CS 240 – Data Structures and Data Management

Module 11: External Memory

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References: Goodrich & Tamassia 20.1-20.3, Sedgewick 16.4

Outline

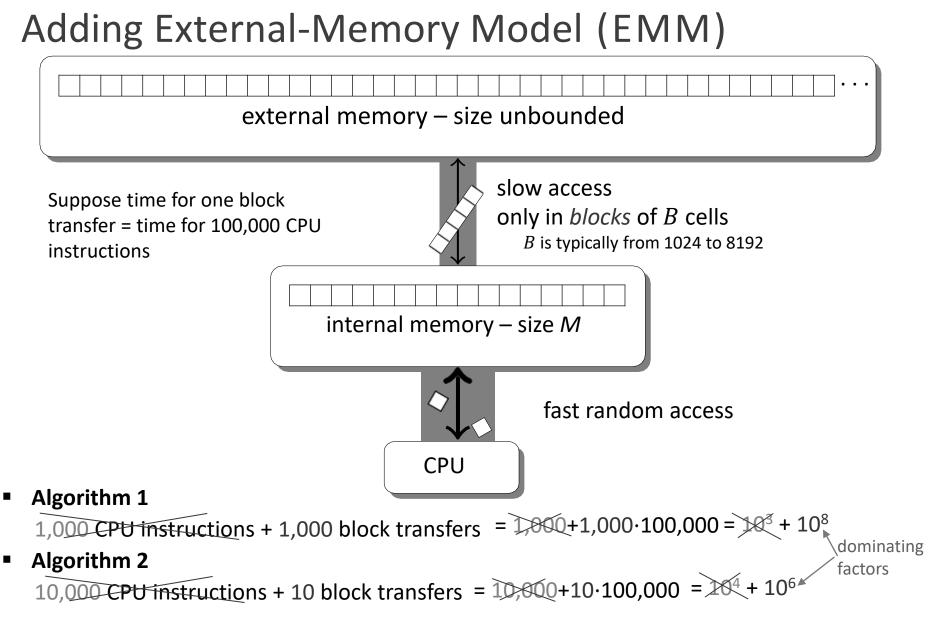
- External Memory
 - Motivation
 - External sorting
 - External Dictionaries
 - 2-4 Trees
 - (*a*, *b*)-Trees
 - B-Trees

Outline

- External Memory
 - Motivation
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 - (*a*, *b*)-Trees
 - B-Trees

Different levels of memory

- Memory hierarchy for current computer architectures
 - Registers: super fast, very small
 - cache L1, L2: very fast, less small
 - main memory: fast, large
 - disk or cloud: slow, very large
 - from 1000 to 1,000,000 times slower than main memory
- Desirable to minimize transfer between slow/fast memory
- Focus on main (internal) memory and disk or cloud (external) memory
 - accessing a single location in external memory automatically loads a whole block (or "page")
 - one block access can take as much time as executing 100,000 CPU instructions
 - need to care about the number of block accesses
 - new objective
 - revisit ADTs/problems with the objective of minimizing block transfers ("probes", "disk transfers", "page loads")



• **Cost of computation:** number of blocks transferred between internal and external memory

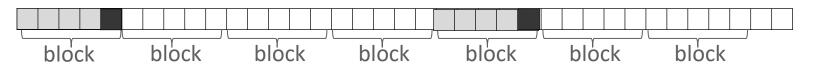
Outline

External Memory

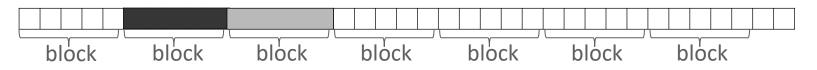
- Motivation
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- External Dictionaries
 - 2-4 Trees
 - (*a*, *b*)-Trees
 - B-Trees
- Extendible Hashing

Sorting in external memory

- Sort array *A* of *n* numbers
 - assume n is huge so that A is stored in blocks in external memory
- Heapsort was optimal in time and space in RAM model
 - poor memory locality: each iteration can access far apart indices of A



