable for larger datasets

# Proposed Formulation

- Enforces model parameters (weights) to be similar to the parent in regularization
- Proposed state-of-the-art: HR-SVM and HR-LR global formulation

## HR-SVM

$$\min_{\mathbf{w}} \sum_{t \in \mathcal{N}} \frac{1}{2} \|\mathbf{w}_t - \mathbf{w}_{\pi(t)}\|_2^2 + C \sum_{k \in L} \sum_{i=1}^n \left[ 1 - \mathbf{Y}_{ik} \mathbf{w}_k^T \mathbf{x}_i \right]_+$$

### Internal Node

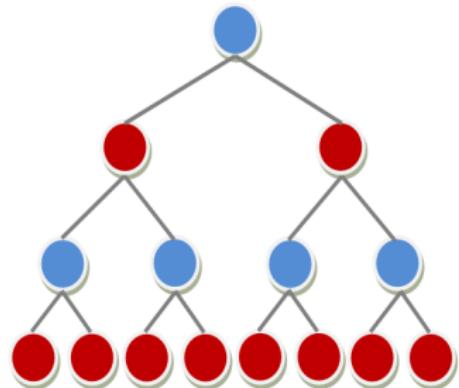
$$\min_{\mathbf{w}_t} \frac{1}{2} \|\mathbf{w}_t - \mathbf{w}_{\pi(t)}\|_2^2 + \frac{1}{2} \sum_{c \in \mathcal{C}(t)} \|\mathbf{w}_c - \mathbf{w}_t\|_2^2$$

### Leaf Node

$$\min_{\mathbf{w}_t} \frac{1}{2} \|\mathbf{w}_t - \mathbf{w}_{\pi(t)}\|_2^2 + \frac{1}{2} \sum_{i=1}^n \left[ 1 - \mathbf{Y}_{it} \mathbf{w}_t^T \mathbf{x}_i \right]_+$$

# Proposed Parallel Implementation

- Each node is independent of all other nodes except its neighbours
- Objective function is block separable. Therefore, Parallel Block Coordinate Descent (CD) can be used for optimization



Alternate level optimized in each iteration

- 1 Fix odd-levels parameters, optimize even-levels in parallel
- 2 Fix even-levels parameters, optimize odd-levels in parallel
- 3 Repeat until convergence

- Extended to graph by first finding the minimum graph coloring [Np-hard] and repeatedly optimizing nodes with the same color in parallel during each iteration

# Experiments

## Dataset description

- Wide range of single and multi-label dataset with varying number of features and categories were used for model evaluation

Datasets	# Features	# Categories	Type	Avg # labels (per instance)
<b>CLEF</b>	89	87	Single-label	1
<b>RCV1</b>	48,734	137	Multi-label	3.18
<b>IPC</b>	541,869	552	Single-label	1
<b>DMOZ-SMALL</b>	51,033	1,563	Single-label	1
<b>DMOZ-2010</b>	381,580	15,358	Single-label	1
<b>DMOZ-2012</b>	348,548	13,347	Single-label	1
<b>DMOZ-2011</b>	594,158	27,875	Multi-label	1.03
<b>SWIKI-2011</b>	346,299	50,312	Multi-label	1.85
<b>LWIKI</b>	1,617,899	614,428	Multi-label	3.26

Table: Dataset statistics

# Flat Baselines Comparison

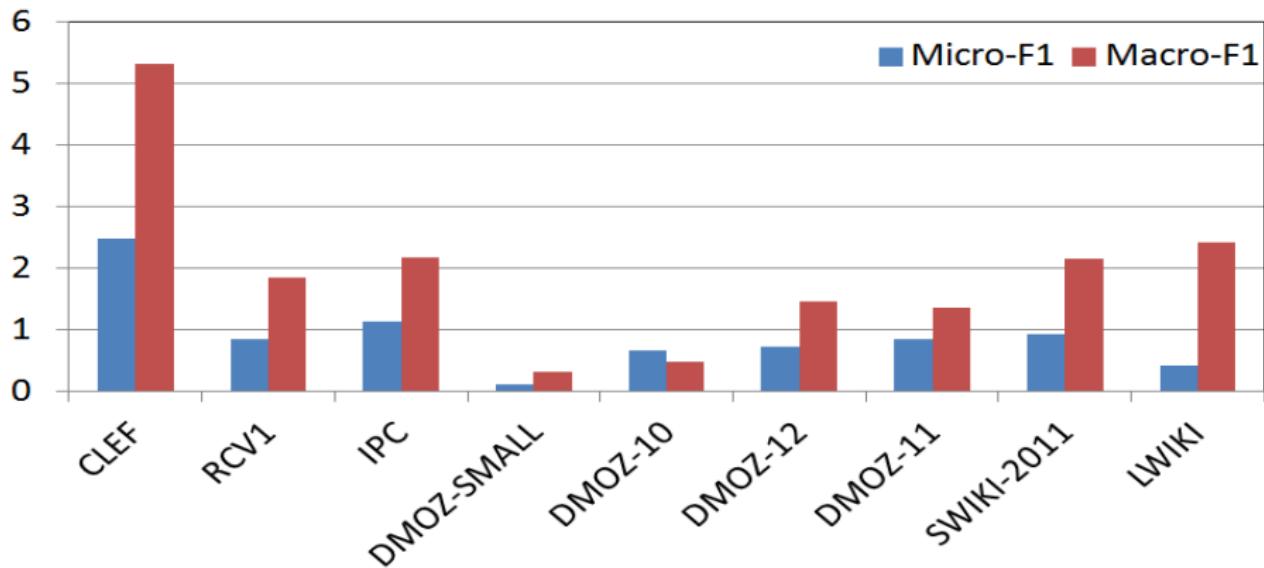


Figure: Performance improvement: HR-SVM vs. SVM

# Hierarchical Baselines Comparison

Datasets	HR-SVM	HR-LR	TD	HSVM	OT	HBLR
<b>CLEF</b>	80.02	80.12	70.11	79.72	73.84	<b>81.41</b>
<b>RCV1</b>	<b>81.66</b>	81.23	71.34	NA	NS	NA
<b>IPC</b>	54.26	55.37	50.34	NS	NS	<b>56.02</b>
<b>DMOZ-SMALL</b>	45.31	45.11	38.48	39.66	37.12	<b>46.03</b>
<b>DMOZ-2010</b>	<b>46.02</b>	45.84	38.64	NS	NS	NS
<b>DMOZ-2012</b>	<b>57.17</b>	53.18	55.14	NS	NS	NS
<b>DMOZ-2011</b>	<b>43.73</b>	42.27	35.91	NA	NS	NA
<b>SWIKI-2011</b>	<b>41.79</b>	40.99	36.65	NA	NA	NA
<b>LWIKI</b>	<b>38.08</b>	37.67	NA	NA	NA	NA

