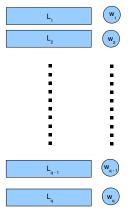
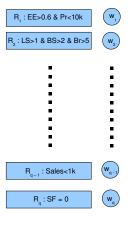
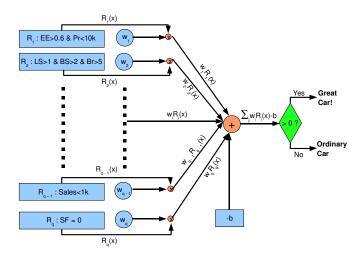
# Efficient Rule Ensemble Learning using Hierarchical Kernels

J. Saketha Nath Collaboration: Pratik J. and Ganesh R.

Indian Institute of Technology — Bombay







# Rule Ensembles — Key Features

- Highly interpretable hypothesis
  - $\blacksquare$  Small set of rules i.e., low q
  - Simple rules e.g., short conjunctive propositions

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  - $\blacksquare$  Small set of rules i.e., low q
  - Simple rules e.g., short conjunctive propositions
- Better generalization than conventional rule learners

## Rule Ensemble Learning — Formal Definition

#### Input:

- Training Set:  $\mathcal{D} = \{ (\mathbf{x}^1, y^1), ..., (\mathbf{x}^m, y^m) \}$ ,  $\mathbf{x}^i \in \mathbb{R}^n$  and  $y^i \in \{-1, 1\}$
- lacktriangle Basic propositions regarding input features (say, p in number)

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Numeric e.g., x_j \geq b and x_j \leq b
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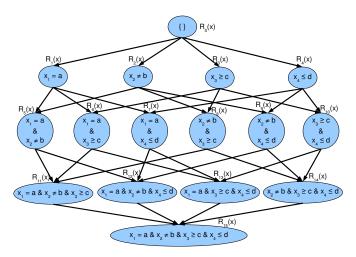
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Nominal e.g., x_i = a and x_i \neq a
Numeric e.g., x_j \geq b and x_j \leq b
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#### Goal:

- Construct conjunctive rules from basic propositions
  - Few in number
  - Short conjunctions
- Compute corresponding weights  $(\mathbf{w}, b)$

# Rule Ensemble Learning — Challenging task

Extremely large, atleast  $O(2^n)$ , rule space!



## Rule Ensembles — Existing Methods

```
\begin{split} & \mathsf{SLIPPER}_{(\mathsf{Cohen\&Singer},\ 99)} \colon \mathsf{AdaBoost} + \mathsf{RIPPER} - \mathsf{greedy} \\ & \mathsf{RuleFit}_{(\mathsf{Friedman\&Popescu},\ 08)} \colon \mathsf{ISLE} + \mathsf{decision}\ \mathsf{tree} - \mathsf{greedy} \\ & \mathsf{ELCS}_{(\mathsf{Gao}\ \mathsf{et.al.},\ 07)} \colon \mathsf{Genetic}\ \mathsf{Alg.} + \mathsf{post-pruning} - \mathsf{sub-optimal} \\ & \mathsf{ENDER}_{(\mathsf{Dembczynski}\ \mathsf{et.al.},\ 10)} \colon \mathsf{Minimization}\ \mathsf{of}\ \mathsf{empirical}\ \mathsf{risk} - \mathsf{greedy} \end{split}