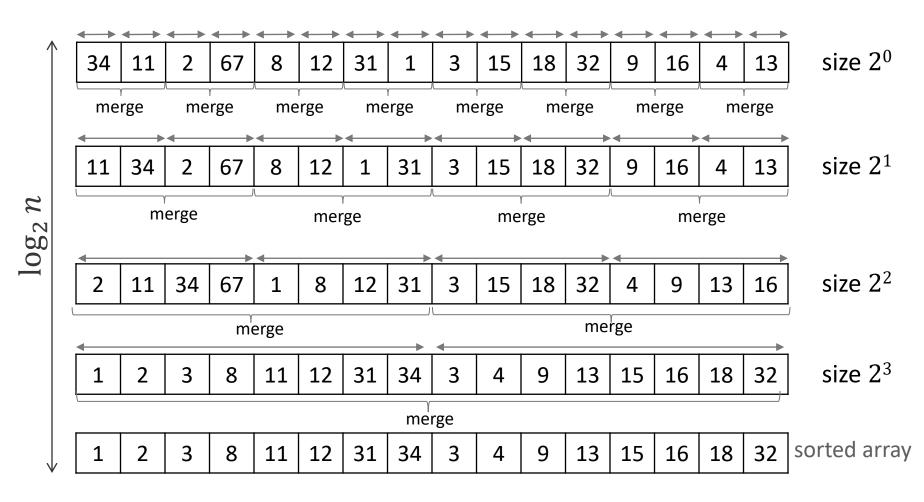
- accesses 2 blocks, but put only 2 elements in order
- and all the other data read in the block is not used
- heapsort does not adapt well to data stored in external memory
- Mergesort adapts well to array stored in external memory
 - access consecutive locations of A, ideal for reading in blocks



accesses 2 blocks, and puts all their elements in order

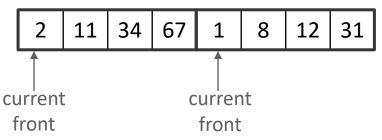
Mergesort: non-recusive view

- Several rounds of merging adjacent pairs of sorted runs (run = subarray)
 - in round *i*, merge sorted runs of size 2ⁱ
- Graphical notation sorted run



2-way Merge

Two sorted runs

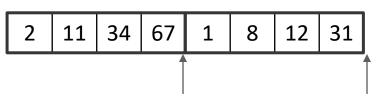


- Put a pointer at the front of each sorted run
 - call it 'current front'
- Repeatedly find the smallest element among current fronts
 - move the smallest element into sorted result array
 - advance current front of corresponding sorted run
- Array to store sorted result

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2-way Merge

Two sorted runs

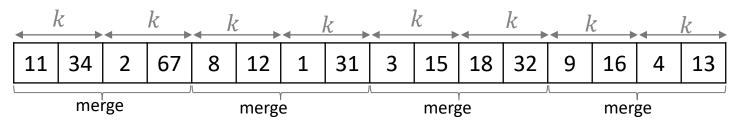


- Put a pointer at the front of each sorted run
 - call it 'current front'
- Repeatedly find the smallest element among current fronts
 - move the smallest element into sorted result array
 - advance current front of corresponding sorted run
- Array to store sorted result

• Time to merge two sequences each of size k is $\Theta(2k)$

Running time of MergeSort with 2-way Merge

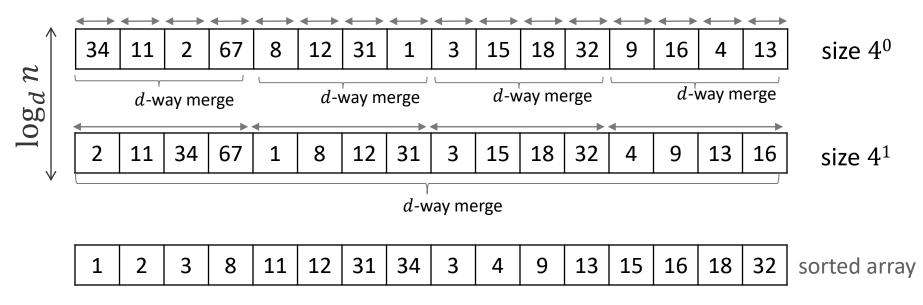
- $\Theta(\log_2 n)$ rounds
- Time for each round
 - time to merge 2 sequences each of size k is $\Theta(2k)$
 - in one round, need to merge n/(2k) sequences pairs



- one round of merge sort takes $\Theta(2k \cdot n/(2k)) = \Theta(n)$ time
- Total time for mergesort is $\Theta(n \log_2 n)$

d-way Mergesort

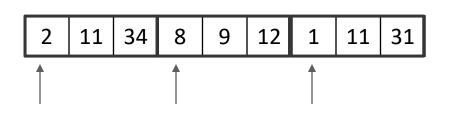
- Can generalize mergesort to merge *d* sorted runs at one time
 - *d* = 2 gives standard mergesort
- Example: d = 4



