I/O-Efficient Algorithms and Data Structures

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8^{th} of September, 2023

AARHUS
UNIVERSITY

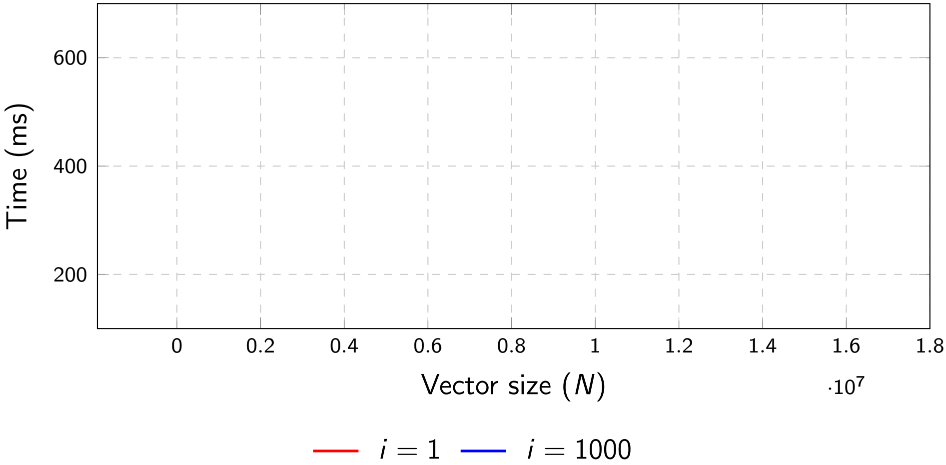
$$0,\ 1,\ 2,\ \cdots\quad i,\ i+1,\ \cdots\ 2i,\ 2i+1,\ \cdots\cdots\quad N-1$$

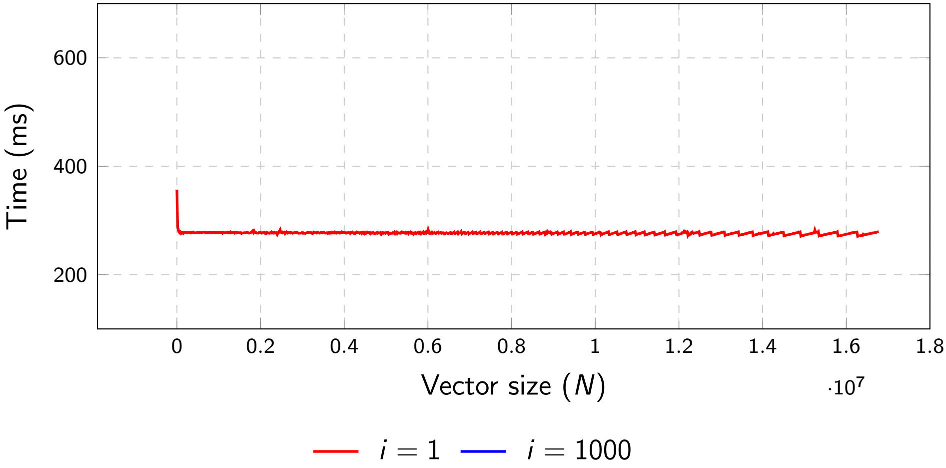
$$0,\ 1,\ 2,\ \cdots\quad i,\ i+1,\ \cdots\ 2i,\ 2i+1,\ \cdots\cdots\quad N-1$$

$$0,\ 1,\ 2,\ \cdots\quad i,\ i+1,\ \cdots\ 2i,\ 2i+1,\ \cdots\cdots\quad N-1$$

$$0,\ 1,\ 2,\ \cdots\ \ i,\ i+1,\ \cdots\ 2i,\ 2i+1,\ \cdots\cdots\ \ N-1$$

$$0,\ 1,\ 2,\ \cdots\ \ i,\ i+1,\ \cdots\ 2i,\ 2i+1,\ \cdots\cdots\ \ N-1$$


Time (ms)
600
400
200
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
Vector size (N)
·10^7
i = 1
i = 1000


Time (ms)
600
400
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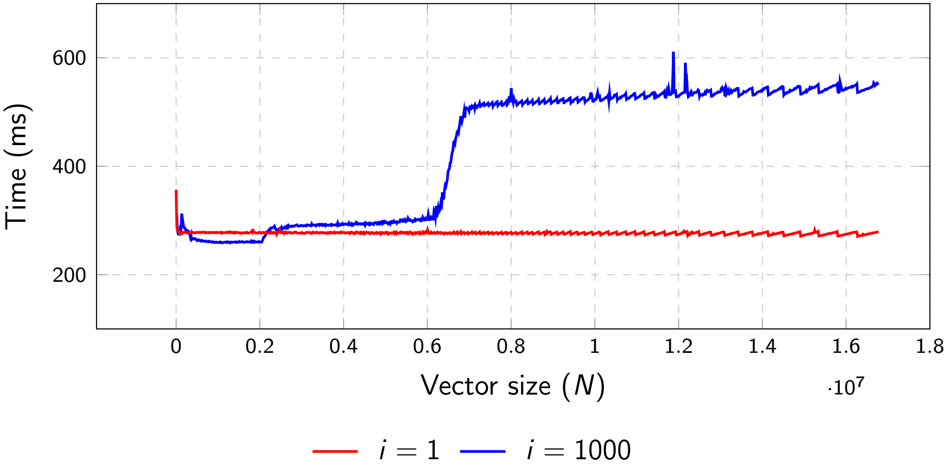
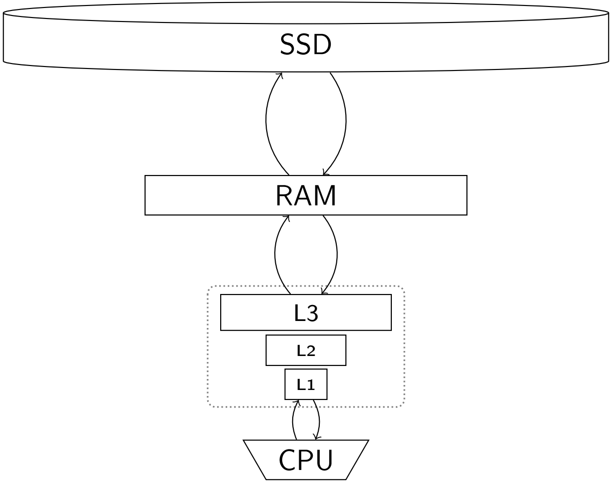
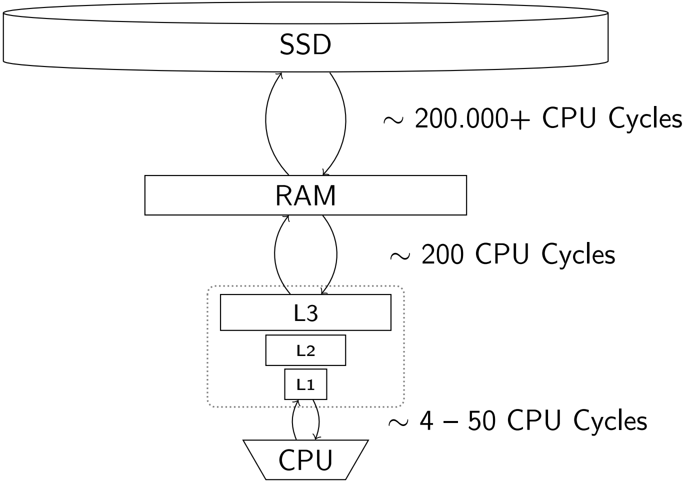
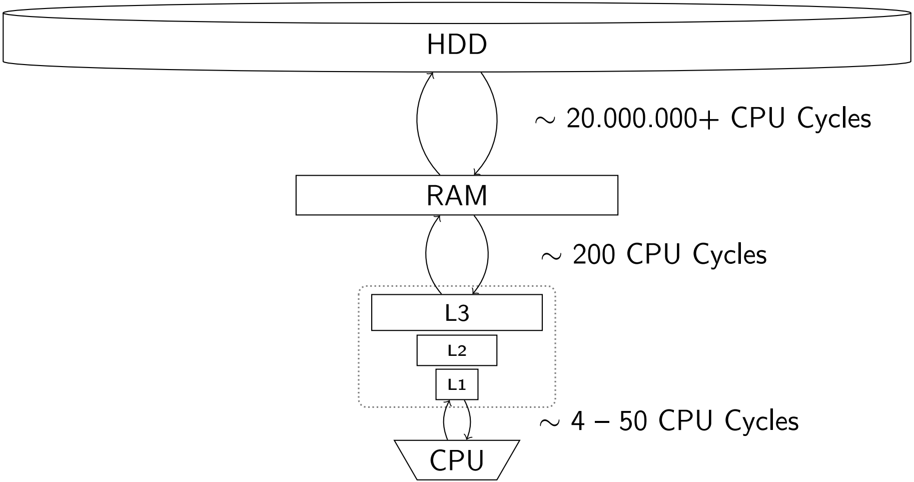
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
Vector size (N)
$\cdot 10^7$
$i = 1$
$i = 1000$

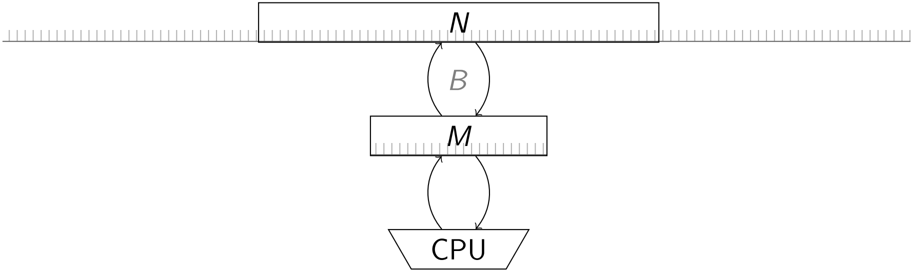

600
400
200
Time (ms)
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
Vector size (N)
·10^7
i = 1
i = 1000