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# Proposed Methodology — Overview

#### Optimal search for rules over all conjunctions

- Regularized loss minimization
- Convex formulation
- Discovers compact ruleset (small set with short rules)

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Efficient mirror-descent based active set method

■ Complexity: polynomial in active set size  $(\ll 2^p)$ 

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■ Complexity: polynomial in active set size  $(\ll 2^p)$ 

#### Key Reason for Efficiency:

(Large) sub-lattices with long rules are avoided

- Decision function<sup>1</sup>: sign  $(\sum_{v \in \mathcal{V}} w_v R_v(\mathbf{x}) b)$
- lacksquare  $l_1$  regularize to force many  $w_v$  to zero

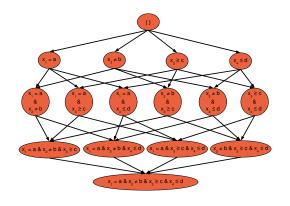
 $<sup>^{1}\</sup>mathcal{V}$  is index set for conjunctive lattice

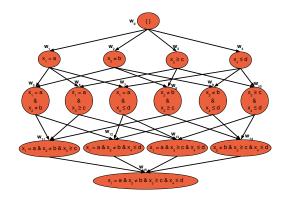
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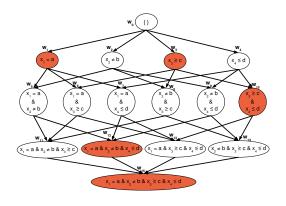
#### $l_1$ regularized formulation:

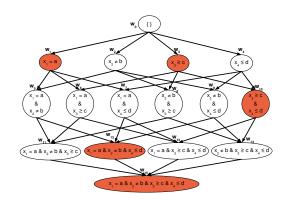
$$\min_{\mathbf{w},b} rac{1}{2} \left( \sum_{v \in \mathcal{V}} |w_v| 
ight)^2 + C \sum_{i=1}^m L \left( y^i, \sum_{v \in \mathcal{V}} w_v R_v(\mathbf{x}^i) - b 
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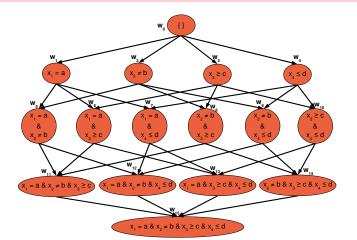


## Short-comings:

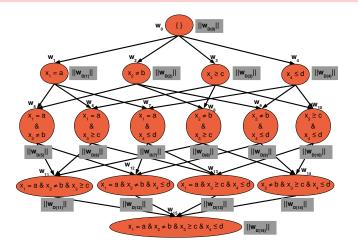
- long rules may be selected
- Computationally difficult problem

## Key Idea:

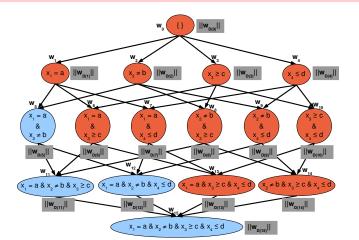
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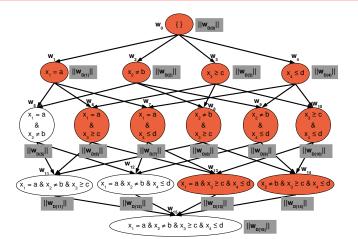
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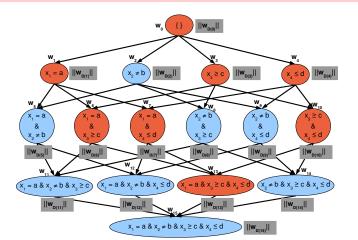
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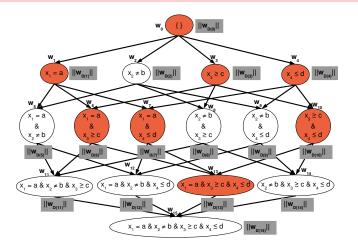
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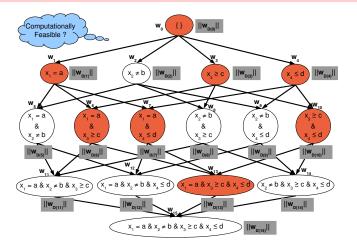