[NA - Not Applicable; NS - Not Scalable]

Table: Micro-F1 performance comparison

## Runtime Comparison - hierarchical baselines

Datasets	HR-SVM	HR-LR	TD	HSVM	OT	HBLR
<b>CLEF</b>	0.42	1.02	0.13	3.19	1.31	3.05
<b>RCV1</b>	0.55	11.74	0.21	NA	NS	NA
<b>IPC</b>	6.81	15.91	2.21	NS	NS	31.20
<b>DMOZ-SMALL</b>	0.52	3.73	0.11	289.60	132.34	5.22
<b>DMOZ-2010</b>	8.23	123.22	3.97	NS	NS	NS
<b>DMOZ-2012</b>	36.66	229.73	12.49	NS	NS	NS
<b>DMOZ-2011</b>	58.31	248.07	16.39	NA	NS	NA
<b>SWIKI-2011</b>	89.23	296.87	21.34	NA	NA	NA
<b>LWIKI</b>	2230.54	7282.09	NA	NA	NA	NA

[NA - Not Applicable; NS - Not Scalable]

Table: Training runtime comparison (in mins) but on several nodes.

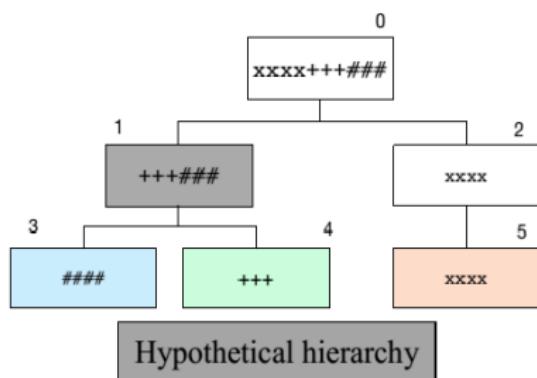
## Motivation

- Drawbacks of Recursive Regularization
  - scalable, but more expensive to train than flat classification
  - requires specialized implementation and communication between processing node
- Does not deal with class imbalance directly

## Objective

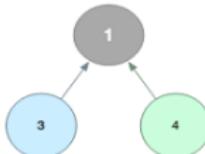
- Decouple models so that they can be trained in parallel without dependencies between models
- Account for class imbalance in the optimization framework

# Hierarchical Regularization Re-examination - I

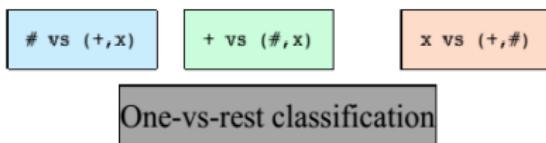


$$\min_{\mathbf{W}} \mathcal{L}(f(\mathbf{X}, \mathbf{W}), \mathbf{Y}) + \lambda \Omega(\mathbf{W})$$

Empirical Loss      Regularization



Regularizer promotes similarity



Loss promotes dissimilarity

# Hierarchical Regularization Re-examination - II

- Opposing learning influences:
  - **loss term** - model for a node is forced to be dissimilar to all other nodes
  - **regularization term** - model is forced to be similar to its neighbors; greater similarity to nearer neighbors
- Resultant effect:
  - Mistakes on negative examples that come from near nodes is less severe than those coming from far nodes while still taking advantage of the hierarchy

# Cost-sensitive Loss

- Consider the loss term for class "t" which is separable over examples

$$\sum_i \text{loss}(y_i, \mathbf{w}_i^T \mathbf{x}_i)$$

- Each loss value is multiplied by importance of the example for this class

$$\sum_i \text{loss}(y_i, \mathbf{w}_i^T \mathbf{x}_i) \times \phi(t, y_i)$$

- This is an example of "instance-based" cost sensitive learning

$$c_i^t = \phi(t, y_i)$$

# Hierarchical Costs

How to define costs based on hierarchy?

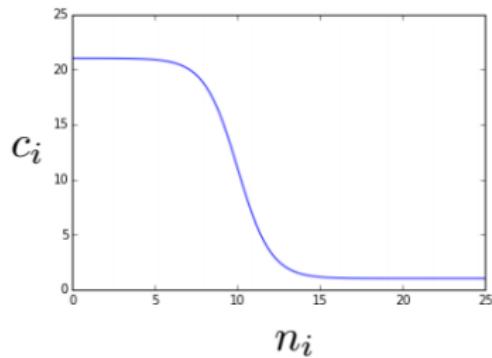
- **Tree Distance (TrD)** - undirected graph distance between nodes
- **Number Common Ancestors (NCA)** - the number of ancestors in common to target class and class label
- **Exponentiated Tree Distance (ExTrD)** - squash tree distance into a suitable range using validation

# Imbalance Costs

- Using the same formulation of cost-sensitive learning, data imbalance can also be addressed

$$c_i = 1 + L/[1 + \exp|n - n_0|]$$

- Due to very large skew, inverse class size can result in extremely large weights. Fix using squashing function shown in Fig.



- Multiply to combine with Hierarchical costs

$n_i$  = num examples  
 $n_0, L$  = user defined constants

# Experiments

## Dataset

- For comparison purpose same dataset has been used as proposed in the paper [**Gopal and Yang, SIGKDD'13**]

## Comparison Methods

### Flat baseline

- LR** - one-vs-rest binary logistic regression is used in the conventional flat classification setting

### Hierarchical baselines

- Top-down Logistic Regression (TD-LR)** - one-vs-rest multi-class classifier trained at each internal node
- HR-LR [Gopal and Yang, SIGKDD'13]** - a recursive regularization approach based on hierarchical relationships

