Improved Parallel Branch-and-Bound solver for Rectangular Maximum Agreement Problem

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RMA Problem Setting

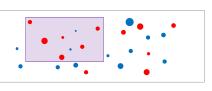
- m observations, each observation has n explanatory variables
- ullet Each observation has a weight $w_i \in \mathbb{R}$
- Explanatory matrix: $X \in \mathbb{R}^{m \times n}$
 - $X_i \in \mathbb{R}^n$ for i = 1, ..., m (row vector of X)
 - $x_j \in \mathbb{R}^m$ for i = 1, ..., n (column vector of X)
 - $x_{ij} \in \mathbb{R}$: $(i,j)^{th}$ element of X

	x_1	 Xj	 Xn	W
X_1				w _i
:				:
X_i		×ij		Wi
: X _m				: : : w _i

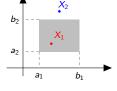
RMA Formulation

- Eliminate zero-weight observations
- Partition observations into

$$\begin{cases} \Omega^+ &= \{i \in \{1, \dots, m\} \mid w_i > 0\} \\ \Omega^- &= \{i \in \{1, \dots, m\} \mid w_i < 0\} \end{cases}$$

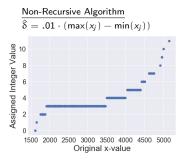


- Goal: Find an axis-parallel box containing the maximum net weight of positive minus negative observations or vice versa
- For any set $S \subseteq \{1, ..., m\}$, let $w(S) = \sum_{i \in S} w_i$
- Coverage contains indices of observations within (a, b), $Cover_X(a, b) = \{i \in \{1, ..., m\} \mid a \le X_i \le b\}$



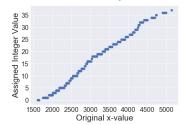
Rectangular Maximum Agreement (RMA) Problem

- Before running RMA, convert $X \in \mathbb{R}^{m \times n} \Rightarrow X \in \mathbb{N}^{m \times n}$
- Assign a natural number to each distinct value of each attribute; aggregation controlled by a parameter $\hat{\delta} = \delta \cdot (\max(x_j) \min(x_j))$
- $\hat{\delta} = \delta \cdot CI_{.95}(x_i)$ to reduce influence of outliers
- If a range of one assigned value is larger than a certain limit, choose smaller δ for the range and split into smaller clusters (Recursive procedure)
- We discretize uniformly distributed large data into L equal intervals



Recursive Algorithm

$$\overline{\hat{\delta} = \delta \cdot CI_{.95}(x_j)}$$
 with $\delta_0 = .1$, $\delta_t = .95\delta_{t-1}$ IntervalLimit $= .05CI_{.95}(x_j)$



RMA MIP Formulation Link: RMA Formulation

s.t.
$$\phi \leq \sum_{i=1}^{m} w_i q_i + (\sum_{i=1}^{m} |w_i|) 2s, \quad \phi \leq -\sum_{i=1}^{m} w_i q_i + (\sum_{i=1}^{m} |w_i|) 2(1-s)$$

$$q_i \leq z_{j,x_{ij}}$$

$$q_i \geq \sum_{i=1}^{m} z_{j,x_{ij}} - (n-1), \quad 0 \leq q_i \leq 1$$

$$\sum_{k=0}^{\ell_j-1} l_{jk} = 1, \quad \sum_{k=0}^{\ell_j-1} u_{jk} = 1, \quad z_{j,-1} = 0, \quad z_{j,\ell_j} = 0$$

$$z_{jk} \le z_{j,k-1} + l_{jk}, \quad z_{jk} \le z_{j,k+1} + u_{jk}, \quad l_{jk} \le z_{jk}, \quad u_{jk} \le z_{jk}$$
 $\forall j, k$
 $l_{jk} \in \{0, 1\}, \quad u_{jk} \in \{0, 1\}, \quad 0 \le z_{jk} \le 1$ $\forall j, k$