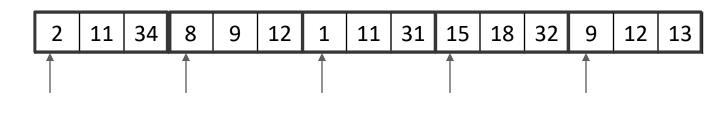
- $\log_d n = \frac{\log_2 n}{\log_2 d}$ rounds
 - the larger is d the less rounds
- How to merge d sorted runs efficiently?
 - *d*-Way merge

d-way Merge

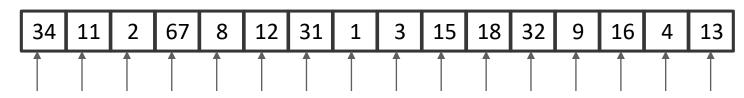
■ *d* = 3



■ *d* = 5



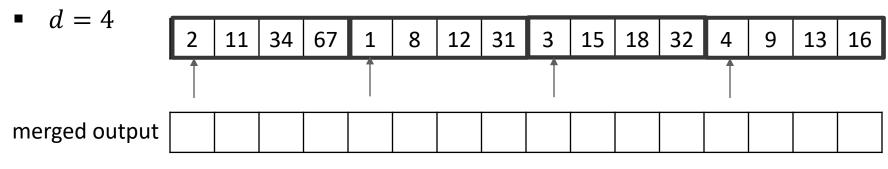
■ *d* = 16



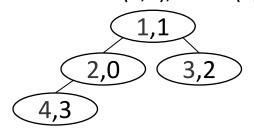
Need efficient data structure to find the minimum among d current fronts

d-way Merge with Min-Heap

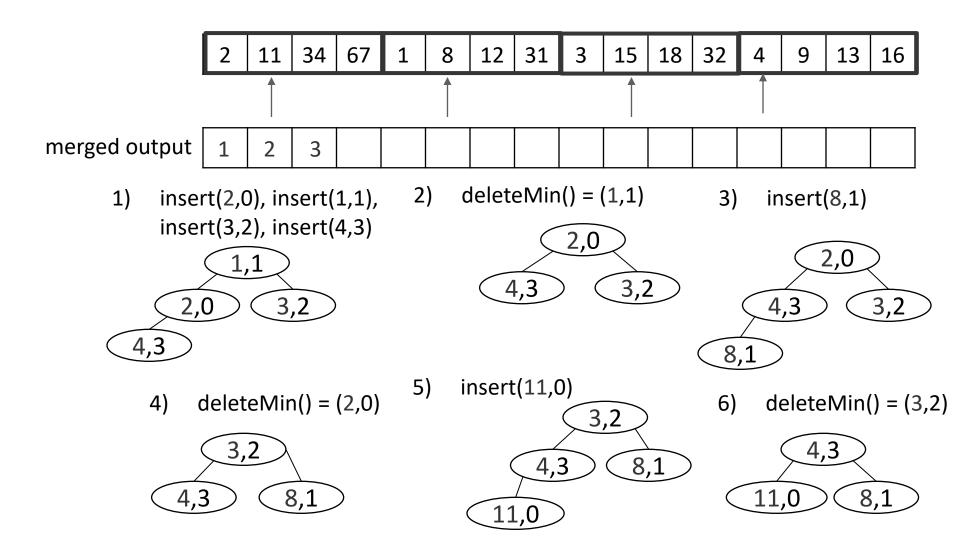
- Use min heap to find the smallest element among of d current fronts
 - (key,value) = (element, sorted run)



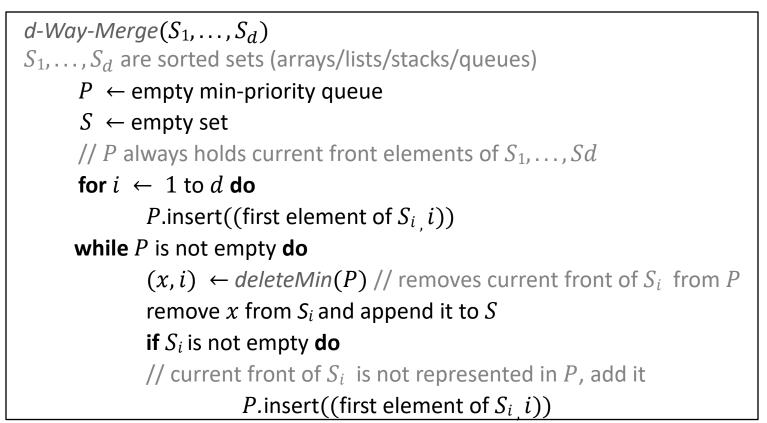
1) insert(2,0), insert(1,1), insert(3,2), insert(4,3)