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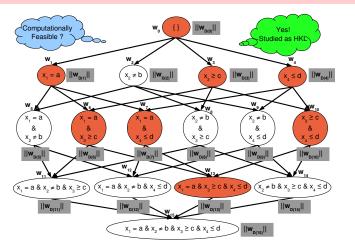
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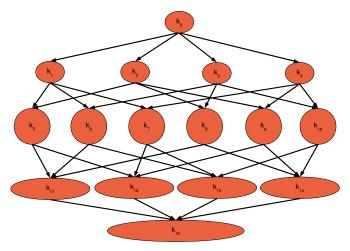


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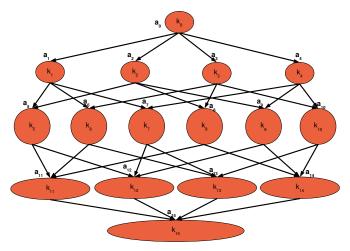


- Multiple Kernel Learning Optimal combination of given kernels
- Kernels arranged on DAG (lattice) are given

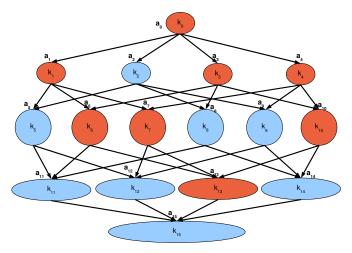
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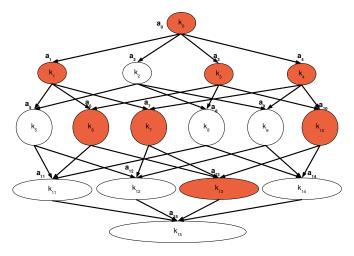
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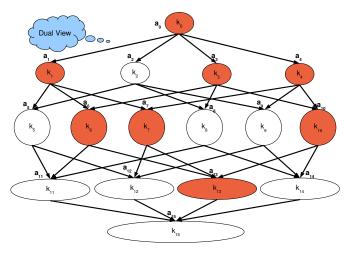
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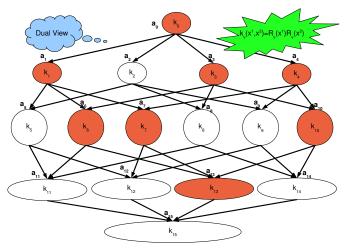


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# Hierarchical Kernel Learning (HKL)(Bach, 08)

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### HKL — Key Result

#### Active Set Algorithm:

- Complexity: Polynomial in number of selected kernels
- Condition: kernels are summable in *linear* time over a sub-lattice

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#### Active Set Algorithm:

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#### Our case:

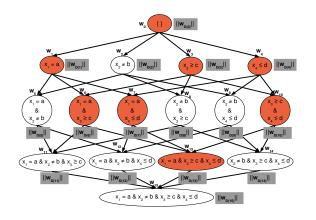
- Kernels indeed easily summable
  - lacksquare  $R_v$  is nothing but product of few base proposition evaluations
  - Sum of exponential no. terms = Product of linear no. terms
  - E.g.,  $1 + R_1 + R_2 + R_1 R_2 = (1 + R_1)(1 + R_2)$
  - Our problem can be solved in reasonable time

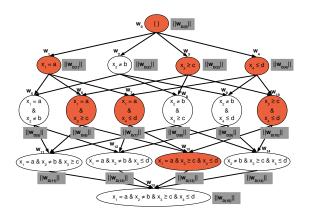
Dataset	RuleFit	SLI	ENDER	HKL
$\begin{array}{l} {\rm TIC\text{-}TAC\text{-}TOE} \\ m = 96, p = 27 \end{array}$	0.652 ± 0.068	$0.747 \pm 0.026$	$0.633 \pm 0.011$	$0.889 \pm 0.029$
$\begin{array}{l} {\tt BALANCE} \\ {\it m} = 28, p = 51 \end{array}$	0.835 ± 0.034	$0.856 \pm 0.027$	$0.827 \pm 0.013$	$0.893 \pm 0.027$
HABERMAN $m = 31, p = 28$	0.512 ± 0.072	$0.565 \pm 0.066$	$0.424 \pm 0.000$	$0.594 \pm 0.056$