- φ objective value
- s 1 for positive objective value and 0 for negative
- q_i 1 if observation i is covered, else 0
- u_{ik} 1 if k is the upper bound of attribute j, else 0
- 1_{jk} 1 if k is the lower bound of attribute j, else 0
- z_{jk} 1 if k is a covered value of attribute j, else 0
- # of variables: $m + 2n + 3 \sum_{j=1}^{n} \ell_j + 2$
- # of constraints: $mn + m + 4n + 4\sum_{j=1}^{n} \ell_j + 2$

 $\forall i, j$

 $\forall i$

Branch-and-Bound Algorithm

The Gurobi MIP solver cannot solve large-scale RMA instances



- Maximum Monomial Agreement (MMA) by Eckstein and Goldberg
 - Convert $X \in \mathbb{R}^{m \times n} \Rightarrow X \in \{0, 1\}^{m \times n}$
 - Binarization is too time consuming
- Solve RMA by a specialized parallel branch-and-bound procedure after preprocessing
- Use PEBBL, a C++ framework for branch-and-bound algorithms (Eckstein, Hart, and Phillips, 2015)

Essential ingredients of all branch-and-bound methods

- A characterization of subproblems
- A bounding function for subproblems
- A branching rule for subdividing subproblems
- 4 An incumbent (best feasible objective seen so far) computation

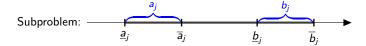
Subproblem Characterization

- $a \in \mathbb{Z}^n$: lower bound of box
- $b \in \mathbb{Z}^n$: upper bound of box
- Each subproblem P has: $\underline{a}, \overline{a}, \underline{b}, \overline{b} \in \mathbb{Z}^n$

Require: $a \le b$ $\underline{a} \le a \le \overline{a}$ $\underline{a} \le \overline{a}$ $\underline{b} \le b \le \overline{b}$ $\underline{b} \le \overline{b}$ $\underline{a} \le \underline{b}$ $\overline{a} \le \overline{b}$

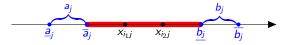
Not Require:

 $\overline{a} \leq \underline{b}$



Root Subproblem: $\begin{array}{c|c} 0 & a_j \leq b_j & \ell_j - 1 \\ \hline \underline{a_j} = \underline{b_j} & \overline{a_j} = \overline{b_j} \end{array}$

Bounding Function and Inseparability



- If either $x_{i_1j}=x_{i_2j}$ or $\overline{a}_j \leq x_{i_1j}, x_{i_2j} \leq \underline{b}_j$ for each $j=1,\ldots,n$, then $X_{i_1}, X_{i_2} \in \mathbb{Z}^n$ are **inseparable** w.r.t. $\overline{a}, \underline{b} \in \mathbb{Z}^n$
- $\mathcal{E}(\overline{a}, \underline{b})$: the **equivalence classes** of observation indices induced by the inseparability
- Any box specified by $(\underline{a}, \overline{a}, \underline{b}, \overline{b})$ must either cover or not cover the entirety of each equivalence class $C \in \mathcal{E}(\overline{a}, \underline{b})$

Bounding Function

$$g(\underline{\underline{a}}, \overline{\underline{a}}, \underline{\underline{b}}, \overline{\underline{b}}) = \max \left\{ \sum_{C \in \mathcal{E}(\overline{\underline{a}}, \underline{\underline{b}})}^{} \left[w(C \cap \mathsf{Cover}_X(\underline{\underline{a}}, \overline{\underline{b}})) \right]_+, \sum_{C \in \mathcal{E}(\overline{\underline{a}}, \underline{\underline{b}})}^{} \left[w(C \cap \mathsf{Cover}_X(\underline{\underline{a}}, \overline{\underline{b}})) \right]_- \right\}$$

- The bound requires computation of the equivalence classes $\mathcal{E}(\overline{a},\underline{b})$
- Bounds not using these equivalence classes are much weaker

Computing Equivalence Classes



- For a subproblem $P = (\underline{a}, \overline{a}, \underline{b}, \overline{b})$, start with $M = \{1, 2, \dots, m\}$
- For j = 1, 2, ..., n, do a stable bucket sort of M on attribute j, but
 - Discard observations with $w_i = 0$
 - Discard observations with $x_{ij} < \underline{a}_i$ or $\overline{b}_j < x_{ij}$
 - Treat x_{i_1j}, x_{i_2j} as equal if $\overline{a}_j \leq x_{i_1j}, x_{i_2j} \leq \underline{b}_j$
- Time O(m) per sort, n attributes $\Rightarrow O(mn)$

$$\textbf{for } j = 1 \dots n \textbf{ do } M \leftarrow \textbf{bucketSortObs}(\underline{a}_j, \overline{a}_j, \underline{b}_j, \overline{b}_j, M, x_j) \qquad \textcolor{red}{\mathsf{O}(\textit{mn})}$$