# Results (Hierarchical Costs)

Datasets		Micro-F1 ( $\uparrow$ )	Macro-F1 ( $\uparrow$ )	hF1 ( $\uparrow$ )	TE ( $\downarrow$ )
CLEF	LR	79.82	53.45	85.24	0.994
	TrD	80.02	55.51	<b>85.39</b>	0.984
	NCA	80.02	57.48	85.34	0.986
	ExTrD	<b>80.22</b>	<b>57.55†</b>	85.34	<b>0.982</b>
DMOZ-SMALL	LR	46.39	30.20	67.00	3.569
	TrD	<b>47.52‡</b>	<b>31.37‡</b>	<b>68.26</b>	<b>3.449</b>
	NCA	47.36‡	31.20‡	68.12	3.460
	ExTrD	47.36‡	31.19‡	68.20	3.456
IPC	LR	55.04	48.99	72.82	1.974
	TrD	55.24‡	50.20‡	73.21	1.954
	NCA	<b>55.33‡</b>	<b>50.29‡</b>	<b>73.28</b>	<b>1.949</b>
	ExTrD	55.31‡	<b>50.29‡</b>	73.26	1.951
RCV1	LR	78.43	60.37	80.16	0.534
	TrD	79.46‡	60.61	82.83	0.451
	NCA	<b>79.74‡</b>	60.76	<b>83.11</b>	<b>0.442</b>
	ExTrD	79.33‡	<b>61.74†</b>	82.91	0.466

Table: Performance comparison of hierarchical costs

# Results (Imbalance Costs)

Datasets		Micro-F1 (↑)	Macro-F1 (↑)	hF1 (↑)	TE (↓)
CLEF	IMB + LR	79.52	53.11	85.19	1.002
	IMB + TrD	79.92	52.84	85.59	0.978
	IMB + NCA	79.62	51.89	85.34	0.994
	IMB + ExTrD	<b>80.32</b>	<b>58.45</b>	<b>85.69</b>	<b>0.966</b>
DMOZ-SMALL	IMB + LR	48.55‡	32.72‡	68.62	3.406
	IMB + TrD	<b>49.03‡</b>	33.21‡	69.41	3.334
	IMB + NCA	48.87‡	33.27‡	69.37	3.335
	IMB + ExTrD	<b>49.03‡</b>	<b>33.34‡</b>	<b>69.54</b>	<b>3.322</b>
IPC	IMB + LR	55.04	49.00	72.82	1.974
	IMB + TrD	55.60‡	<b>50.45†</b>	73.56	1.933
	IMB + NCA	55.33	50.29	73.28	1.949
	IMB + ExTrD	<b>55.67‡</b>	50.42	<b>73.58</b>	<b>1.931</b>
RCV1	IMB + LR	78.59‡	60.77	81.27	0.511
	IMB + TrD	<b>79.63‡</b>	61.04	<b>83.13</b>	<b>0.435</b>
	IMB + NCA	79.61	61.04	82.65	0.458
	IMB + ExTrD	79.22	<b>61.33</b>	82.89	0.469

Table: Performance comparison with imbalance cost included

# Results (our best with other methods)

Datasets		Micro-F1 ( $\uparrow$ )	Macro-F1 ( $\uparrow$ )	hF1 ( $\uparrow$ )	TE ( $\downarrow$ )
CLEF	TD-LR	73.06	34.47	79.32	1.366
	LR	79.82	53.45	85.24	0.994
	HR-LR	80.12	55.83	NA	NA
	HierCost	<b>80.32</b>	<b>58.45†</b>	<b>85.69</b>	<b>0.966</b>
DMOZ-SMALL	TD-LR	40.90	24.15	<b>69.99</b>	<b>3.147</b>
	LR	46.39	30.20	67.00	3.569
	HR-LR	45.11	28.48	NA	NA
	HierCost	<b>49.03‡</b>	<b>33.34‡</b>	69.54	3.322
IPC	TD-LR	50.22	43.87	69.33	2.210
	LR	55.04	48.99	72.82	1.974
	HR-LR	55.37	49.60	NA	NA
	HierCost	<b>55.67‡</b>	<b>50.42†</b>	<b>73.58</b>	<b>1.931</b>
RCV1	TD-LR	77.85	57.80	<b>88.78</b>	0.524
	LR	78.43	60.37	80.16	0.534
	HR-LR	<b>81.23</b>	55.81	NA	NA
	HierCost	79.22‡	<b>61.33</b>	82.89	<b>0.469</b>

Table: Performance comparison of HierCost with other baseline methods

# Runtime comparison

Datasets	TD-LR	LR	HierCost
<b>CLEF</b>	<1	<1	<1
<b>DMOZ-SMALL</b>	4	41	40
<b>IPC</b>	27	643	453
<b>RCV1</b>	20	29	48
<b>DMOZ-2010</b>	196	15191	20174
<b>DMOZ-2012</b>	384	46044	50253

Table: **Total training runtimes (in mins)**

- Freely available for research and education purpose at:
  - <https://cs.gmu.edu/~mlbio/HierCost/>
- Software: implemented in python using **scikit-learn** machine learning and **svmlight-loader** package
- Other prerequisite package:
  - numpy
  - scipy
  - networkx
  - pandas

## Motivation

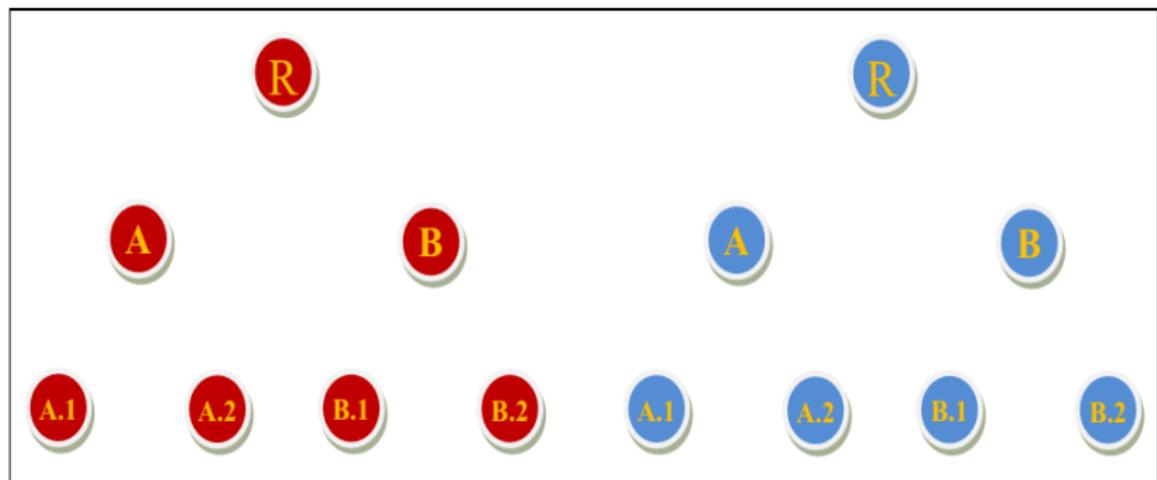
- Hierarchies are so common that sometimes multiple hierarchies classify similar data
- Heterogenous label view provide additional knowledge which should be exploited by learners
- Examples
  - **protein structure classification** - several hierarchical schemes for organizing proteins based on curation process or 3D structure
  - **web-page classification** - several hierarchy exist for categorizing such as DMOZ and wikipedia datasets