CAR $m=159, p=21$	0.913 ± 0.033	$0.895 \pm 0.024$	$0.755 \pm 0.028$	$0.943 \pm 0.024$
BLOOD TRANS. $m=75, p=32$	0.549 ± 0.092	$0.559 \pm 0.100$	$0.489 \pm 0.054$	$0.594 \pm 0.009$
CMC m = 114, p = 38	0.632 ± 0.013	$0.601 \pm 0.041$	0.644 ± 0.026	<b>0.656</b> ± 0.014

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BALANCE $m=28, p=51$	0.835 ± 0.034 ( 2.18)	$0.856 \pm 0.027 \\ (\qquad 1.88)$	$0.827 \pm 0.013 \ (1.99)$	$0.893 \pm 0.027 \ (1.65)$
HABERMAN $m=31, p=28$	0.512 ± 0.072 ( 1.68)	$0.565 \pm 0.066 \ (1.14)$	$0.424 \pm 0.000 \ (1.87)$	0. <b>594</b> ± 0.056 ( 1.27)
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$\begin{array}{c} \text{CMC} \\ m = 114, p = 38 \end{array}$	0.632 ± 0.013 ( 2.41)	$0.601 \pm 0.041 \\ ( 2.13)$	0.644 ± 0.026 ( 2.65)	0.656 ± 0.014 ( 1.96)

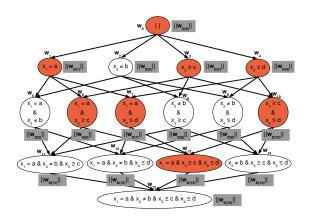
Dataset	RuleFit	SLI	ENDER	HKL
TIC-TAC-TOE $m=96,p=27$	0.652 ± 0.068 ( <b>40</b> , 2.51)	$0.747 \pm 0.026 \\ (59, 2.35)$	$0.633 \pm 0.011 \ (111, 2.46)$	$0.889 \pm 0.029 \ (129, 1.85)$
BALANCE $m=28, p=51$	0.835 ± 0.034 (17, 2.18)	$0.856 \pm 0.027 \\ (25, 1.88)$	$0.827 \pm 0.013 \\ (64, 1.99)$	0.893 ± 0.027 (65, 1.65)
HABERMAN $m=31$ , $p=28$	0.512 ± 0.072 ( <b>6</b> , 1.68)	$0.565 \pm 0.066$ (8, <b>1.14</b> )	$0.424 \pm 0.000 \\ (18, 1.87)$	$0.594 \pm 0.056 \\ (32, 1.27)$
$\begin{array}{l} \mathtt{CAR} \\ m = 159, p = 21 \end{array}$	0.913 ± 0.033 ( <b>34</b> , 3.12)	$0.895 \pm 0.024 \\ (141, 2.27)$	$0.755 \pm 0.028 \\ (80, 1.85)$	$0.943 \pm 0.024 \\ (87, 1.78)$
BLOOD TRANS. $m=75, p=32$	0.549 ± 0.092 (18, 1.99)	$0.559 \pm 0.100$ (6, 1.07)	$0.489 \pm 0.054 \\ (58, 1.5)$	$0.594 \pm 0.009 $ (242, 1.64)
$\begin{array}{c} \text{CMC} \\ m = 114, p = 38 \end{array}$	0.632 ± 0.013 (39, 2.41)	$0.601 \pm 0.041$ (13, 2.13)	0.644 ± 0.026 (74, 2.65)	0.656 ± 0.014 (127, <b>1.96</b> )

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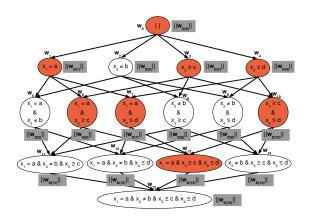




■ Node selected only if all its ancestors are!



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- $\blacksquare$   $l_1$  promotes sparsity.