SSD
RAM
L3
L2
L1
CPU


SSD
∼ 200.000+ CPU Cycles
RAM
∼ 200 CPU Cycles
L3
L2
L1
∼ 4 – 50 CPU Cycles
CPU


HDD
~ 20.000.000+ CPU Cycles
RAM
~ 200 CPU Cycles
L3
L2
L1
~ 4 – 50 CPU Cycles
CPU

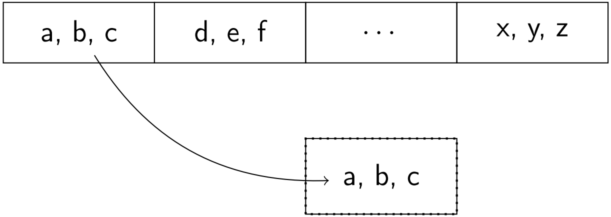
I/O Model
Aggarwal and Vitter '87



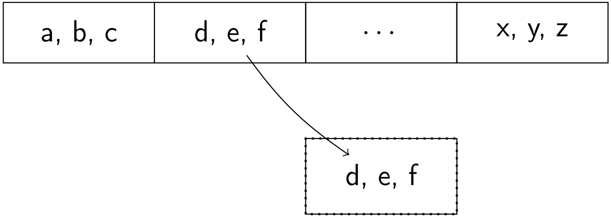
I/O Model : Sequential Access
Aggarwal and Vitter '87

a, b, c	d, e, f	$\cdots$	x, y, z

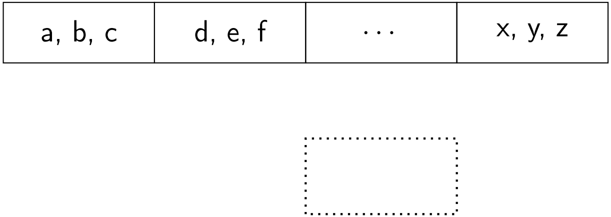
I/O Model : Sequential Access
Aggarwal and Vitter '87



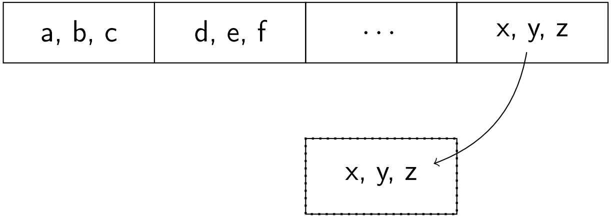
I/O Model : Sequential Access
Aggarwal and Vitter '87



I/O Model : Sequential Access
Aggarwal and Vitter '87



I/O Model : Sequential Access
Aggarwal and Vitter '87



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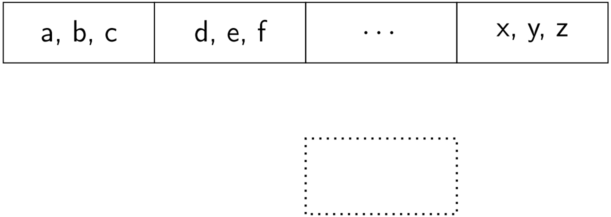

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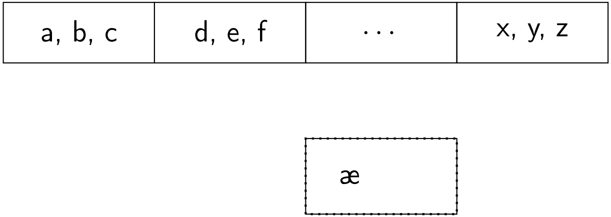
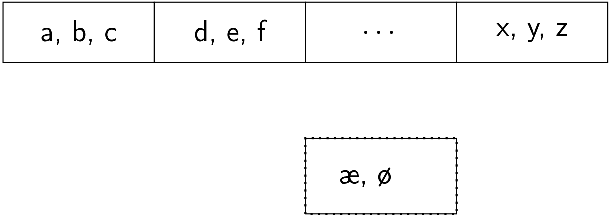
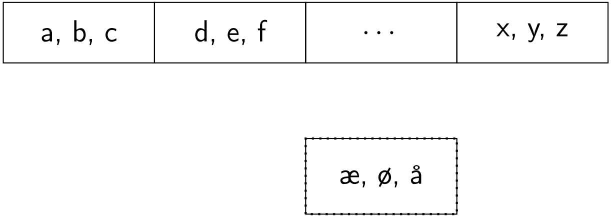


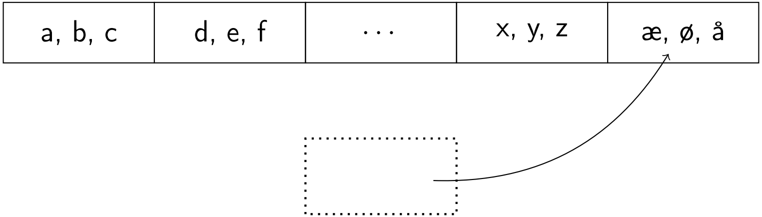
I/O Model : Sequential Access
Aggarwal and Vitter '87



I/O Model : Sequential Access
Aggarwal and Vitter '87



I/O Model : Sequential Access
Aggarwal and Vitter '87

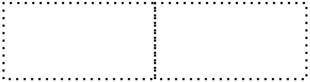


I/O Model : Sequential Access
Aggarwal and Vitter '87

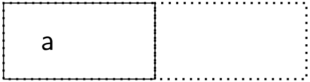
a, b, c	d, e, f	$\cdots$	x, y, z	æ, ø, å

Time	:	N
I/O	:	N/B
Memory	:	B

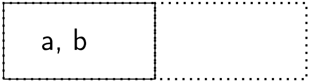
I/O Model : Stack



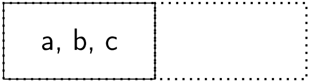
I/O Model : Stack



I/O Model : Stack



I/O Model : Stack



I/O Model : Stack

a, b, c	d

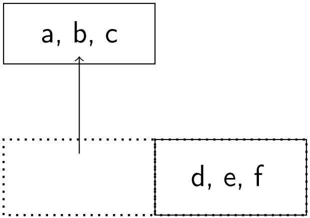
I/O Model : Stack

a, b, c	d, e

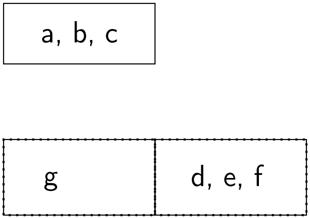
I/O Model : Stack

a, b, c	d, e, f

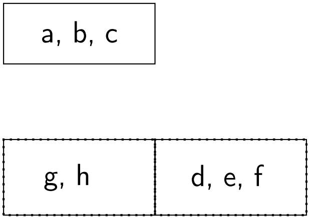
I/O Model : Stack



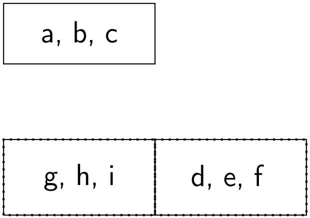
I/O Model : Stack



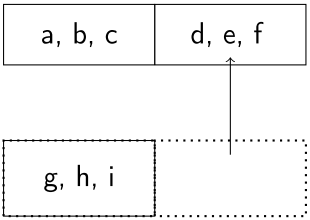
I/O Model : Stack



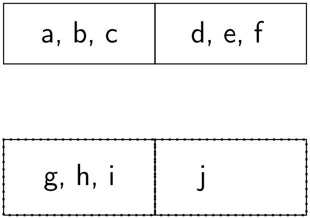
I/O Model : Stack



I/O Model : Stack



I/O Model : Stack



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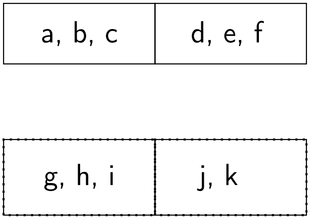
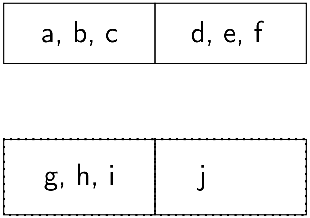
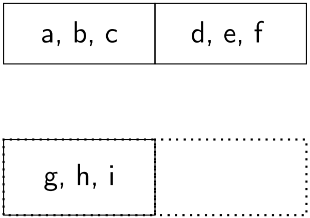


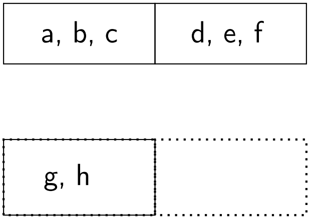
I/O Model : Stack



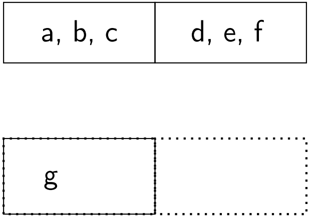
I/O Model : Stack



I/O Model : Stack



I/O Model : Stack



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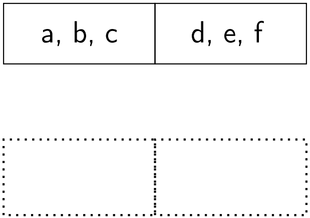
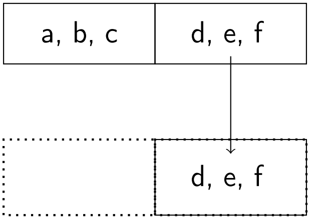
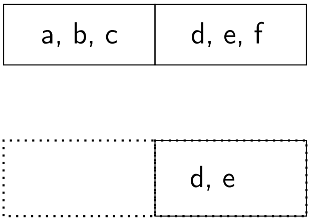


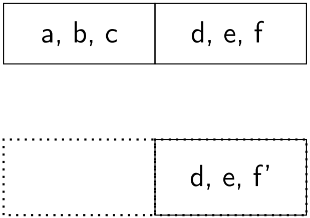
I/O Model : Stack



I/O Model : Stack



I/O Model : Stack



I/O Model : Stack

a, b, c	d, e, f

g'	d, e, f'

I/O Model : Stack

a, b, c	d, e, f

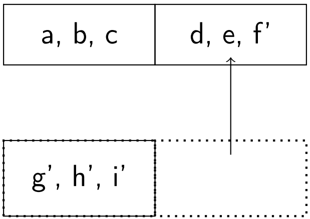
g', h'	d, e, f'