## Objective

- Utilize multiple hierarchical label views in multi-task learning context to improve classification performance

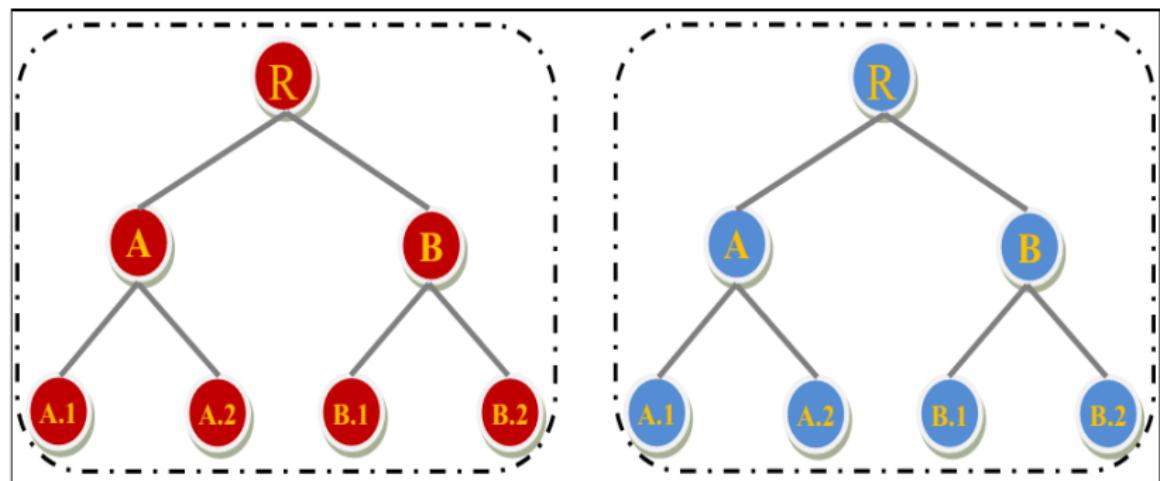
# Three Different Learning Settings - I

- (i) **Single Task Learning (STL)** - each task model parameters learned independently



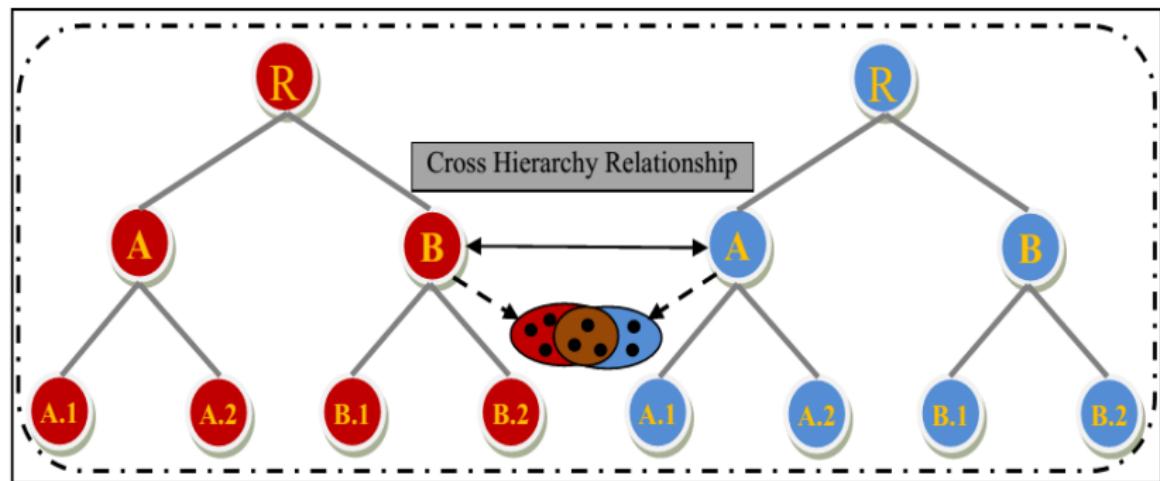
## Three Different Learning Settings - II

- (ii) **Single Hierarchy Multi-Task Learning (SHML)** - relationship between tasks within a hierarchy are combined individually



## Three Different Learning Settings - III

(iii) **Multiple Hierarchy Multi-Task Learning (MHMTL)** - relationship between tasks from different hierarchies are extracted using common examples



# MTL Formulations

- General MTL formulation:

$$\sum_{t=1}^T \sum_{i=1}^{n_t} \mathcal{L}(f(\mathbf{x}_i, \mathbf{W}_t), y_i) + \lambda \Omega\left(\{\mathbf{W}_t\}_{t=1}^T\right)$$

Empirical Loss

Regularization

- Different MTL formulation based on regularization:

- Sparse** - All tasks share a single set of useful features

$$\Omega(\mathbf{W}) = \|\mathbf{W}\|_{2,1}$$

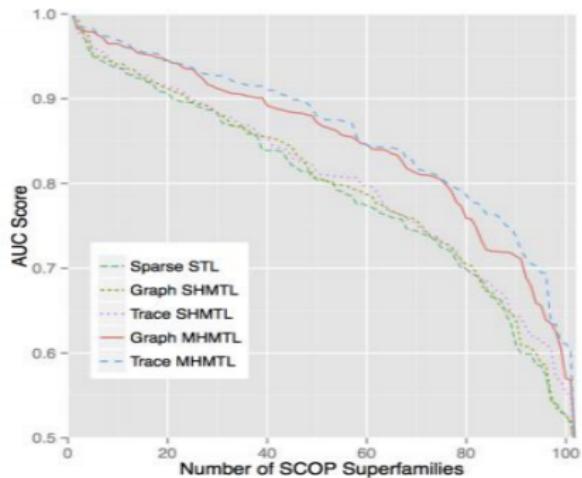
- Graph Regularization** - Related tasks have similar parameters

$$\Omega(\mathbf{W}) = \sum_{(a,b) \in \mathcal{E}} \|\mathbf{W}_a - \mathbf{W}_b\|_2^2$$