• Scanning through M in order will now yield the equivalence classes: O(mn) work (but often much less)

$$E \leftarrow \mathsf{createInitEquivClass}(\underline{a}, \overline{a}, \underline{b}, \overline{b}, M, X) \qquad \mathsf{O}(mn)$$

First Visual Example: $\underline{b} \leq \overline{a}$

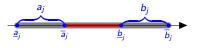


Suppose $\underline{b} \leq \overline{a}$, so that observations are inseparable only if they are identical

	Observation											
Attribute	i_1	i_2	<i>i</i> 3	i_4	<i>i</i> ₅	i 6	<i>i</i> 7	i 8	i 9	i_{10}	i_{10}	i_{12}
<i>j</i> ₃	0	0	0	0	0	0	1	1	1	1	1	1
j 2	0	0	1	1	2	2	0	0	1	1	2	2
j_1	0	1	0	1	0	1	0	1	0	1	0	1
					_	(\mathbf{R})						
			<u> </u>									
<i>j</i> ₃ :			0						$\sqrt{1}$.)_		
<i>j</i> ₂ :	0	(1	7	2		0		1)	2	
j_1 : 0	1	0	1	0)	0) (1	0	1	0	1
$M: i_1$	i_2	<i>i</i> 3	<i>i</i> ₄	<i>i</i> ₅	<i>i</i> ₆	i	7	i ₈	i 9	i_{10}	i_{11}	i_{12}
$E: e_1$	e_2	e ₃	e_4	e_5	e_6	ϵ	₽7	e 8	e 9	e_{10}	e_{11}	e_{12}

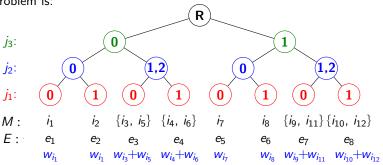
- M: a vector of sorted covered observations
- E: a vector of sorted covered equivalence class indices

Second Visual Example: $\bar{a}_j < \underline{b}_j$



Attribute	<u>a</u>	ā	<u>b</u>	\overline{b}
j ₃	0	1	0	1
j_2	0	1	2	2
j_1	0	1	0	1

- Values of attribute j_2 are in the same bucket if within $[\overline{a}_{j_2},\underline{b}_{j_2}]=[1,2]$
- The initial equivalence class tree for this subproblem is:



- Each equivalence class maintains the sum of observations weights
- At this point, computing the bound is just O(|E|) additional work

Branching scheme Link: Branching

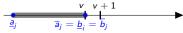
Branching of a subproblem $P = (\underline{a}, \overline{a}, \underline{b}, \overline{b})$ is based on:

• Pick some feature j and "cut value" $v \in \{\underline{a}_j, \dots, \overline{b}_j - 1\}$

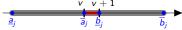
Parent: $\underline{\underline{a}_j}$ $\underline{\underline{b}_j}$ $\underline{\underline{b}_j}$ $\underline{\underline{b}_j}$ $\underline{\underline{b}_j}$

is partitioned into:

1 Down Child — the box is below v in feature j



2 Middle Child — the box straddles [v, v+1] in feature j



3 Up Child — the box is above v + 1 in feature j

$$\begin{array}{c|c}
v & v+1 \\
\underline{a_j} = \overline{a_j} = \underline{b_j} & \overline{b_j}
\end{array}$$

- Except that if $v < \underline{b}_i$, then "down child" is not possible $(b_i \le v < \underline{b}_i)$
- Else if $\overline{a}_j < v+1$, then "up child" is not possible $(\overline{a}_j < v+1 \le a_j)$
- If $\underline{b}_j < \overline{a}_j$ and $v \in \{\underline{b}_j, \dots, \overline{a}_j 1\}$, then 3 children, otherwise 2 children