I/O Model : Stack

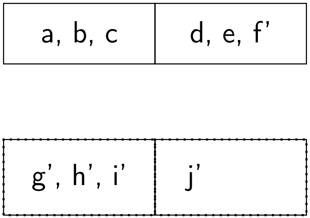
a, b, c	d, e, f

g', h', i'	d, e, f'

I/O Model : Stack



I/O Model : Stack



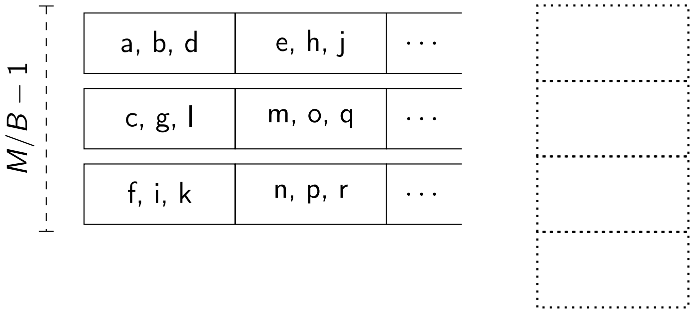
I/O Model : Stack

a, b, c	d, e, f’

g’, h’, i’	j’

Time	:	$O(N)$
I/O	:	$O(N/B)$
Memory	:	$2B$

I/O Model : M/B-way Mergesort
Aggarwal and Vitter '87



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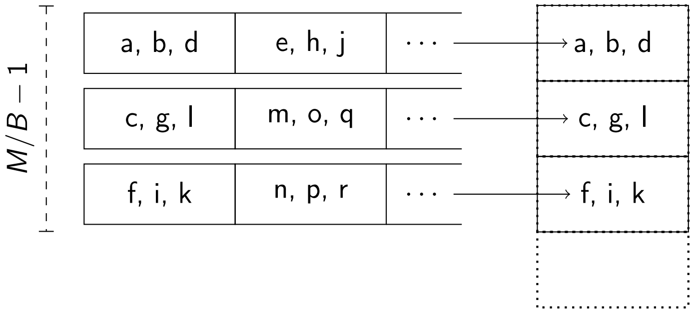

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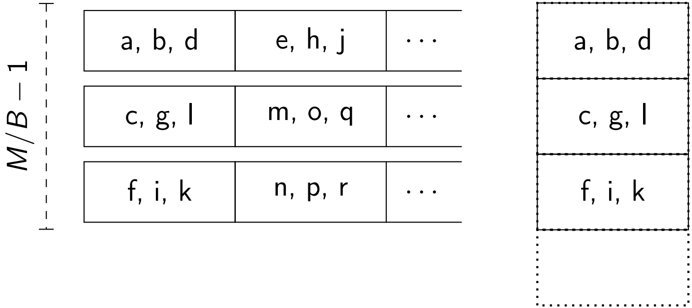

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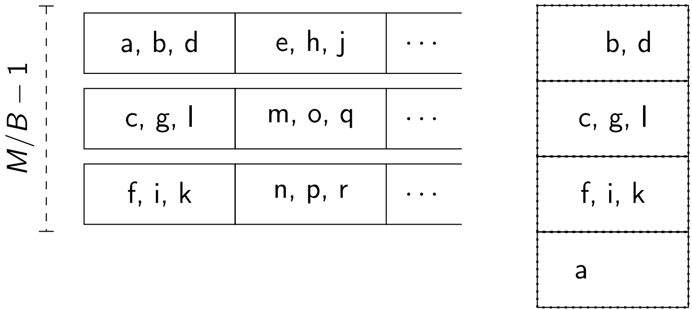
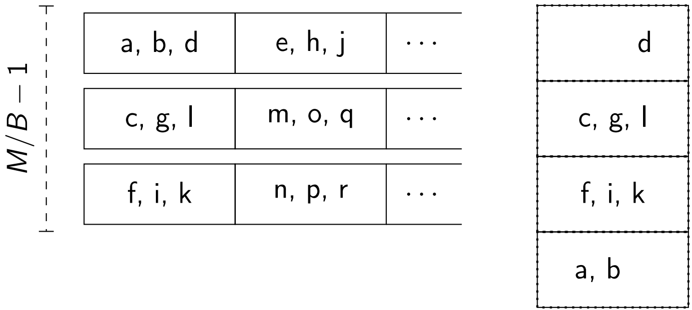
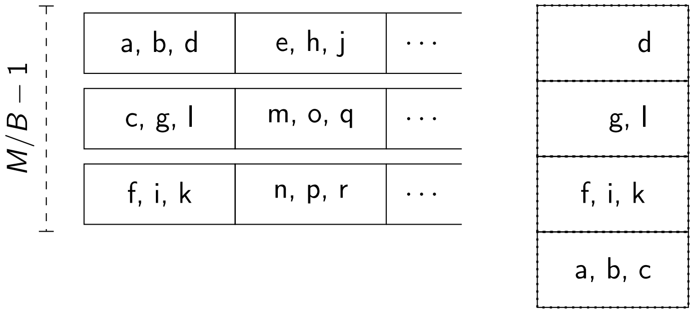
Aggarwal and Vitter '87



I/O Model : M/B-way Mergesort
Aggarwal and Vitter '87



I/O Model : M/B-way Mergesort
Aggarwal and Vitter '87



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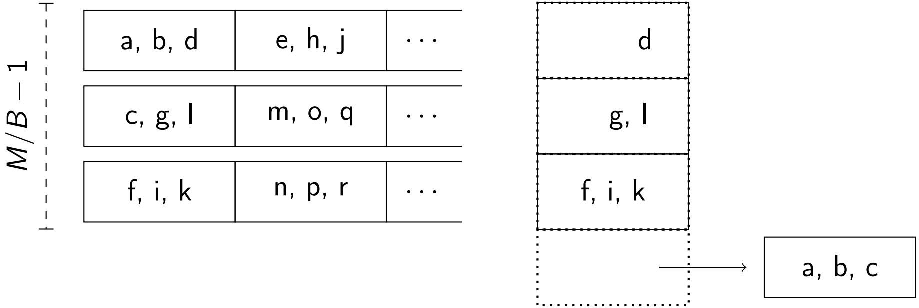

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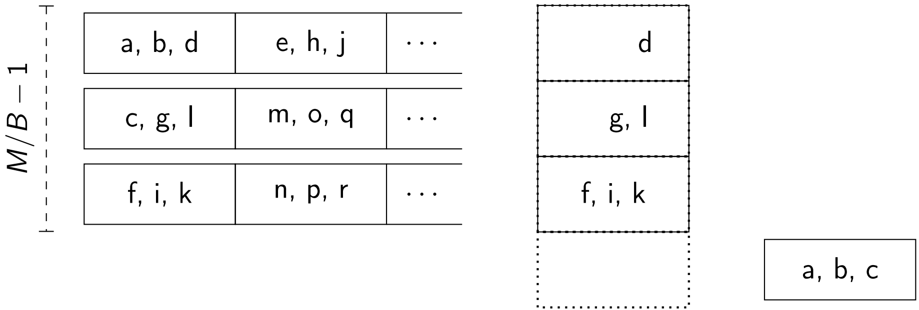

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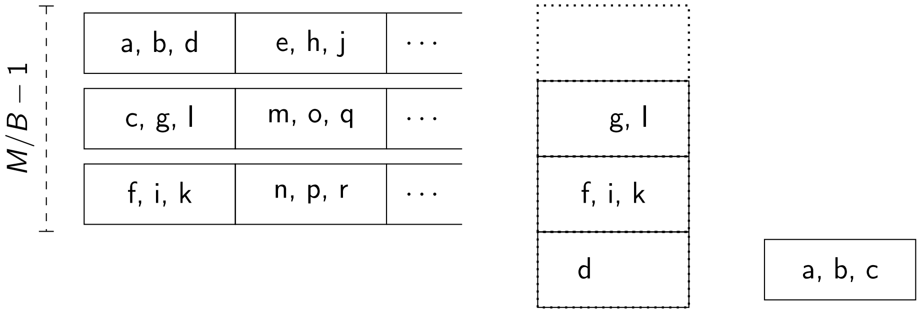

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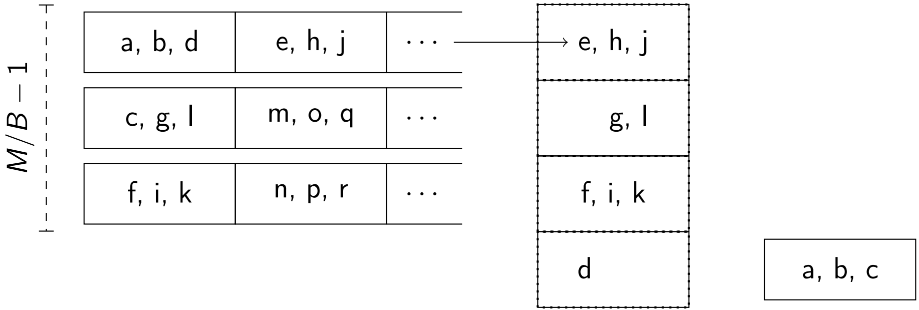

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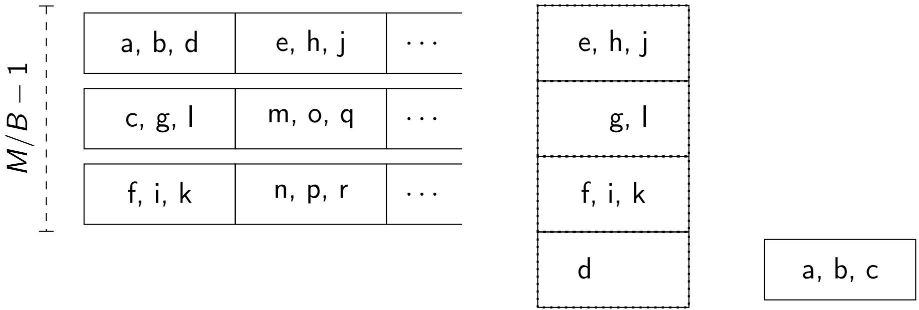