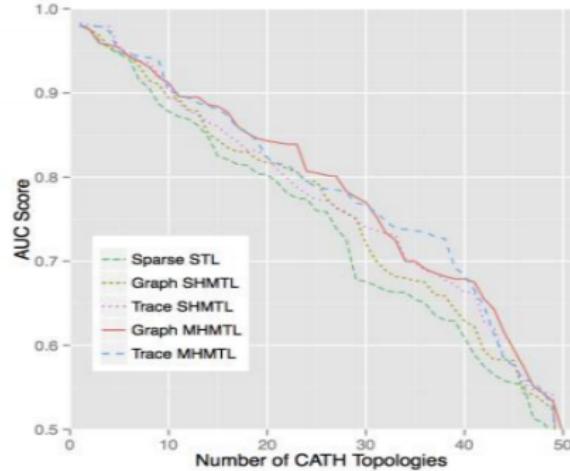
- Trace** - Task parameters are drawn from a low dimensional sub-space

$$\Omega(\mathbf{W}) = \|\mathbf{W}\|_* = \text{TraceNorm}(\mathbf{W})$$

# Performance: AUC Comparison

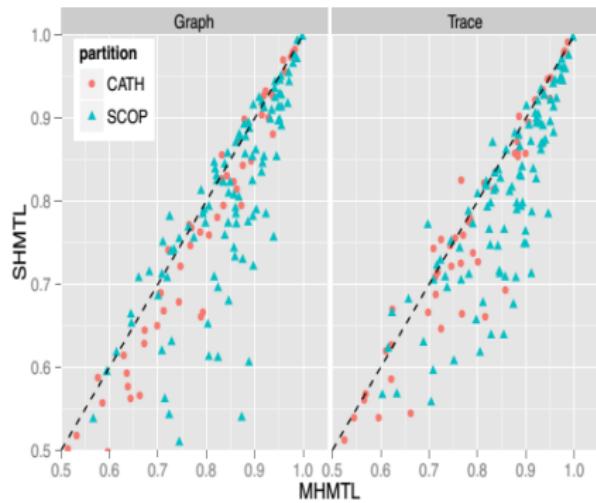
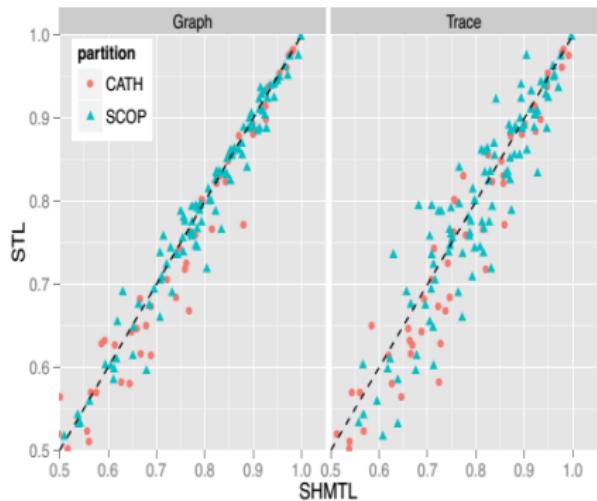


**SCOP**



**CATH**

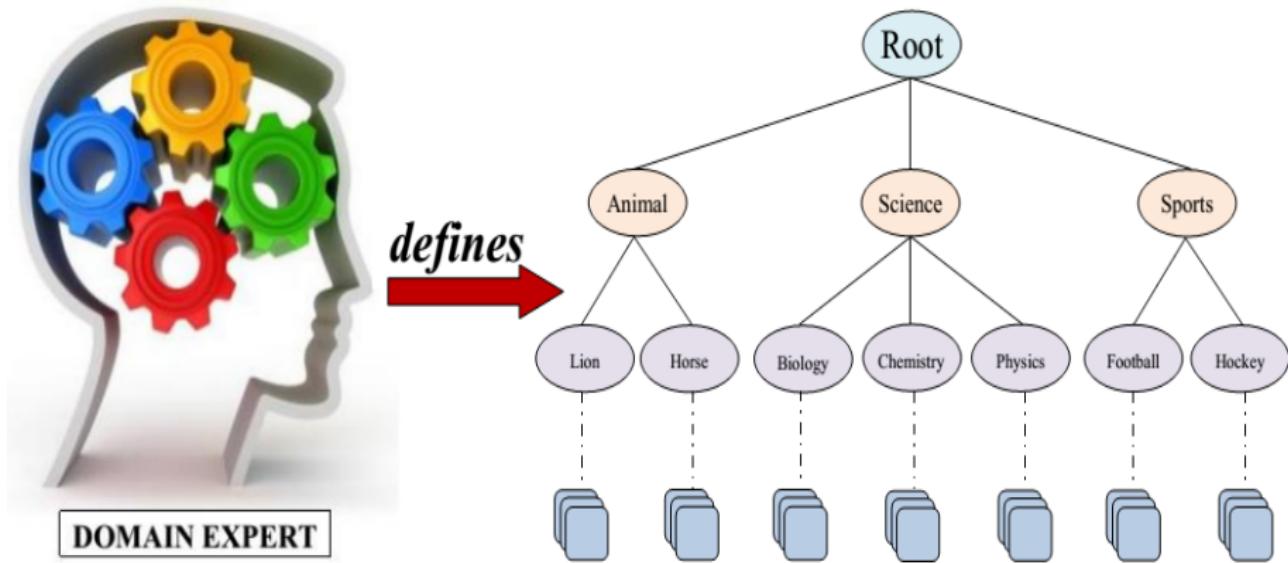
# STL, SHMTL and MHMTL Comparison



# Motivation

## Predefined Hierarchy

- Hierarchy defined by the domain experts
- Reflects human-view of the domain - may not be optimal for machine learning classification algorithms



# Case Study

## Question

- Can we trust the predefined expert's hierarchy for achieving the good classification performance?
- Can we tweak (adjust) the hierarchy to improve the performance?