d-way Merge with Min-Heap

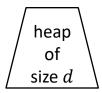


d-way Merge with Min Heap Pseudo Code



d-way Merge with Min Heap Time Complexity

- Merging d sequences each of size k
- *dk* iterations, at each iteration
 - one deleteMin() on heap of size d
 - $\Theta(\log_2 d)$
 - one insert() on heap of size *d*
 - $\Theta(\log_2 d)$
- Total time is $\Theta(dk \log_2 d)$



d-way Mergesort Complexity In Internal Memory

- log_d n rounds
- Time complexity for one round
 - time to merge d sequences of size is k is $\Theta(kd \log_2 d)$
 - for one round of mergesort , have to do n/(dk) of these merges
 - time for one round is $\Theta\left(\frac{n}{dk}kd \log_2 d\right) = \Theta(n \log_2 d)$

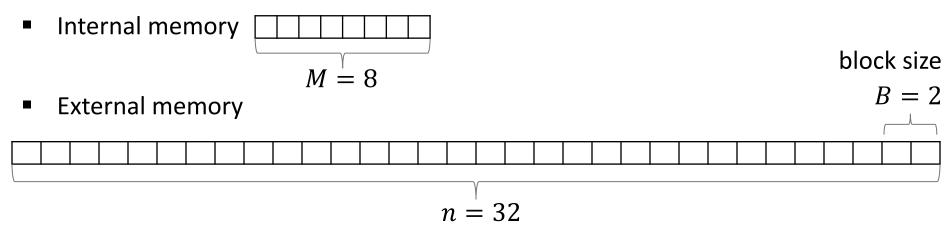
• Total time
$$\Theta(\log_d n \cdot n \log_2 d) = \Theta\left(\frac{\log_2 n}{\log_2 d} \cdot n \log_2 d\right) = \Theta(n \log_2 n)$$

no advantage in internal memory

d-way Mergesort Complexity In External Memory

- How do we gain advantage in external memory?
 - we only count block accesses
- $\log_d n$ rounds
 - time for each round is $\Theta(n \log_2 d) \quad \Theta(n)$, or better, in block accesses
- Total time $\Theta(\log_d n \cdot n \log_2 d) = \Theta(n \log_2 n)$ $\Theta(n)$ block $\Theta(n \log_d n)$ accesses block accesses

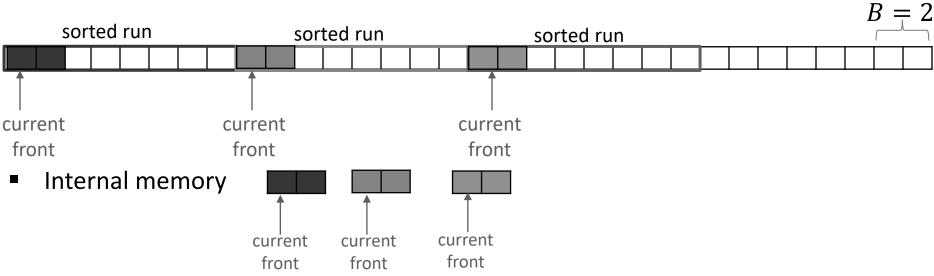
d-Way Mergesort in External Memory



- Cannot merge in external memory directly, have to transfer to internal memory
 - only internal memory has access to CPU
- Algorithm is largely the same, but for maximum block access efficiency
 - make d as large as possible
 - less rounds of mergesort
 - for any transferred block, all data from that block should be used for sorting

d-Way Merge in External Memory

External memory



- Key observation
 - do not need to transfer the full sorted run in internal memory to do d-way merge
 - at some point sorted runs will become so large that even one sorted run will not fit into the internal memory

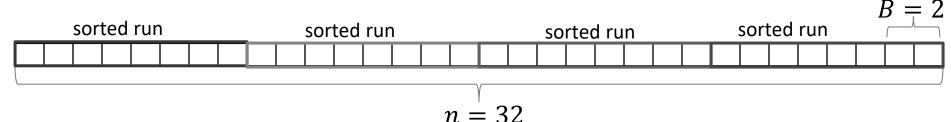
block size

- enough to transfer the block that contains current front from each sorted run
 - let is call it the *active block*
- could transfer more than one block, but transferring exactly one block lets us perform *d*-way merge with a larger *d*