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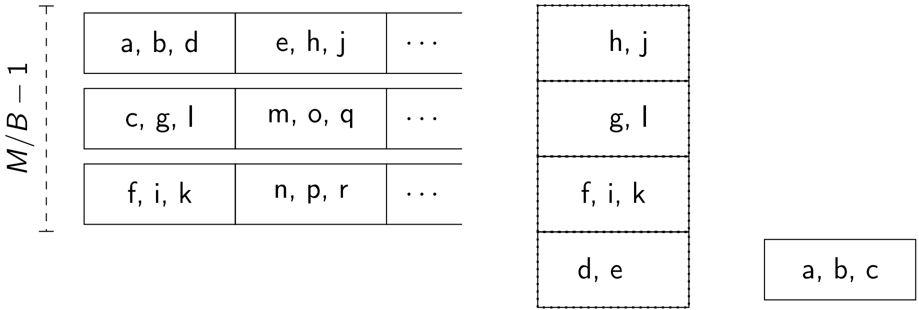
Aggarwal and Vitter '87



I/O Model : M/B-way Mergesort
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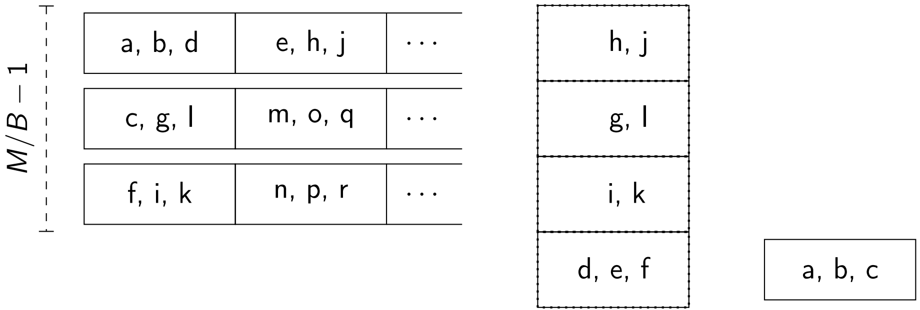
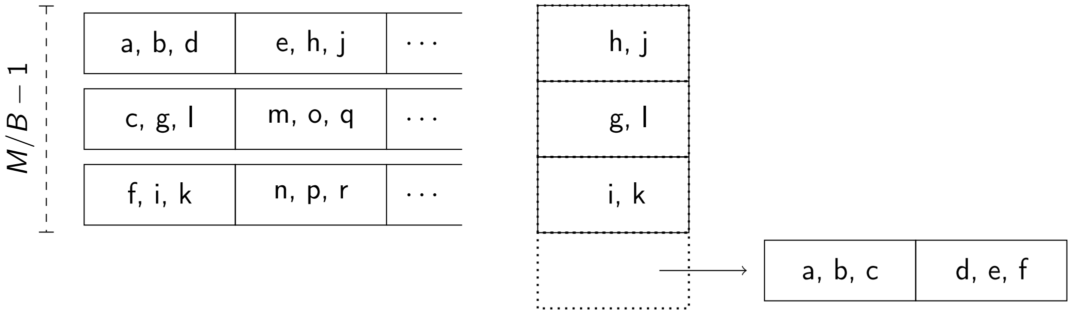
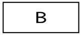


I/O Model : M/B-way Mergesort
Aggarwal and Vitter '87



I/O Model : M/B-way Mergesort
Aggaarwal and Vitter '87

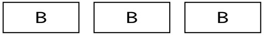
I/O Model : M/B-way Mergesort
Aggarwal and Vitter '87



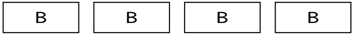
I/O Model : M/B-way Mergesort
Aggarwal and Vitter '87

B	B

I/O Model : M/B-way Mergesort
Aggarwal and Vitter '87



I/O Model : M/B-way Mergesort
Aggarwal and Vitter '87



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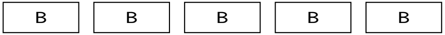

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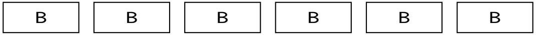

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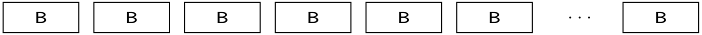

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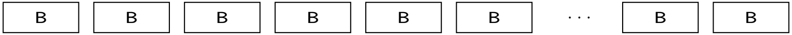

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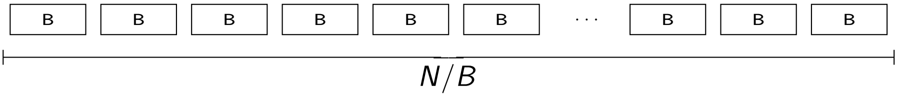
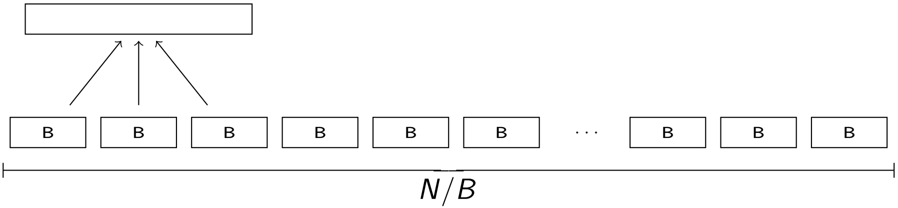


I/O Model : M/B-way Mergesort
Aggarwal and Vitter '87



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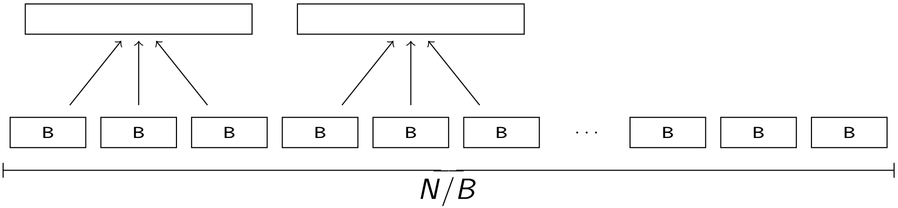

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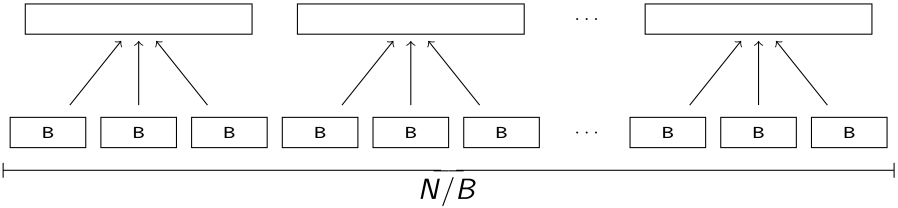

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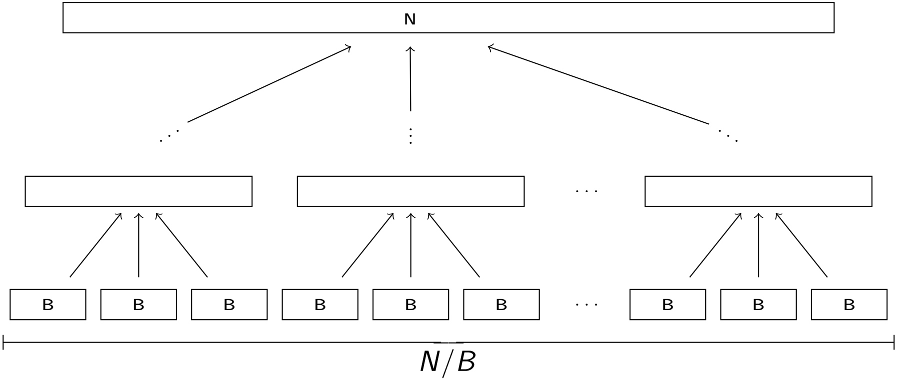

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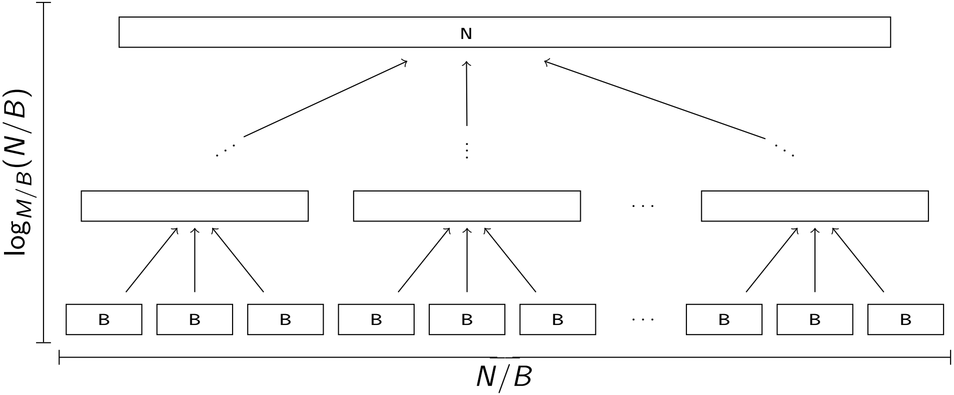


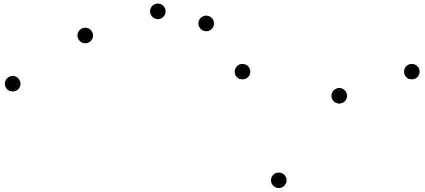
I/O Model : M/B-way Mergesort
Aggarwal and Vitter '87

Theorem
N elements can be sorted in $\Theta(N/B \cdot \log_{M/B}(N/B))$ I/Os.

Convex Hull : Graham Scan
Graham '72

Convex Hull

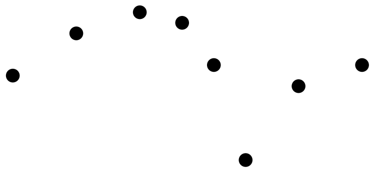
Compute the *convex hull* for N points in the plane.