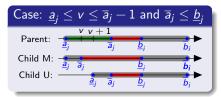
Graphical View of Branching Scheme 4

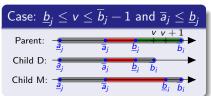
Link: Branching

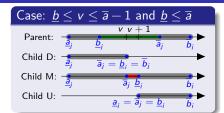
Child D: Down Child (Box below v)

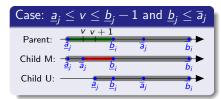
Child M: Middle Child (Box straddles [v, v + 1])

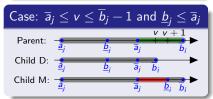
Child U: Up Child (Box above v + 1)











More about Branching

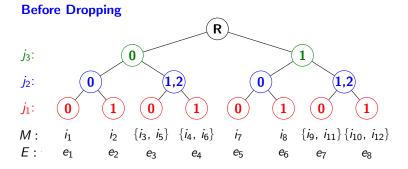
• "Cutpoint": each possible attribute / cut value pair (j, v)

How to choose a cutpoint (j, v)

- Strong branching: check all possible cutpoints (j, v) and pick the one that $\min_{(j,v)} \{\max\{\text{bounds of 2 or 3 children}\}\}$
- Randomly choose one among cutpoints with tied bounds
- Brute-force implementation (recomputing all the equivalence classes) is $O(mnV) \preceq O(m^2n^2)$ work
 - *V* is the number of cutpoints $(V \leq mn)$
 - but only $O(mn^2)$ in the binary-data case
- Instead, exploit relationship between parent and child equivalence classes and use "rotation algorithm"

Down Child Bound: Drop Equivalence Classes

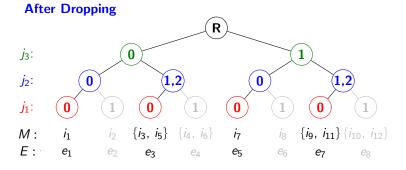
- If a child's \underline{a}_i or \overline{b}_j changes, drop equivalence classes no longer covered
- In most recent example, suppose $j = j_1$, v = 0
- "Down" child is then: $(\underline{a}_{j_1}, \overline{a}_{j_1}, \underline{b}_{j_1}, \overline{b}_{j_1}) = (0, 0, 0, 0)$



$$\widehat{E} \leftarrow \mathsf{dropEquivClass}(\underline{a}_i, v, E, x_j) \qquad \mathsf{O}(|E|) \leq \mathsf{O}(m)$$

Down Child Bound: Drop Equivalence Classes

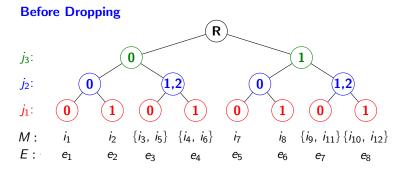
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$$\widehat{E} \leftarrow \mathsf{dropEquivClass}(\underline{a}_i, v, E, x_i) \qquad \mathsf{O}(|E|) \preceq \mathsf{O}(m)$$

Up Child Bound: Also Drop Equivalence Classes

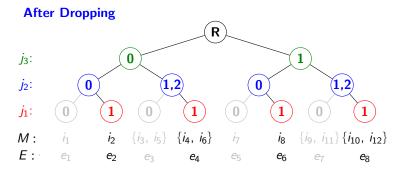
• In the same situation, "up" child is $(\underline{a}_{j_1}, \overline{a}_{j_1}, \underline{b}_{j_1}, \overline{b}_{j_1}) = (1, 1, 1, 1)$, so drop different uncovered equivalence classes to obtain



$$\widehat{E} \leftarrow \mathsf{dropEquivClass}(v+1, \overline{b}_j, E, x_j) \qquad \mathsf{O}(|E|) \preceq \mathsf{O}(m)$$

Up Child Bound: Also Drop Equivalence Classes

• In the same situation, "up" child is $(\underline{a}_{j_1}, \overline{a}_{j_1}, \underline{b}_{j_1}, \overline{b}_{j_1}) = (1, 1, 1, 1)$, so drop different uncovered equivalence classes to obtain



$$\widehat{E} \leftarrow \mathsf{dropEquivClass}(v+1, \overline{b}_j, E, x_j) \qquad \mathsf{O}(|E|) \preceq \mathsf{O}(m)$$