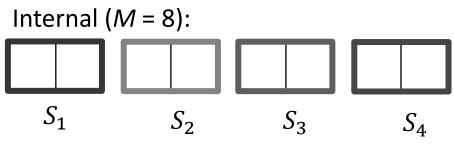
d-Way Merge in External Memory

External memory





Partition internal memory

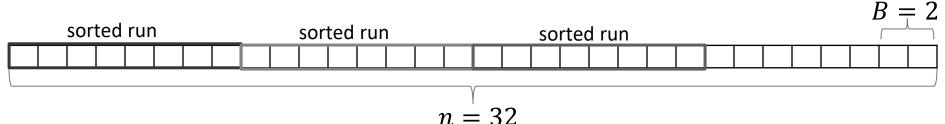


- In our example, looks like can perform 4-way merge (d = 4)
- But no, need to have some space for merged result
 - again, one block of memory is enough

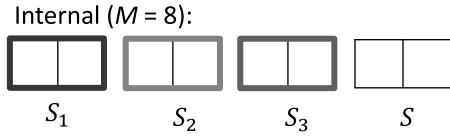
d-Way Merge in External Memory

External memory





- Partition internal memory

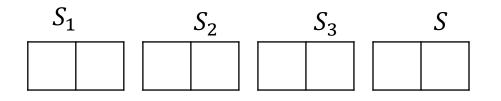


- In the example, can perform 3-way merge
- In general
 - partition in approximately $\frac{M}{B}$ sequences
 - perform $d \approx \frac{M}{B} 1$ way merge
 - first d sequences for storing active blocks of sorted runs
 - last sequence for storing results of the merged result

d-Way merge in External Memory

• External (B = 2)

4																											
5	10	22	28	29	33	37	39	8	21	30	31	40	45	52	54	11	12	13	35	36	42	49	53				

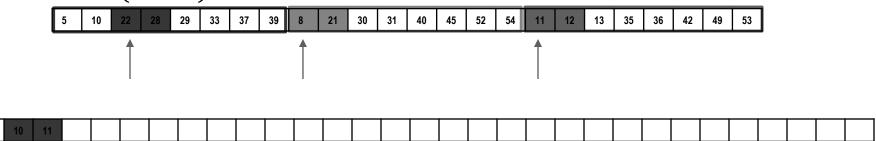


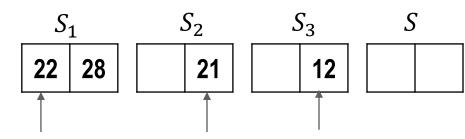
(d = 3, priority queue not shown)

- Example: 3-way merge
 - always bring elements from/to external memory in full blocks

d-Way merge in External Memory

• External (B = 2)





(d = 3, priority queue not shown)

Example: 3-way merge

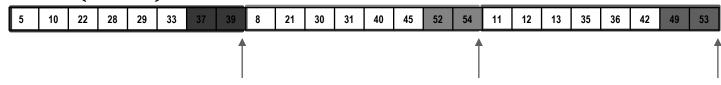
8

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- always bring elements from/to external memory in full blocks
- merge in internal memory until any sequence becomes full/empty

d-Way merge in External Memory

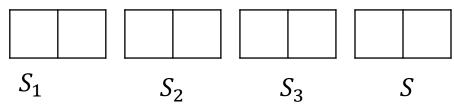
• External (B = 2)





sorted

Internal (M = 8):



(d = 3, priority queue not shown)

- Example: 3-way merge
 - always bring elements from/to external memory in full blocks
 - merge in internal memory until any sequence becomes full/empty
- Done with the first 3 sorted runs, continue with all other sorted runs in sets of 3
 - until all sorted runs are processed
- Total number of block transfers for one round is $\Theta(n/B)$
 - external array has size n, brought into internal memory in full blocks of size B
 - copied back to external memory in full blocks of size B