Theorem
Convex Hull can be computed in $O(N/B \cdot \log_{M/B}(N/B))$ *I/Os.*

Convex Hull : Graham Scan
Graham '72

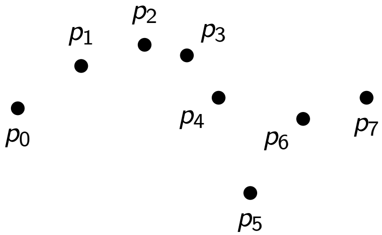
Upper Hull:



Convex Hull : Graham Scan
Graham '72

Upper Hull:

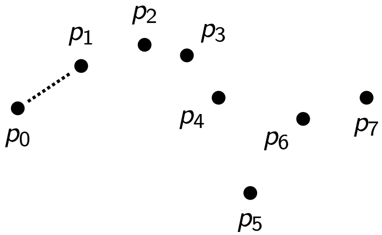
- Sort input points by x-axis



Convex Hull : Graham Scan
Graham '72

Upper Hull:

- Sort input points by x-axis
- Initialize stack $S = [p_0, p_1]$



Convex Hull : Graham Scan
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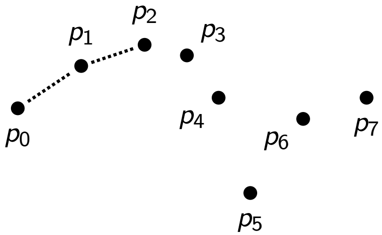
Upper Hull:

- Sort input points by x-axis
- Initialize stack $S = [p_0, p_1]$
- For remaining points $p_i \in p_2, p_3, \ldots, p_{N-1}$:
  1. Let p_s, p_t be the two top-most points of S
  2. While $p_s - p_t - p_i$ is a "left-turn":
     - Pop p_t and go-to 1
  3. Push p_i onto S



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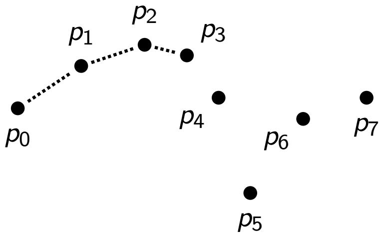

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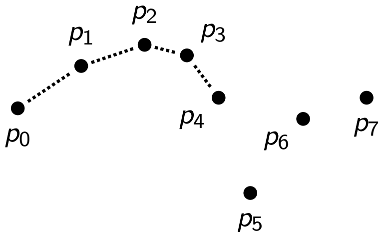

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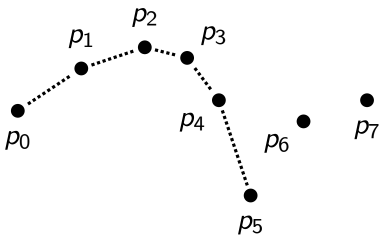

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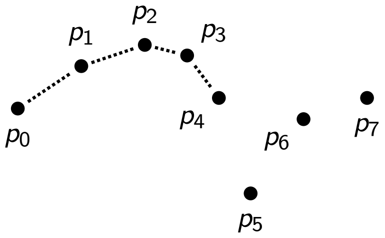

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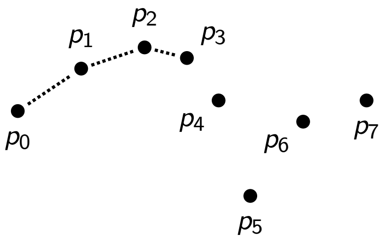

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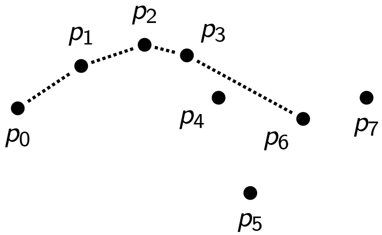

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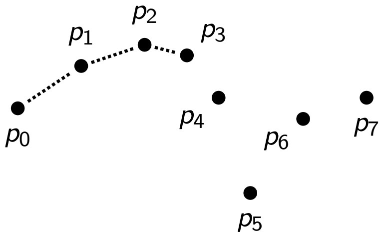

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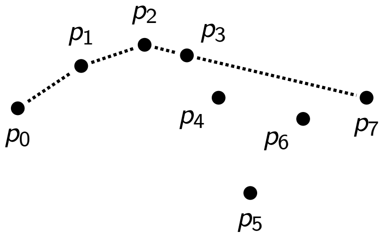

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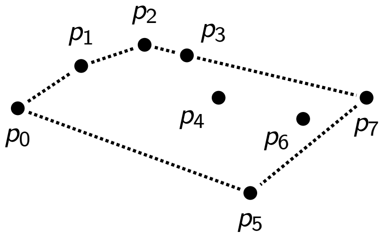
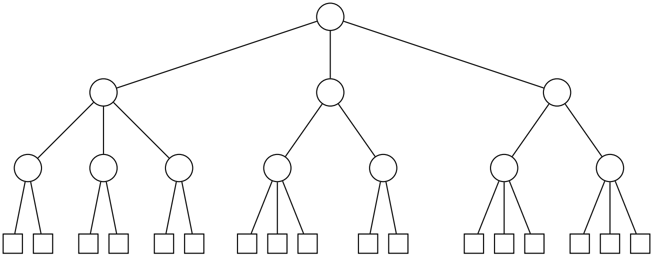


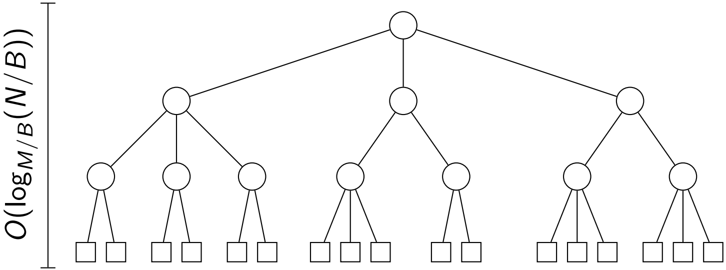
Lower Hull:

- Symmetric...

a–b Tree
Huddleston and Mehlhorn '82



Buffer Tree
Arge '95



$$a = \frac{1}{4}M/B, \qquad b = M/B, \qquad \text{Leaf Size} = B$$

Buffer Tree
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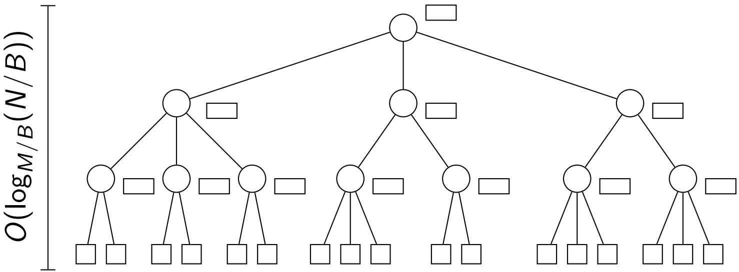

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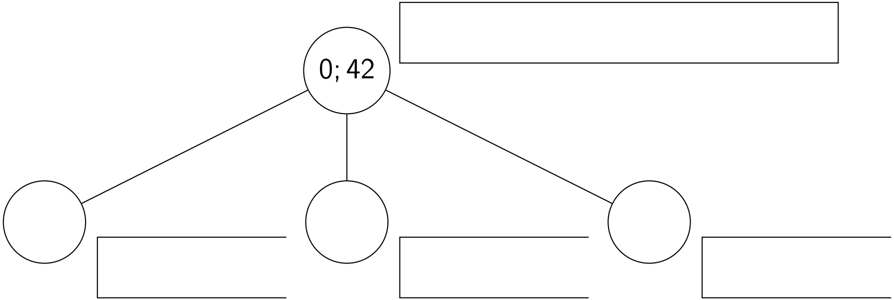

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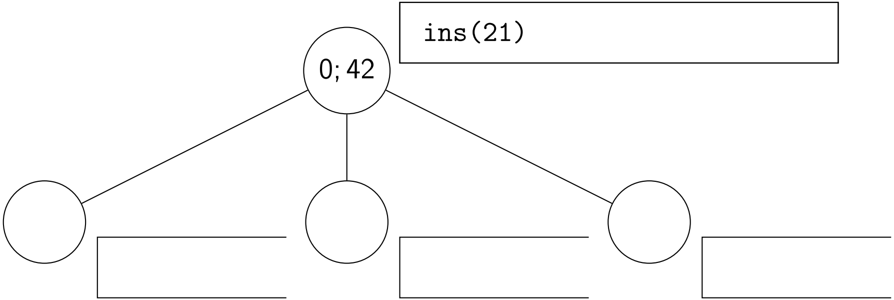

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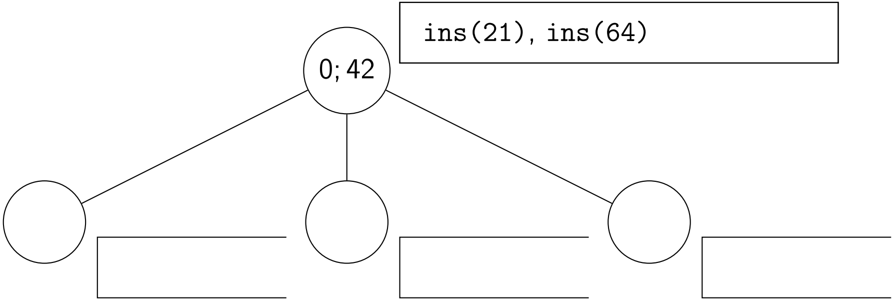

Buffer Tree
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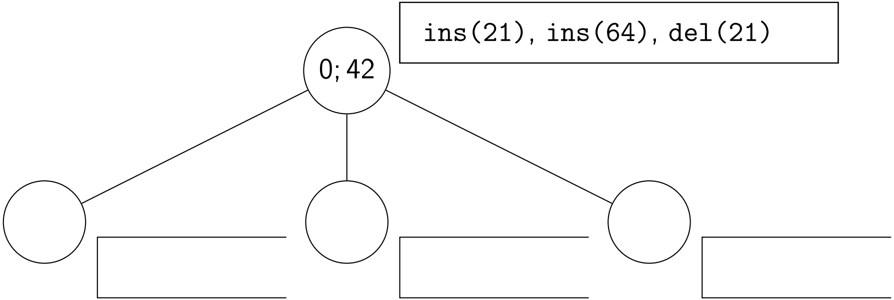