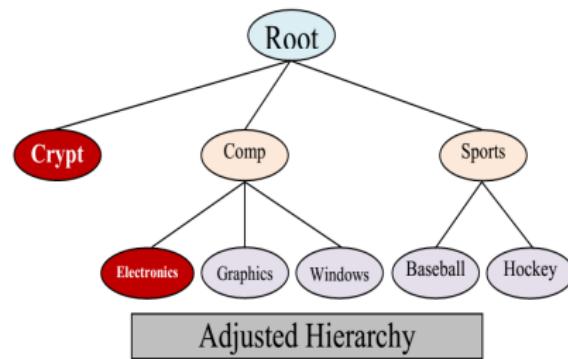
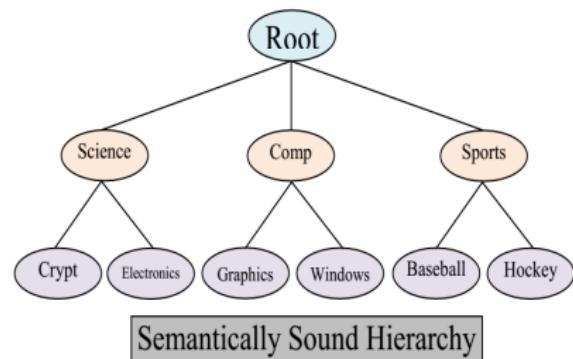
# Case Study

## Question

- Can we trust the predefined expert's hierarchy for achieving the good classification performance?
- Can we tweak (adjust) the hierarchy to improve the performance?

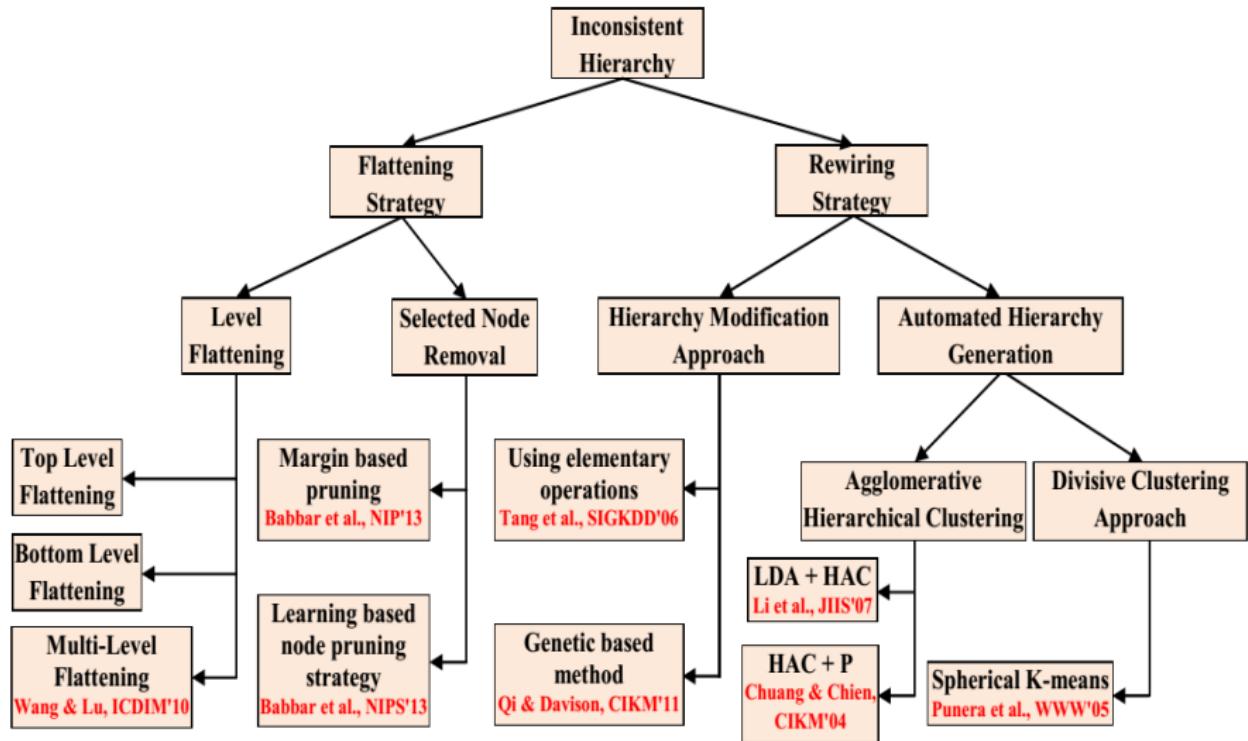
## Answer

- Case study on subset of newsgroup dataset



"Adjusted hierarchy classification performance **comparatively better** than semantically sound hierarchy"

# Literature Overview



# Hierarchy Modification Strategy

## Motivation

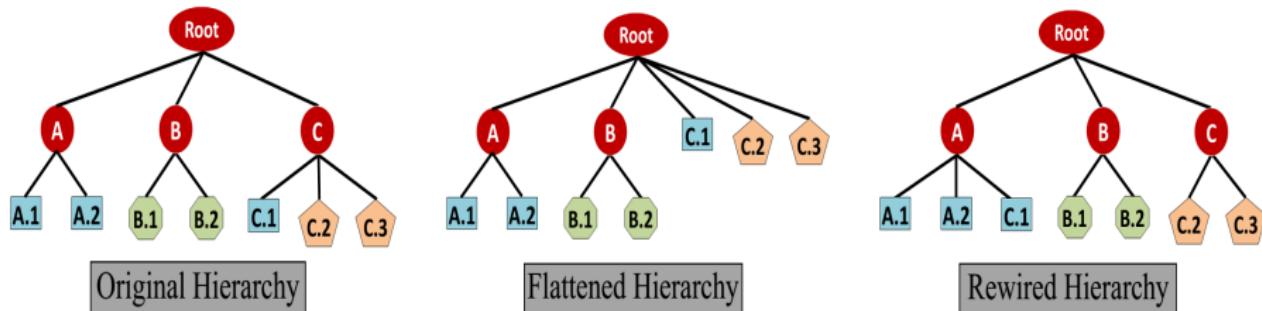
- For large scale datasets top-down (TD) hierarchical models are preferred over flat models due to computational benefit (training and prediction time)
- TD models performance suffers due to **error propagation** i.e. compounding of errors from misclassifications at higher levels which cannot be rectified at the lower levels

## Objective

- Modify predefined hierarchy by removing (flattening) or rewiring inconsistent nodes to improve the classification performance of TD models
- Reduces top-down error propagation due to less number of decisions for classifying unlabeled examples