- l<sub>2</sub> promotes non-sparsity. Employ sparsity inducing norm!



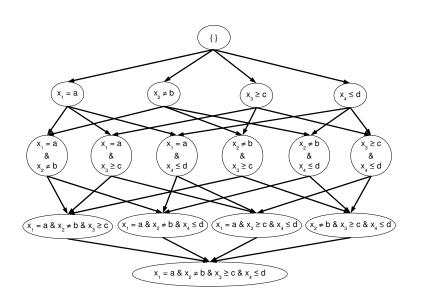
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### **Proposed Formulation**

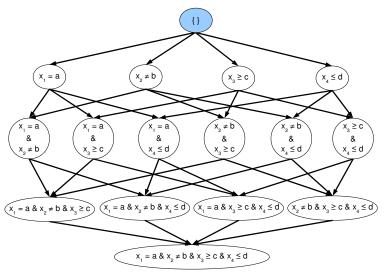
#### Generalized HKL

$$\min_{\mathbf{w},b} rac{1}{2} \left( \sum_{v \in \mathcal{V}} d_v \|\mathbf{w}_{D(v)}\|_{
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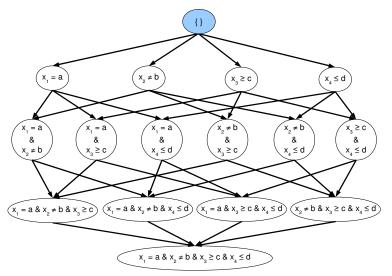
where  $1 < \rho < 2$ .



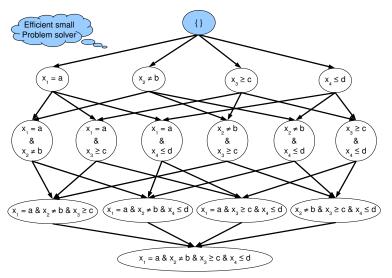
Initialize active set with root node ( $W = \{0\}$ ).



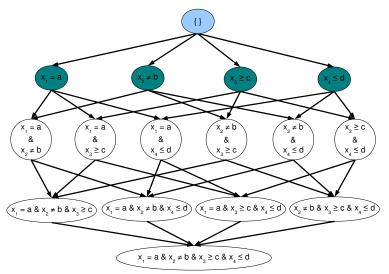
### Solve small problem



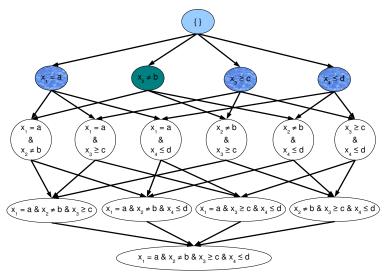
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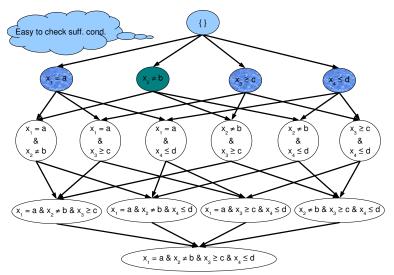
Identify potential active set entries (i.e.,  $sources(\mathcal{W}^c)$ )



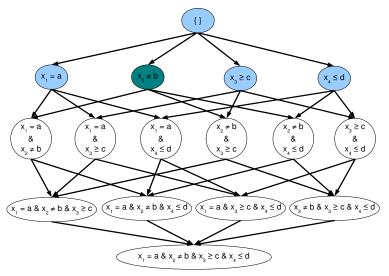
Among them, optimality condition violators



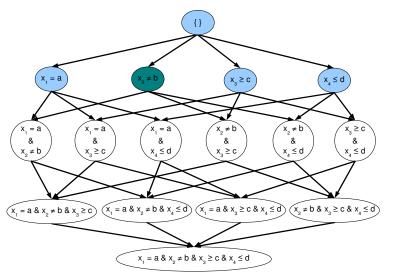
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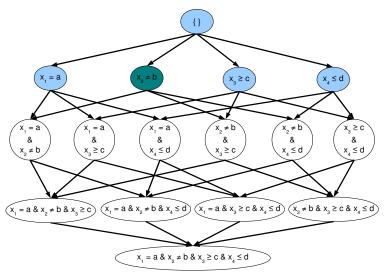
Append them to active set  $(W = \{0, 1, 3, 4\})$ .