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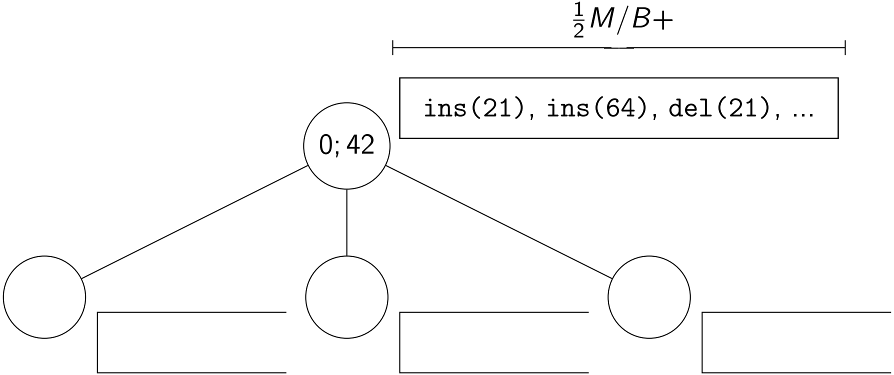

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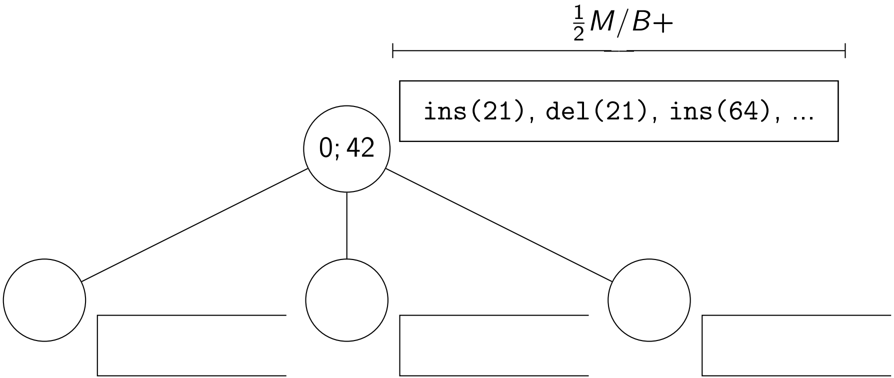

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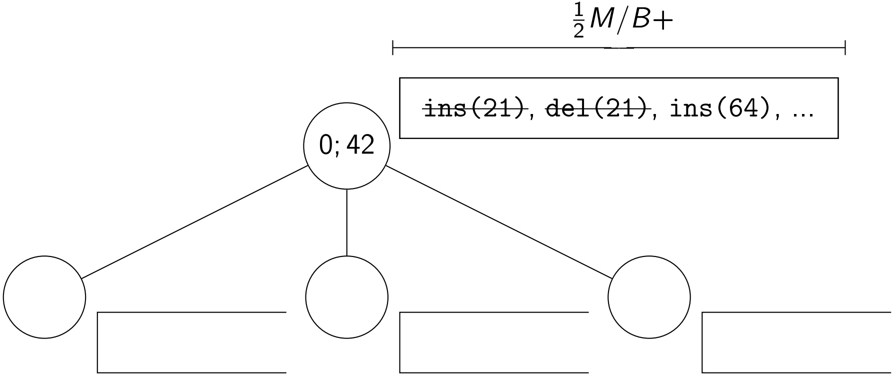

Buffer Tree
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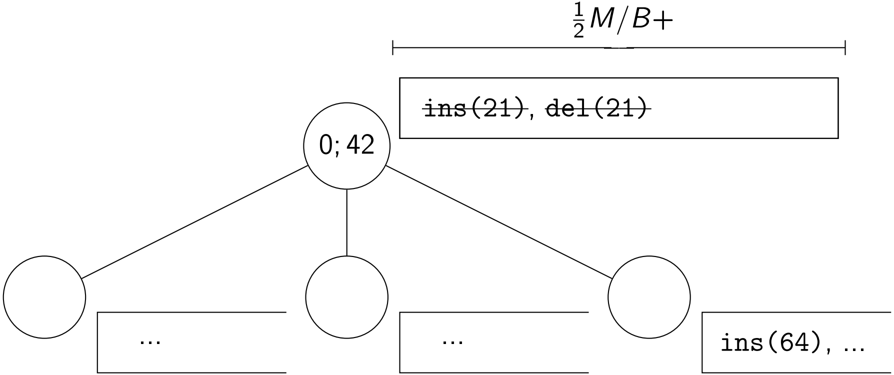

Buffer Tree
Arge '95

Theorem
A Buffer Tree can resolve N `inserts` and `deletes` in $\Theta(N/B \cdot \log_{M/B}(N/B))$ I/Os.

Buffer Tree
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A Buffer Tree can resolve N $\mathtt{inserts}$ and $\mathtt{deletes}$ in $\Theta(N/B \cdot \log_{M/B}(N/B))$ I/Os.

Theorem
A Buffer Tree with N requests can empty all its buffers, and output all remaining sorted elements, in $\Theta(N/B)$ I/Os.

Buffer Tree
Arge '95

Theorem
A Buffer Tree can resolve N `inserts` and `deletes` in $\Theta(N/B \cdot \log_{M/B}(N/B))$ *I/Os.*

Theorem
A Buffer Tree with N requests can empty all its buffers, and output all remaining sorted elements, in $\Theta(N/B)$ *I/Os.*

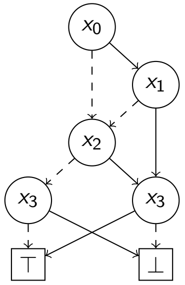
Corollary
An I/O-efficient Priority Queue can resolve N `push` and `deletemin` operations in $\Theta(N/B \cdot \log_{M/B}(N/B))$ *I/Os.*

Proof.
Use an $M/2$ sized internal memory priority queue, `pq`. If `pq` overflows, move $M/4$ the largest elements to a Buffer Tree, `t`. If `pq` underflows, obtain the $M/4$ smallest elements from `t`. □

Binary Decision Diagrams
Arge '96, Sølvsten '22

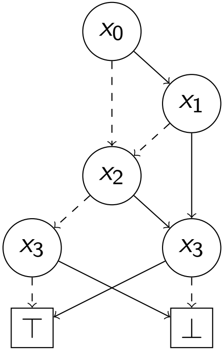
#Paths
Given a Binary Decision Diagram of N nodes, compute the number of paths from the root to the $\top$ terminal.

Theorem
#Paths can be computed in $O(N/B \cdot \log_{M/B}(N/B))$ *I/Os.*



(a) $(x_0 \land x_1 \land x_3) \lor (x_2 \oplus x_3)$

Binary Decision Diagrams
Arge '96, Sølvsten '22



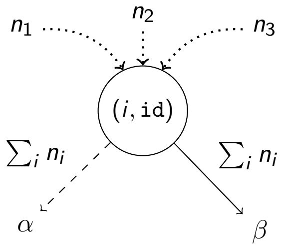
Decision Diagram

$$
\begin{array}{lcr}
[& ((0,0),(2,0),(1,0)) & , \\
  & ((1,0),(2,0),(3,1)) & , \\
  & ((2,0),(3,0),(3,1)) & , \\
  & ((3,0),\top,\bot) & , \\
  & ((3,1),\bot,\top) &]
\end{array}
$$

On-Disk Format

(a) $(x_0 \wedge x_1 \wedge x_3) \vee (x_2 \oplus x_3)$

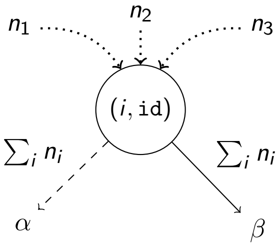
Binary Decision Diagrams
Arge '96, Sølvsten '22



Idea

Count the number of in-going paths to each node.

Binary Decision Diagrams
Arge '96, Sølvsten '22

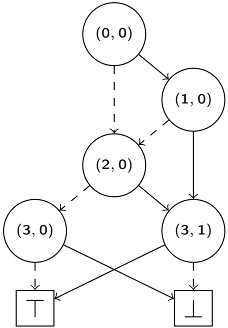


Time-Forward Processing

Defer work with Q_{count} : $\texttt{PriorityQueue}\langle(s \to t, \quad \mathbb{N})\rangle$ sorted on t in ascending order.

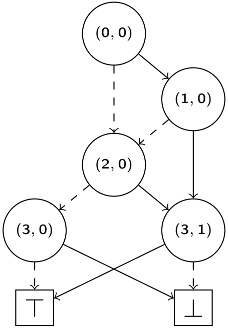
$$((i, \texttt{id}) \xrightarrow{\perp} \alpha, \quad \textstyle\sum_i n_i), \qquad ((i, \texttt{id}) \xrightarrow{\top} \beta, \quad \textstyle\sum_i n_i)$$

Binary Decision Diagrams
Arge '96, Sølvsten '22



(a) $(x_0 \land x_1 \land x_3) \lor (x_2 \oplus x_3)$

Binary Decision Diagrams
Arge '96, Sølvsten '22



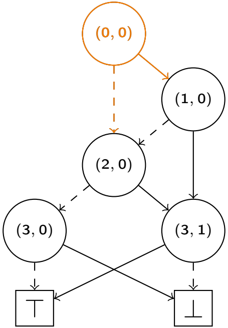
(a) $(x_0 \wedge x_1 \wedge x_3) \vee (x_2 \oplus x_3)$

Priority Queue: Q_{count}:

[

]

Binary Decision Diagrams
Arge '96, Sølvsten '22



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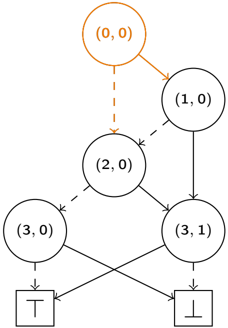