Middle Child: Merge Equivalence Classes

- If a child's \overline{a}_j or \underline{b}_i changes, merge some equivalence classes
- If $j = j_1$, the classes to be merged are adjacent in E
- "Middle" child of our example: $(\underline{a}_{j_1}, \overline{a}_{j_1}, \underline{b}_{j_1}, \overline{b}_{j_1}) = (0, 0, 1, 1)$, and so

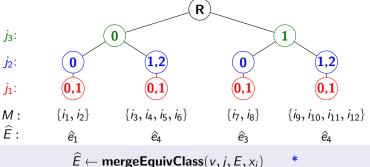
Before Merging *j*3: j_2 : 0 1 0 $\{i_3, i_5\} \{i_4, i_6\} i_7$ *M* : $\{i_9, i_{11}\}\{i_{10}, i_{12}\}$ F· e_5 **e**₇ e_8 $\widehat{E} \leftarrow \mathsf{mergeEquivClass}(v, j, E, x_i)$

* "Amortized" complexity analysis for this step Helps to have mergeable classes adjacent

Middle Child: Merge Equivalence Classes

- If a child's \overline{a}_i or \underline{b}_i changes, merge some equivalence classes
- If $j = j_1$, the classes to be merged are adjacent in E
- "Middle" child of our example: $(\underline{a}_{j_1}, \overline{a}_{j_1}, \underline{b}_{j_1}, \overline{b}_{j_1}) = (0, 0, 1, 1)$, and so

After Merging



* "Amortized" complexity analysis for this step Helps to have mergeable classes adjacent

Evaluate all Potential Children from Cutting on j_1

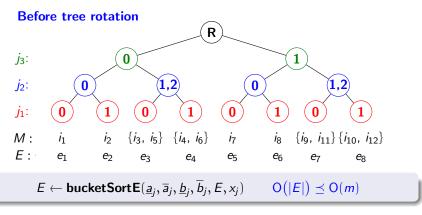
- For each possible cutpoint (j, v) with $j = j_1$, repeat the above procedures to evaluate the bounds of the 2 or 3 possible children
- ullet There are at most ℓ_i-1 such cutpoints

bound
$$\leftarrow$$
 boundComputation $(j, \underline{a}_j, \overline{a}_j, \underline{b}_j, \overline{b}_j, E, X)$ $O(mn + m^2)$

• To deal with cutpoints with $j \neq j_1 \Rightarrow$ "rotate" the tree

Rotate the Tree: Bucket Sort by j_1

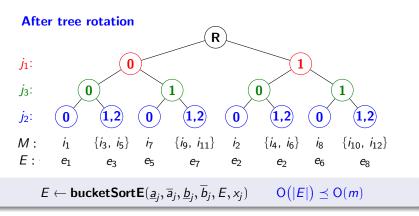
ullet Perform a stable bucket sort of the equivalence classes by attribute j_1



• Similarly, evaluate all children obtained by cutting on j_2

Rotate the Tree: Bucket Sort by j_1

ullet Perform a stable bucket sort of the equivalence classes by attribute j_1



• Similarly, evaluate all children obtained by cutting on j_2

Efficiency of Tree Rotation Algorithm

Repeat this procedure for $j = 1, \dots n-1$

- Skip for attributes with no possible cutpoints
- Evaluate every possible cutpoint
- Overall Running Time per Subproblem:

$$O\left(\underbrace{n \atop n \text{ attributes}} \cdot \underbrace{(mn+m^2)}_{\text{per each attribute}}\right) = O(mn^2 + m^2 n)$$

- Usually faster than that: this bound is very pessimistic
 - but still better than $O(m^2n^2)$ for brute-force strong branching

Alternatives to Strong Branching

Strong Branching: (checking all possible cutpoints)

— greatly accelerated by the tree rotation technique but still time consuming

Alternative Branching Ideas:

- Randomly choose some percentage of the total cutpoints
 - Did not work well due massive inflation of the branch-and-bound tree
- **2** Binary-style search for a good cutpoint within each feature
 - Only beneficial for attributes with a large number ℓ_i of distinct values
- **3** Cutpoint caching:
 - Many cutpoints are never used
 - Same cutpoints are repeatedly chosen in different parts of the tree

Store cutpoints already chosen in earlier subproblems

- if (# applicable cached cutpoints)
 - \geq (t% of total cutpoins) **then** select the best of them
- else perform strong branching
- ullet Can combine with binary-style search, depending on ℓ_j

Initially, no constraint $(a,b)=(0,\ell-1),\ j^*=-1,\ z^*_{max}=0$ for each iteration $t=1,\ldots,T$

- For each $j \in \{1, \dots n\} \setminus j^*$, **Kadane's algorithm** finds the range (a_j^t, b_j^t) that optimizes the sum weight z_j^t of covered observations if we narrow the box bounds for attribute j
- $j^* \leftarrow \arg\max_{j} \{z_j^t\}$
- **3** if $z_{i^*}^t \leq z_{max}^*$ then stop (no improvement)
- $\textbf{4} \ \mathsf{Update} \ z_{\mathit{max}}^* \leftarrow z_{j^*}^t \ \mathsf{and} \ (a_{j^*}, b_{j^*}) \leftarrow (a_{j^*}^t, b_{j^*}^t)$

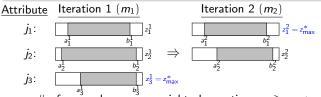
Attribute Iteration $1 (m_1)$



of covered non-zero weight observation: $m \geq m_1$

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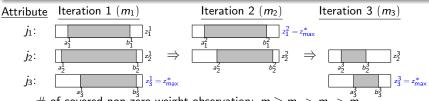
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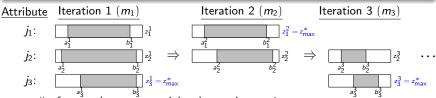
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of covered non-zero weight observation: $m \geq m_1 > m_2 > \vec{m}_3$

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- $j^* \leftarrow \arg\max_{j} \{z_j^t\}$
- **3 if** $z_{j^*}^t \leq z_{max}^*$ **then stop** (no improvement)
- $\textbf{4} \ \mathsf{Update} \ z^*_{\mathit{max}} \leftarrow z^t_{j^*} \ \mathsf{and} \ (a_{j^*}, b_{j^*}) \leftarrow (a^t_{j^*}, b^t_{j^*})$



of covered non-zero weight observation: $m \ge m_1 > m_2 > m_3 > \dots$

Repeat this process for the maximum and minimum cases

(incumbent, (a, b)) \leftarrow initialGuess(X, y, w) $O(mnT) \leq O(m^2n)$

Incumbent Heuristic for Each Subproblem

- Kadane's algorithm to finds a largest-sum contiguous subvector of any given vector in linear time
- For each attribute *j*, apply Kadane's algorithm twice (for positive and negative)
- Each Kadane run can be reduced to O(|E|)

(incumbent,
$$(a_j, b_j)$$
) \leftarrow **checkIncumbent** (j, E, x_j, w) $O(|E|) \leq O(m)$

- Repeat for each attribute (so 2n runs of Kadane in total)
- Total time for checking all attributes $O(n|E|) \leq O(mn)$

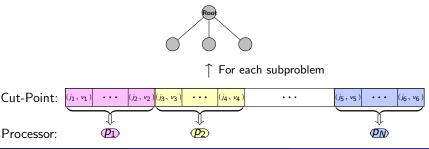
Parallel Implementation: Ramp-up Phase

- Using PEBBL, easy to upgrade the implementation from serial to parallel
- PEBBL's built-in ramp-up / crossover feature

Ramp-up near the tree root,

- Only strong branching and
- All processors cooperate synchronously on evaluating each branch-and-bound node
- 1 Distributes nearly equal number of cutpoints to each processor
- **2** Each processor computes the bounds for its assigned cutpoints

Initial B&B Tree



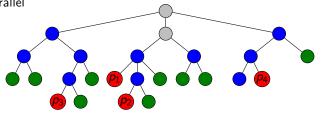
Parallel Implementation: Crossing Over

Crossover to standard asynchronous search mode:

If (# of active search nodes of B&B tree) \geq (# of processors)

or (# of active search nodes of B&B tree) > (# of cutpoints) then

- PEBBL automatically distributes the current search tree evenly across the available processors
- Processors start asynchronously evaluating different tree nodes, in parallel

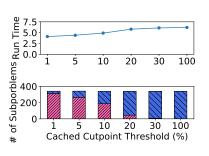


- bounded during ramp-up
- already bounded by asynchronous search
- currently being bounded by asynchrnous search
- created but not yet bounded

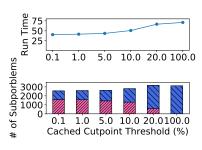
Computational Results: Benefits of Cutpoint Caching (in Serial)

- Implemented our algorithm in C++ with PEBBL
- ullet Run time improved as we decreased the cutpoint threshold t
- ullet # of total bounded subproblem did not change significantly
- Compute bounds for cutpoitns in cache if there is at least 1 applicable cupoint for each subrpoblem

Data: cmc_bin



Data: parkinson



Strong branching
Cutpoints from the cache

Results: Benefits of Tree Rotation and Cutpoint Caching

RMA: RMA with the rotation method and with the strong branching RMA_CC: RMA with the rotation method and with the cutpoint caching

RMA_BF: RMA with brute-force strong branching

MMA: Binary case of RMA (old implementation by Goldberg)

MIP: The MIP formulation solved by Gurobi

Serial Run time in seconds for BINARY data sets

Method	cleveland	diabetes	hungheart	cmc_bin	spam	spam75
RMA_CC	0.5	1.0	2.0	4.1	5.2	130.2
RMA	0.5	1.1	3.5	6.1	5.9	154.8
MIP	8.5	14.8	11.5	199.8	276.6	829.4
MMA	20.5	43.6	147.3	909.6	554.4	18966.0
RMA_BF	11.2	70.5	310.0	1104.8	2053.9	(2)

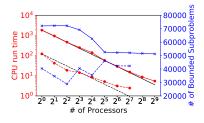
Serial and Parallel Run time in seconds for INTEGER data sets

Method	Р	cmc_int	climate	indian	parkinson	skin (245K×3)
RMA_CC	1	0.7	21.8	38.4	40.4	65.9
RMA	1	1.0	25.3	315.2	68.1	1978.8
MIP	1	64.1	14.4	16.4	5.9	(2)
RMA_CC	16	0.2	17.9	4.2	25.1	26.7
RMA	16	0.2	4.1	26.0	9.5	221.4
MIP	16	12.1	16.2	15.5	6.3	@

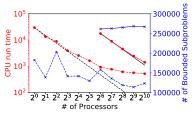
- Gurobi generates cutting plans at the root nodes
- PEBBL parallel speedup is much better than Gurobi
- P: # of processors
- Average over 5 runs

Parallel Speedups

Data: indian $(583 \times 10:628)$



 $\textbf{Data: credit_card } \big(30\textit{K} \times 23:1931\big)$

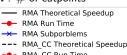


 $(m \times n : V)$

m: # of observations

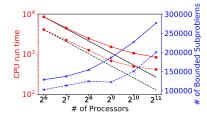
n: # of attributes

V: # of cutpoints



--- RMA_CC Run Time
--- RMA_CC Subporblems

Data: poker $(1M \times 10 : 85)$



- Parallel PEBBL runs nondeterministically
- Average over 5 runs

Conclusion and Planned Improvements/Extensions

Conclusion

 Constructed an improved parallel branch-and-bound procedure and greedy heuristic to solve RMA

Improvement

- Dimensional reduction
- More parallel procedures

Major Contributions

- Developed a branch-and-bound algorithm for RMA in C++ programming language with PEBBL, a C++ framework for branch-and-bound algorithms (Eckstein, Hart, and Phillips, 2015)
 - an efficient algorithm to compute an improved bounding function
 - non-strong branching methods
- Built a greedy heuristic to solve RMA
- Invented a recursive data discretization method
 - Reduces the level of difficulty for RMA