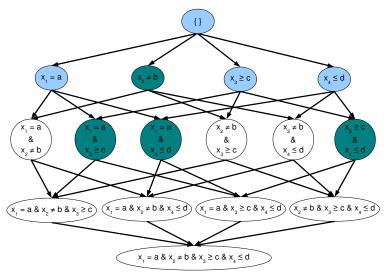
Append them to active set  $(\mathcal{W}=\{0,1,3,4\})$ . (repeat until suff. cond. satisfied)



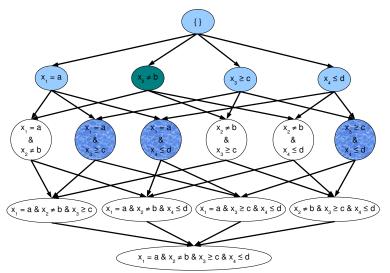
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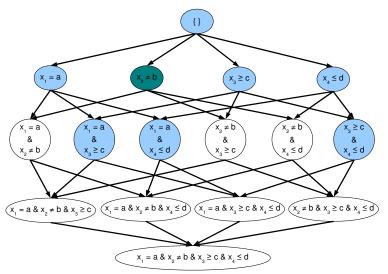
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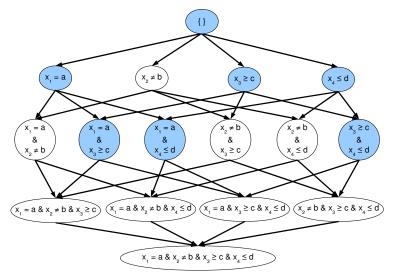
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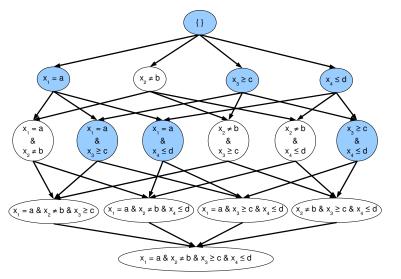
Append them to active set  $(\mathcal{W} = \{0, 1, 3, 4, 6, 7, 10\})$ 



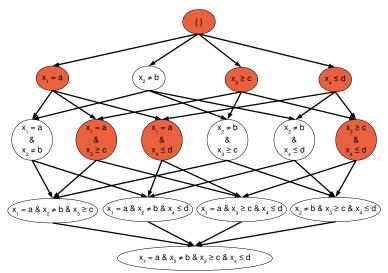
Final active set:  $W = \{0, 1, 3, 4, 6, 7, 10\}$ 



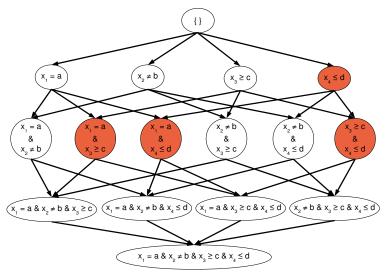
Final active set:  $\mathcal{W} = \{0, 1, 3, 4, 6, 7, 10\}$  (Complexity: Polynomial in active set size)



#### Solution with HKL



Key difference from HKL: Node selected without its ancestor!