# Flattening and Rewiring Strategy

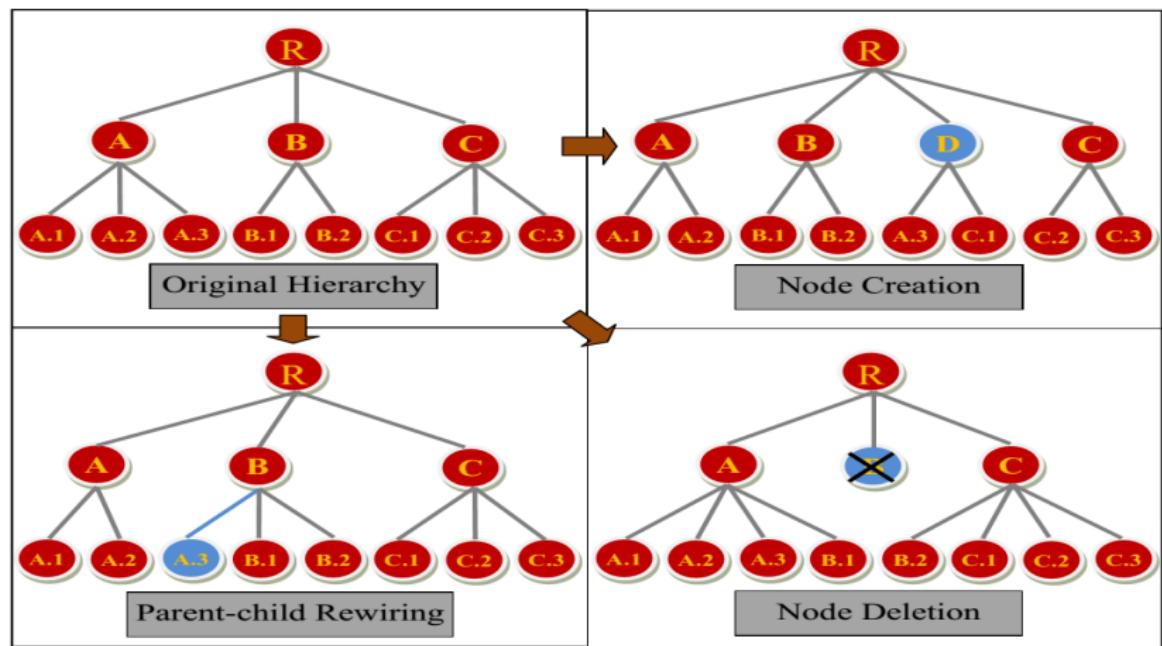
- Flattening strategy although useful upto certain extent has few limitations
  - Inability to deal with inconsistencies in different branches of the hierarchy



- Rewiring strategy can be used to resolve inconsistencies that occurs in different branch

# Proposed Rewiring Strategy

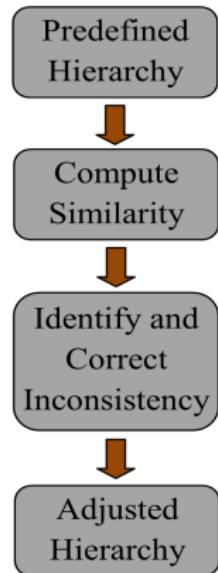
- Elementary operation: **node creation, parent-child rewiring, node deletion**



# Proposed Rewiring Strategy Algorithm

- Filter based approach for hierarchy modification

**Input:** Predefined hierarchy ( $H_0$ ), Train data ( $\mathcal{D}_t$ )



- 1 Compute pairwise similarity between classes defined in  $H_0$  on  $\mathcal{D}_t$
- 2 Group together most similar classes
- 3 Identify inconsistencies within the hierarchy
- 4 Apply elementary operations: node creation or parent-child rewiring to correct inconsistencies and obtain new hierarchy  $H_1$
- 5 Perform post-processing step (node deletion) on  $H_1$  to obtain new hierarchy  $H_2$
- 6 Train and evaluate hierarchical classification models on  $H_2$

# Performance Results

Datasets		Flattening Best TD Model (Flattening)	Rewiring Tang et al.	Rewiring Proposed Filter Model
CLEF	$\mu F_1(\uparrow)$	77.14 (0.01)	<b>78.12 (0.16)</b>	78.00 (0.22)
	$MF_1(\uparrow)$	46.54 (0.06)	<b>48.83<sup>‡</sup> (0.08)</b>	47.10 (0.03)
	$hF_1(\uparrow)$	79.06 (0.01)	<b>81.43 (0.03)</b>	80.14 (0.02)
DIATOMS	$\mu F_1(\uparrow)$	61.31 (0.53)	<b>62.34<sup>‡</sup> (0.28)</b>	62.05 <sup>‡</sup> (0.10)
	$MF_1(\uparrow)$	51.85 (0.23)	<b>53.81<sup>‡</sup> (0.11)</b>	52.14 <sup>‡</sup> (0.14)
	$hF_1(\uparrow)$	62.80 (0.04)	<b>64.28 (0.22)</b>	63.24 (0.13)
IPC	$\mu F_1(\uparrow)$	52.30 (0.12)	53.94 <sup>†</sup> (0.24)	<b>54.28<sup>†</sup> (0.18)</b>
	$MF_1(\uparrow)$	45.65 (0.11)	<b>46.10<sup>†</sup> (0.21)</b>	46.04 <sup>†</sup> (0.22)
	$hF_1(\uparrow)$	64.73 (0.12)	67.23 (0.24)	<b>68.34 (0.18)</b>
DMOZ-SMALL	$\mu F_1(\uparrow)$	46.61 (0.28)		<b>48.25<sup>‡</sup> (0.13)</b>
	$MF_1(\uparrow)$	31.26 (0.64)	NS	<b>33.92<sup>‡</sup> (0.22)</b>
	$hF_1(\uparrow)$	63.37 (0.44)		<b>66.18 (0.15)</b>
DMOZ-2010	$\mu F_1(\uparrow)$	42.37 (0.27)	NS	<b>43.10 (0.28)</b>
	$MF_1(\uparrow)$	30.11 (0.64)		<b>31.21 (0.34)</b>
DMOZ-2012	$\mu F_1(\uparrow)$	50.64 (0.22)		<b>51.82 (0.02)</b>
	$MF_1(\uparrow)$	30.58 (0.28)	NS	<b>31.24 (0.12)</b>
	$hF_1(\uparrow)$	73.19 (0.02)		<b>74.21 (0.03)</b>