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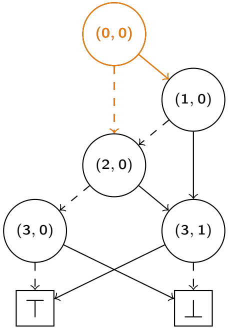
Priority Queue: Q_{count}:

$$
[\quad ((0,0) \xrightarrow{\top} (1,0),\quad 1)\quad ,
$$
$$
((0,0) \xrightarrow{\bot} (2,0),\quad 1)\quad ,
$$
$$
]
$$

Binary Decision Diagrams
Arge '96, Sølvsten '22



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Seek	Sum	Result
$(1, 0)$	0	0

Priority Queue: Q_{count}:

$$[\quad ((0,0) \xrightarrow{\top} (1,0),\quad 1)\quad ,$$
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$$]$$

Binary Decision Diagrams
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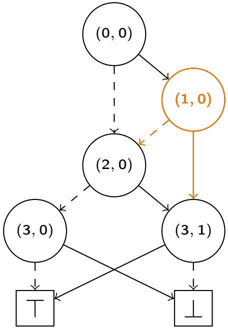

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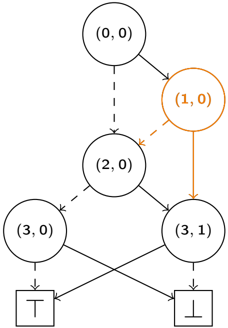
Binary Decision Diagrams
Arge '96, Sølvsten '22



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Priority Queue: Q_{count}:

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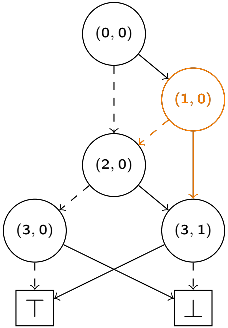
$((0,0) \xrightarrow{\perp} (2,0), \quad 1)$,

]

Binary Decision Diagrams
Arge '96, Sølvsten '22



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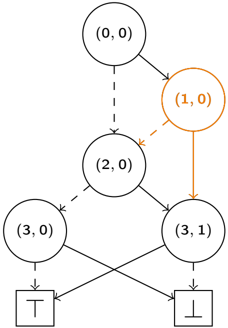
Binary Decision Diagrams
Arge '96, Sølvsten '22



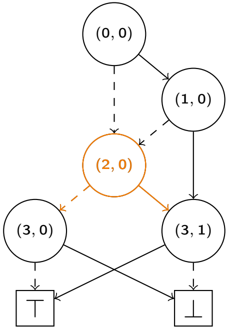
(a) $(x_0 \wedge x_1 \wedge x_3) \vee (x_2 \oplus x_3)$

Seek	Sum	Result
$(2,0)$	0	0

Priority Queue: Q_{count}:

$$
\begin{aligned}
[\; & \\
& ((0,0) \xrightarrow{\perp} (2,0), \quad 1) \quad , \\
& ((1,0) \xrightarrow{\perp} (2,0), \quad 1) \quad , \\
& \\
& ((1,0) \xrightarrow{\top} (3,1), \quad 1) \quad , \\
& \;]
\end{aligned}
$$

Binary Decision Diagrams
Arge '96, Sølvsten '22



(a) $(x_0 \wedge x_1 \wedge x_3) \vee (x_2 \oplus x_3)$

Seek	Sum	Result
$(2, 0)$	0	0

Priority Queue: Q_{count}:

$$
\begin{array}{l}
[\\
\quad ((0,0) \xrightarrow{\perp} (2,0), \quad 1) \quad , \\
\quad ((1,0) \xrightarrow{\perp} (2,0), \quad 1) \quad , \\
\\
\quad ((1,0) \xrightarrow{\top} (3,1), \quad 1) \quad , \\
]
\end{array}
$$

Binary Decision Diagrams
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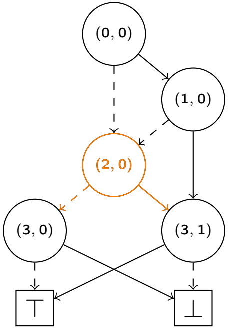


(a) $(x_0 \wedge x_1 \wedge x_3) \vee (x_2 \oplus x_3)$

Seek	Sum	Result
$(2, 0)$	1	0

Priority Queue: Q_{count}:

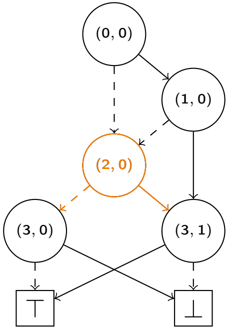
[

$((1,0) \xrightarrow{\perp} (2,0),\quad 1)$,

$((1,0) \xrightarrow{\top} (3,1),\quad 1)$,

]

Binary Decision Diagrams
Arge '96, Sølvsten '22



(a) $(x_0 \wedge x_1 \wedge x_3) \vee (x_2 \oplus x_3)$

Seek	Sum	Result
$(2, 0)$	2	0

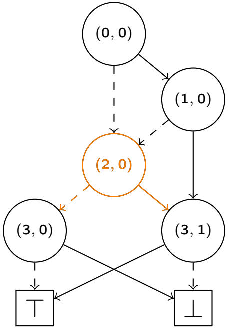
Priority Queue: Q_{count}:

[

$((1,0) \xrightarrow{\top} (3,1), \quad 1)$,

]

Binary Decision Diagrams
Arge '96, Sølvsten '22



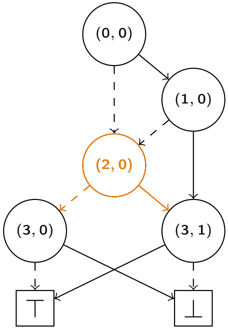
(a) $(x_0 \land x_1 \land x_3) \lor (x_2 \oplus x_3)$

Seek	Sum	Result
$(2, 0)$	2	0

Priority Queue: Q_{count}:

$$
\begin{aligned}
[\ & \\
&((2,0) \xrightarrow{\perp} (3,0), \quad 2) \quad , \\
&((1,0) \xrightarrow{\top} (3,1), \quad 1) \quad , \\
&((2,0) \xrightarrow{\top} (3,1), \quad 2) \quad]
\end{aligned}
$$

Binary Decision Diagrams
Arge '96, Sølvsten '22



(a) $(x_0 \wedge x_1 \wedge x_3) \vee (x_2 \oplus x_3)$

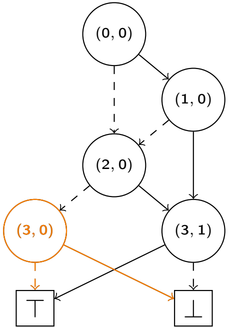
Seek	Sum	Result
$(3, 0)$	0	0

Priority Queue: Q_{count}:

[

$((2,0) \xrightarrow{\perp} (3,0),\quad 2)$,
$((1,0) \xrightarrow{\top} (3,1),\quad 1)$,
$((2,0) \xrightarrow{\top} (3,1),\quad 2)$]

Binary Decision Diagrams
Arge '96, Sølvsten '22



(a) $(x_0 \land x_1 \land x_3) \lor (x_2 \oplus x_3)$

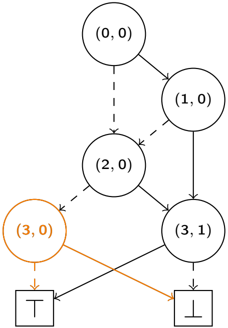
Seek	Sum	Result
$(3, 0)$	0	0

Priority Queue: Q_{count}:

[

$((2,0) \xrightarrow{\bot} (3,0),\quad 2)$,
$((1,0) \xrightarrow{\top} (3,1),\quad 1)$,
$((2,0) \xrightarrow{\top} (3,1),\quad 2)$]

Binary Decision Diagrams
Arge '96, Sølvsten '22



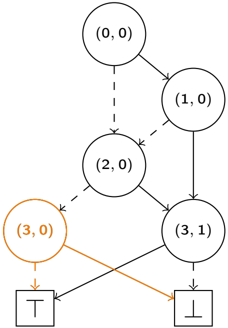
(a) $(x_0 \land x_1 \land x_3) \lor (x_2 \oplus x_3)$

Seek	Sum	Result
$(3, 0)$	2	0

Priority Queue: Q_{count}:

$$[\; ((1,0) \xrightarrow{\top} (3,1),\quad 1) \;,\; ((2,0) \xrightarrow{\top} (3,1),\quad 2) \;]$$

Binary Decision Diagrams
Arge '96, Sølvsten '22



(a) $(x_0 \wedge x_1 \wedge x_3) \vee (x_2 \oplus x_3)$

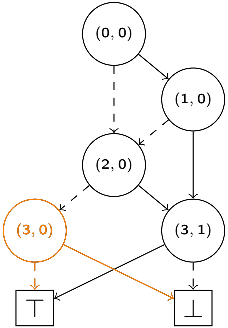
Seek	Sum	Result
$(3, 0)$	2	2

Priority Queue: Q_{count}:

[

$((1, 0) \xrightarrow{\top} (3, 1), \quad 1)$,
$((2, 0) \xrightarrow{\top} (3, 1), \quad 2)$]

Binary Decision Diagrams
Arge '96, Sølvsten '22



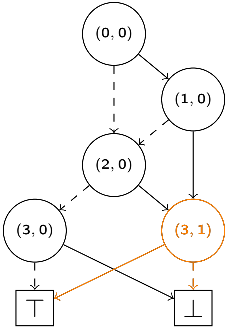
(a) $(x_0 \wedge x_1 \wedge x_3) \vee (x_2 \oplus x_3)$

Seek	Sum	Result
$(3, 1)$	0	2

Priority Queue: Q_{count}:

$$[\; ((1,0) \xrightarrow{\top} (3,1),\quad 1) \;,\; ((2,0) \xrightarrow{\top} (3,1),\quad 2) \;]$$

Binary Decision Diagrams
Arge '96, Sølvsten '22



(a) $(x_0 \wedge x_1 \wedge x_3) \vee (x_2 \oplus x_3)$

Seek	Sum	Result
$(3, 1)$	0	2

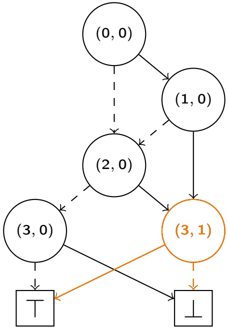
Priority Queue: Q_{count}:

[

$((1,0) \xrightarrow{\top} (3,1), \quad 1)$,

$((2,0) \xrightarrow{\top} (3,1), \quad 2)$]

Binary Decision Diagrams
Arge '96, Sølvsten '22



(a) $(x_0 \wedge x_1 \wedge x_3) \vee (x_2 \oplus x_3)$

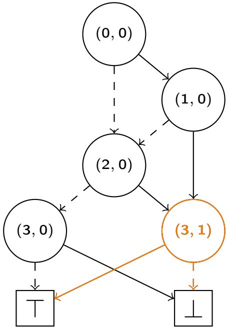
Seek	Sum	Result
(3, 1)	1	2

Priority Queue: Q_{count}:

[

$((2,0) \xrightarrow{\top} (3,1),\quad 2)$]

Binary Decision Diagrams
Arge '96, Sølvsten '22



(a) $(x_0 \wedge x_1 \wedge x_3) \vee (x_2 \oplus x_3)$

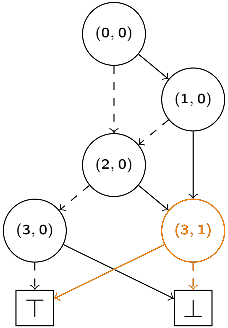
Seek	Sum	Result
$(3, 1)$	3	2

Priority Queue: Q_{count}:

[

]

Binary Decision Diagrams
Arge '96, Sølvsten '22



(a) $(x_0 \wedge x_1 \wedge x_3) \vee (x_2 \oplus x_3)$

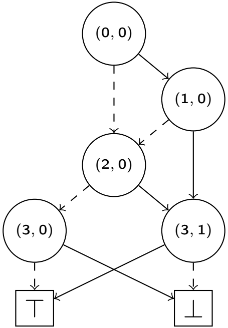
Seek	Sum	Result
$(3,1)$	3	5

Priority Queue: Q_{count}:

[

]

Binary Decision Diagrams
Arge '96, Sølvsten '22



(a) $(x_0 \wedge x_1 \wedge x_3) \vee (x_2 \oplus x_3)$

Result

5

Priority Queue: Q_{count}:

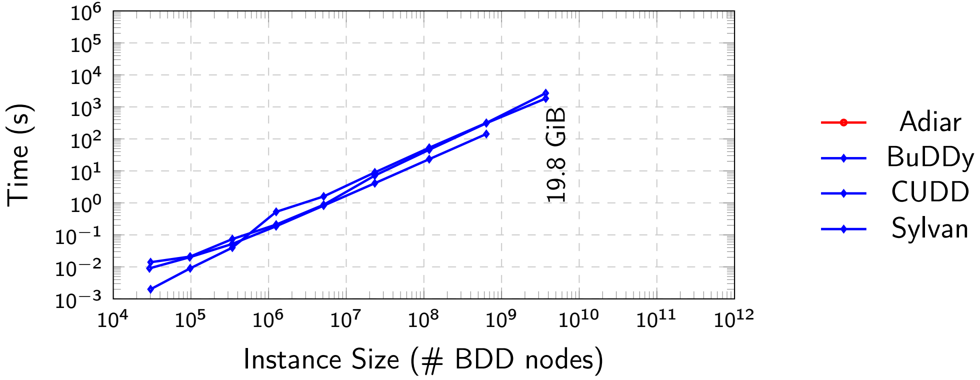
[

]

Adiar

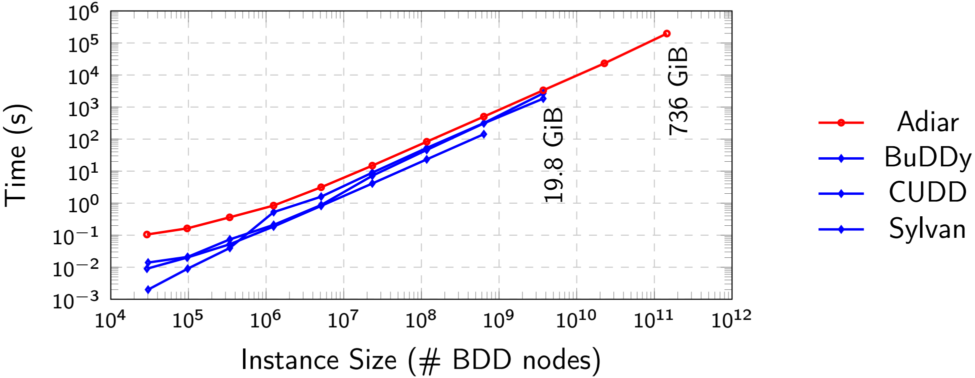
github.com/ssoelvsten/adiar

Binary Decision Diagrams
Arge '96, Sølvsten '22



Running time for the *N-Queens* problems.

Binary Decision Diagrams
Arge '96, Sølvsten '22



Running time for the *N-Queens* problems.

Further Reading : Foundations

- **Aggarwal and Vitter (1987)**
  "The Input/Output Complexity of Sorting and Related Problems"
  The I/O-model, Sorting, Permutation, FFT, and Matrix transposition.
- **Arge, Goodrich, Nelson, and Sitchinava (2008)**
  "Fundamental Parallel Algorithms for Private-cache Chip Multiprocessors."
  The I/O-model for Multi-Threading.

Further Reading : Data Structures

- **Arge (1995)**
  "The Buffer Tree: A new technique for Optimal I/O-algorithms"
  An I/O-efficient Tree, Priority Queue, and Range Tree.
- **Sanders (2002)**
  "Fast Priority Queues for Cached Memory"
  A much faster I/O-efficient Priority Queue.
- **Agarwal, Arge and Yi (2006)**
  "I/O-Efficient Batched Union-Find and Its Applications to Terrain Analysis"
  An I/O-efficient (Lazy) Union-Find.

Further Reading : Algorithms

- **Goodrich, Tsay, Vengroff, and Vitter (1993)**
  "External-Memory Computational Geometry"
  Distribution Sweeping and other algorithms.
- **Chiang, Goodrich, Grove, Tamassia, Vengroff, and Vitter (1995)**
  "External-memory Graph Algorithms"
  Time-forward Processing and other algorithms.
- **Arge, Toma, Vitter (2001)**
  "I/O-Efficient Algorithms for Problems on Grid-Based Terrains"
  The TerraFlow algorithm.

Further Reading : Libraries (C++)

- **TPIE : Templated Portable I/O Environment**
  `github.com/thomasmoelhave/tpie`
  Duke University and Aarhus University
- **STXXL : Standard Template library for XXL data sets**
  `github.com/stxxl/stxxl`
  University of Karlsruhe

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ssoelvsten.github.io

Adiar

github.com/ssoelvsten/adiar

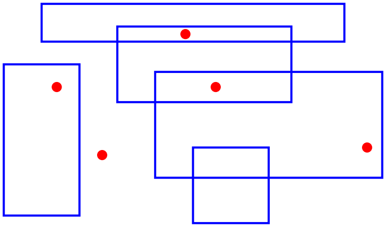
ssoelvsten.github.io/adiar

AARHUS UNIVERSITY

Distribution Sweeping
Goodrich, Tsay, Vengroff, and Vitter '93

Batched Range Searching

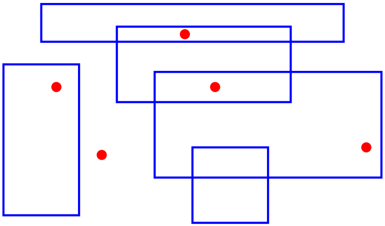
Given N axis-parallel rectangles and N points in the plane, compute for each point p all rectangles containing p.



Theorem
Batched Range Searching can be solved in $O(sort(N) + scan(T))$ I/Os.

Distribution Sweeping
Goodrich, Tsay, Vengroff, and Vitter '93

Preprocessing:

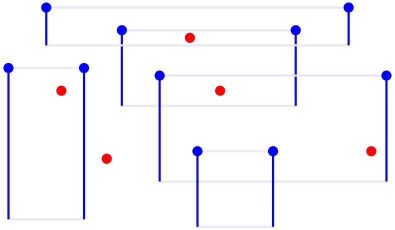


Algorithm:

Distribution Sweeping
Goodrich, Tsay, Vengroff, and Vitter '93

Preprocessing:

- Split each rectangle into two vertical lines.



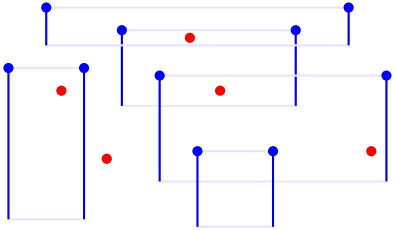
Algorithm:

Distribution Sweeping
Goodrich, Tsay, Vengroff, and Vitter '93

Preprocessing:

- Split each rectangle into two vertical lines.
- Sort all lines and points by their x-value.

Algorithm:



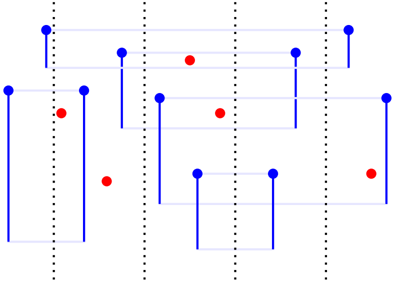
Distribution Sweeping
Goodrich, Tsay, Vengroff, and Vitter '93

Preprocessing:

- Split each rectangle into two vertical lines.
- Sort all lines and points by their x-value.

Algorithm:

- Split all data into $\Theta(\sqrt{M/B})$ *slabs*. Solve these recursively; output is given sorted by y-value.



Distribution Sweeping
Goodrich, Tsay, Vengroff, and Vitter '93

Preprocessing:

- Split each rectangle into two vertical lines.
- Sort all lines and points by their x-value.

Algorithm:

- Split all data into $\Theta(\sqrt{M/B})$ *slabs*. Solve these recursively; output is given sorted by y-value.
- Merge slabs together, report points between line segments outside its slab.
  - Use $\Theta(\sqrt{M/B}^2) = \Theta(\sqrt{M/B})$ multi-slabs to maintain each *active* rectangle.
  - Output points and un-matched line segments.