## Key Technical Result

#### **Theorem**

A highly specialized partial dual of generalized HKL is:

$$egin{array}{ll} \min & g(\eta) \ ext{s.t.} & \eta \geq 0, \; \sum_{v \in \mathcal{V}} \eta_v = 1 \end{array}$$

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where  $g(\eta)$  is the optimal objective value of the following convex problem:

$$\max_{\boldsymbol{\alpha} \in \mathcal{R}^m} \sum_{i=1}^m \alpha_i - \frac{1}{2} \left( \sum_{v \in \mathcal{V}} \zeta_v(\eta) \left( \boldsymbol{\alpha}^\top \mathbf{K}_v \boldsymbol{\alpha} \right)^{\bar{\rho}} \right)^{\frac{1}{\bar{\rho}}} \text{ s.t. } 0 \leq \alpha_i \leq C, \sum_{i=1}^m \alpha_i y^i = 0.$$

where  $\zeta_v(\eta) = \left(\sum_{u \in A(v)} d_u^{\rho} \eta_u^{1-\rho}\right)^{\frac{1}{1-\rho}}$ ,  $\bar{\rho} = \frac{\rho}{2(\rho-1)}$  and  $\mathbf{K}_v$  is matrix with entries:  $y^i y^j k_v(\mathbf{x}^i, \mathbf{x}^j)$ .

# Solving small problem

- Dual is min. of convex, Lipschitz conts., sub-differential objective over a simplex.
- Mirror-descent highly scalable alg. for such problems.
- Sub-gradient solve  $l_p$ -MKL (Vishwanathan et.al., 10).

## Key Technical Result

#### **Theorem**

Suppose the active set W is such that W = A(W). Let the reduced solution with this W be  $(\mathbf{w}_{W}, b_{W})$  and the corresponding dual variables be  $(\eta_{W}, \alpha_{W})$ . Then the reduced solution is a solution to the full problem with a duality gap less than  $\epsilon$  if:

$$\max_{t \in sources(\mathcal{W}^c)} \left( \sum_{v \in D(t)} \left( \frac{\alpha_{\mathcal{W}}^{\top} \mathbf{K}_v \alpha_{\mathcal{W}}}{\left( \sum_{u \in A(v) \cap D(t)}^{d_u} d_u \right)^2} \right)^{\tilde{\rho}} \right)^{\tilde{\rho}} \leq (\Omega(\mathbf{w}_{\mathcal{W}}))^2 + 2(\epsilon - \epsilon_{\mathcal{W}})$$

where  $\epsilon_W$  is a duality gap term associated with the computation of the reduced solution.

$$\max_{t \in sources(\mathcal{W}^c)} \left( \sum_{v \in D(t)} \left( rac{lpha_{\mathcal{W}}^{ op} \mathbf{K}_v lpha_{\mathcal{W}}}{\left( \sum_{u \in A(v) \cap D(t)} rac{d_u}{d_u} 
ight)^2} 
ight)^{ar{ar{
ho}}} \stackrel{ar{ar{
ho}}}{=} \leq (\Omega(\mathbf{w}_{\mathcal{W}}))^2 + 2(\epsilon - \epsilon_{\mathcal{W}})$$

#### **Sufficiency Condition:**

$$\max_{t \in sources(\mathcal{W}^c)} \left( \sum\nolimits_{v \in D(t)} \left( \frac{\alpha_{\mathcal{W}}^\top \mathbf{K}_v \alpha_{\mathcal{W}}}{\left(\sum\nolimits_{u \in A(v) \cap D(t)} \frac{du}{}\right)^2} \right)^{\bar{\rho}} \right)^{\frac{1}{\bar{\rho}}} \leq (\Omega(\mathbf{w}_{\mathcal{W}}))^2 + 2(\epsilon - \epsilon_{\mathcal{W}})$$

 $ightharpoonup 
ho o 1 \ (\bar{
ho} o \infty)$ , suff. cond. tight

$$\max_{t \in sources(\mathcal{W}^c)} \left( \sum_{v \in D(t)} \left( \frac{lpha_{\mathcal{W}}^{ op} \mathbf{K}_v lpha_{\mathcal{W}}}{\left( \sum_{u \in A(v) \cap D(t)} rac{d_u}{d_u} 
ight)^2} 
ight)^{ar{
ho}} \int_{ar{
ho}}^{ar{
ho}} \leq (\Omega(\mathbf{w}_{\mathcal{W}}))^2 + 2(\epsilon - \epsilon_{\mathcal{W}})$$

- $ho \rightarrow 1 \ (\bar{\rho} \rightarrow \infty)$ , suff. cond. tight
- $ho = 2 \ (\bar{\rho} = 1)$ , suff. cond. loose; computationally feasible

$$\max_{t \in sources(\mathcal{W}^c)} \left( \sum_{v \in D(t)} \left( \frac{lpha_{\mathcal{W}}^{ op} \mathbf{K}_v lpha_{\mathcal{W}}}{\left( \sum_{u \in A(v) \cap D(t)} rac{d_u}{d_u} 
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  - Not much: As kernels near bottom are extremely sparse!