# Runtime Comparison

Datasets	Flattening	Rewiring	
	Best TD Model (Flattening)	Tang et al.	Proposed Filter Model
<b>CLEF</b>	3.5	59	7.5
<b>DIATOMS</b>	10	268	24
<b>IPC</b>	830	26432	1284
<b>DMOZ-SMALL</b>	65	NS	168
<b>DMOZ-2010</b>	25600	NS	42000
<b>DMOZ-2012</b>	63000	NS	94800

Table: Total training runtimes (in mins)

# Conclusion

- Large scale hierarchical classification is an important research problem in machine learning community due to its wide applicability across several domains
- Discussed various challenges associated with the hierarchical classification
- Discussed various state-of-the-art existing approaches;
- Discussed Multiple Hierarchy MTL and Approaches for Resolving Inconsistencies
- Emerging topics:
  - Large-scale classification with deep hierarchies
  - Orphan node prediction

## References - I

- Gopal, Siddharth, and Yiming Yang. "Recursive regularization for large-scale classification with hierarchical and graphical dependencies." SIGKDD, 2013.
- Charuvaka, Anveshi, and Huzefa Rangwala. "HierCost: Improving Large Scale Hierarchical Classification with Cost Sensitive Learning." ECML, 2015.
- Tang, Lei, Jianping Zhang, and Huan Liu. "Acclimatizing taxonomic semantics for hierarchical content classification." SIGKDD, 2006.
- Li, Tao, Shenghuo Zhu, and Mitsunori Ogihara. "Hierarchical document classification using automatically generated hierarchy." Journal of Intelligent Information Systems 29.2 (2007): 211-230.
- Charuvaka, Anveshi, and Huzefa Rangwala. "Multi-task learning for classifying proteins using dual hierarchies." ICDM, 2012.
- Punera, Kunal, Suju Rajan, and Joydeep Ghosh. "Automatically learning document taxonomies for hierarchical classification." WWW, 2005.
- Qi, Xiaoguang, and Brian D. Davison. "Hierarchy evolution for improved classification." CIKM, 2011.
- Bennett, Paul N., and Nam Nguyen. "Refined experts: improving classification in large taxonomies." SIGIR, 2009.

## References - II

- Silla Jr, Carlos N., and Alex A. Freitas. "A survey of hierarchical classification across different application domains." DMKD, 2011.
- Naik, Azad, A. Charuvaka, and H. Rangwala. "Classifying documents within multiple hierarchical datasets using multi-task learning." ICTAI, 2013.
- Babbar, Rohit, et al. "On flat versus hierarchical classification in large-scale taxonomies." NIPS, 2013.
- Wang, Xiao-Lin, and Bao-Liang Lu. "Flatten hierarchies for large-scale hierarchical text categorization." ICDIM, 2010.
- Chuang, Shui-Lung, and Lee-Feng Chien. "A practical web-based approach to generating topic hierarchy for text segments." CIKM, 2004.
- Fagni, Tiziano, and Fabrizio Sebastiani. "On the selection of negative examples for hierarchical text categorization." LTC, 2007.
- Clare, Amanda, and Ross D. King. "Predicting gene function in *Saccharomyces cerevisiae*." Bioinformatics, 2003.
- Koller, Daphne, and Mehran Sahami. "Hierarchically Classifying Documents Using Very Few Words." ICML, 1997.

## References - III

- Xue et al. "Deep classification in large-scale text hierarchies." SIGIR, 2008.
- Tzanetakis, G., and P. Cook. "Musical genre classification of audio signals." IEEE transactions on Speech and Audio Processing, 2007.
- Gopal, Siddharth, et al. "Bayesian models for large-scale hierarchical classification." NIPS, 2012.
- Xiao, Lin, Dengyong Zhou, and Mingrui Wu. "Hierarchical classification via orthogonal transfer." ICML, 2011.
- Naik, Azad, and Huzefa Rangwala. "A ranking-based approach for hierarchical classification." DSAA, 2015.
- Tsochantaridis, Ioannis, et al. "Large margin methods for structured and interdependent output variables." JMLR, 2005.
- Liu, Tie-Yan, et al. "Support vector machines classification with a very large-scale taxonomy." SIGKDD, 2005.
- Caruana, Rich. "Multitask learning." Machine learning, 1997.
- Anveshi Charuvaka and Huzefa Rangwala. "Approximate block coordinate descent for large scale hierarchical classification." SAC, 2015.

## References - IV

- Dumais, Susan, and Hao Chen. "Hierarchical classification of Web content." SIGIR, 2000.
- Mineiro, Paul, and Karampatziakis, Nikos. "A Hierarchical Spectral Method for Extreme Classification." eprint arXiv:1511.03260 (NIPS workshop), 2015.
- Choromanska, Anna, et al. "Extreme Multi Class Classification." NIPS Workshop: eXtreme Classification, 2013.
- McCallum, Andrew, et al. "Improving Text Classification by Shrinkage in a Hierarchy of Classes." ICML, 1998.
- Babbar, Rohit, et al. "Maximum-margin framework for training data synchronization in large-scale hierarchical classification." NIP, 2013.
- Choromanska, Anna E., and John Langford. "Logarithmic time online multiclass prediction." NIPS, 2015.
- Prabhu, Yashoteja, and Manik Varma. "FastXML: a fast, accurate and stable tree-classifier for extreme multi-label learning." SIGKDD, 2014.
- Bhatia, Kush, et al. "Sparse Local Embeddings for Extreme Multi-label Classification." NIPS, 2015.

## References - V

- Naik, A., and Rangwala, H. "Filter based taxonomy modification for improving hierarchical classification." <http://arxiv.org/abs/1603.00772>, 2016.
- Peng, Hanchuan, Fuhui Long, and Chris Ding. "Feature selection based on mutual information criteria of max-dependency, max-relevance, and min-redundancy." PAMI, 2005.
- Ding, Chris, and Hanchuan Peng. "Minimum redundancy feature selection from microarray gene expression data." Journal of bioinformatics and computational biology, 2005.

# Thanks



## Ph.D. Students:



**Anveshi Charuvaka**



**Azad Naik**

Slides available for download at:

<https://cs.gmu.edu/~mlbio/sdm2016tutorial.html>