#### Final Sufficiency Condition:

$$\max_{t \in sources(\mathcal{W}^c)} \left( \sum_{v \in D(t)} \left( \frac{\alpha_{\mathcal{W}}^{ op} \mathbf{K}_v \alpha_{\mathcal{W}}}{\left( \sum_{u \in A(v) \cap D(t)}^{d_u} d_u \right)^2} \right) \right) \leq (\Omega(\mathbf{w}_{\mathcal{W}}))^2 + 2(\epsilon - \epsilon_{\mathcal{W}})$$

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Dataset	RuleFit	SLI	ENDER	HKL	$HKL^2_{\rho=1.1}$
TIC-TAC-TOE	$0.652 \pm 0.068 $ (40, 2.51)	$0.747 \pm 0.026 \\ (59, 2.35)$	$0.633 \pm 0.011 \ (111, 2.46)$	$0.889 \pm 0.029 \\ (129, 1.85)$	0.935 ± 0.043 (79, 1.77)
BLOOD TRANS.	$0.549 \pm 0.092 \\ (18, 1.99)$	$0.559 \pm 0.100 \ (6, 1.07)$	$0.489 \pm 0.054 \ (58, 1.5)$	$0.594 \pm 0.009 $ (242, 1.64)	$0.593 \pm 0.011 \\ (7,1.40)$
BALANCE	$0.835 \pm 0.034 \ (17, 2.18)$	$0.856 \pm 0.027 \\ (25, 1.88)$	$0.827 \pm 0.013 \\ (64, 1.99)$	$0.893 \pm 0.027 \\ (65, 1.65)$	0.899 ± 0.023 (28,1.23)
HABERMAN	$0.512 \pm 0.072 \ (6, 1.68)$	$0.565 \pm 0.066 \ (8, 1.14)$	$0.424 \pm 0.000 \\ (18, 1.87)$	$0.594 \pm 0.056$ (32, 1.27)	$0.594 \pm 0.056$ $(12,1.20)$
CAR	$0.913 \pm 0.033$ (34, 3.12)	$0.895 \pm 0.024 \\ (141, 2.27)$	$0.755 \pm 0.028 \\ (80, 1.85)$	<b>0.943</b> ± 0.024 (87, 1.78)	0.935 ± 0.036 (50, <b>1.68</b> )
CMC	$0.632 \pm 0.013$ (39, 2.41)	$0.601 \pm 0.041$ (13, 2.13)	$0.644 \pm 0.026$ (74, 2.65)	$0.656 \pm 0.014$ (127, 1.96)	$0.659 \pm 0.008$ $(43,1.70)$

 $<sup>^2</sup> Code \ at \ http://www.cse.iitb.ac.in/~pratik.j/REL-HKL.tar.gz$ 

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  - Applicable elsewhere
- Efficient mirror-descent based active set method
  - Complexity: polynomial in active set size  $\ll O(2^n)$
  - Searched rule space size  $\sim 2^{50}$  in  $\sim 10$  min.

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# Questions?