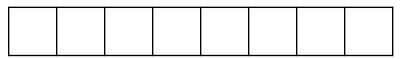
d-way Mergesort In External Memory

- $\log_d n = \frac{\log_2 n}{\log_2 d}$ rounds
- Each round makes $\Theta(n/B)$ external memory block accesses
 - with *d*-way merge sort, $\Theta\left(\frac{n}{B} \cdot \log_d n\right) = \Theta\left(\frac{n}{B} \cdot \frac{\log_2 n}{\log_2 d}\right)$ block accesses
 - 2-way (standard) mergesort, $\Theta\left(\frac{n}{B} \cdot \log_2 n\right)$ block accesses
 - *d*-way mergesort has savings factor $\log_2 d$ over 2-way mergesort
 - we made d as large as possible so that one round makes Θ(n/B) block accesses
 - n/B is the smallest number of block accesses needed to do one round of mergesort
 - if we made d any larger would need more than n/B block accesses for each round

• External (B = 2)

_																															
39	5	28	22	10	33	29	37	8	30	54	40	31	52	21	45	35	11	42	53	13	12	49	36	4	14	27	9	44	3	32	15

Internal (M = 8):



- Smart initialization can further reduce block transfers
- Mergesort starts with initial runs of size 1 and creates sorted runs of size d after one round

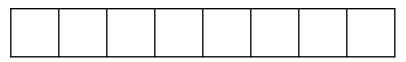


- cost of one round is $\Theta(n/B)$ block transfers
- The larger the initial sorted runs are, the less rounds mergesort takes
- Can we create sorted runs of size larger than d using only Θ(n/B) of block transfers?
 - i.e. the same computational cost as the first round of mergesort

• External (B = 2)

39	5	28	22	10	33	29	37	8	30	54	40	31	52	21	45	35	11	42	53	13	12	49	36	4	14	27	9	44	3	32	15
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Internal (M = 8):



• Can created sorted runs of size M using only $\Theta(n/B)$ of block transfers

•
$$M > d \approx \frac{M}{B} - 1$$

• Sort external memory chunks that fit into internal memory (size *M* chunks)

• External (B = 2)

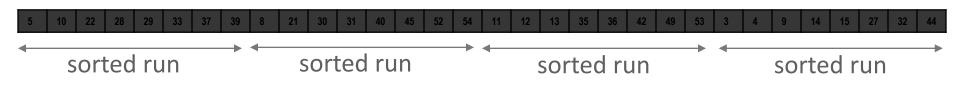
5 10 22 28 29 33 37 39	8 21 30 31 40 45 52 54	35 11 42 53 13 12 49 36 4 14 27 9 44 3 32 15
sorted run	sorted run	

Internal (M = 8):

8	21	30	31	40	45	52	54	
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- Smart initialization can further reduce block transfers
- Sort external memory chunks that fit into internal memory (size *M* chunks)
 - copy the next chunk
 - sort in internal memory
 - copy back to external memory
- Copy, sort, copy back the rest of them

• External (B = 2)



Internal (M = 8):

- Smart initialization creates sorted runs of length M
 - $\Theta(n/B)$ block transfers
 - each chunk of size M is copied in full blocks of size B

Mergesort in External Memory: Total Cost in Block Transfers

- Initialization creates n/M sorted runs of length M
 - $\Theta(n/B)$ block transfers
- Each round increases size of a sorted run by a factor of *d*

$$M \cdot \underbrace{d \cdot d \cdot \dots \cdot d}_{d^{t}} = n \quad \Rightarrow \quad d^{t} = \frac{n}{M} \quad \Rightarrow \quad t = \log_{d} \frac{n}{M}$$

- At most $\log_d n/M$ rounds of merging create sorted array
 - each round $\Theta(n/B)$ block transfers
- Total number of block transfers: $O\left(\frac{n}{B}\log_d n/M\right)$
 - better than $\Theta\left(\frac{n}{B} \cdot \log_d n\right)$ without smart initialization
- Can show that *d*-way Mergesort with $d \approx M/B$ is optimal to minimize block transfers for sorting in external memory
 - up to constant factors

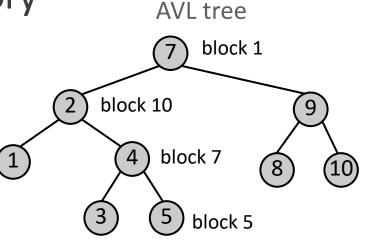
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External Memory

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 - 2-4 Trees
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Dictionaries in External Memory

- Tree-based dictionary implementations have poor *memory locality*
 - if an operation accesses *m* nodes, it must access *m* spaced-out memory locations



- In an AVL tree, $\Theta(\log n)$ blocks are loaded in the worst case
- Better solution
 - trees that store more keys inside a node, smaller height
 - B-trees is one example
 - first consider special case of B-trees: 2-4 trees
 - 2-4 trees also used for dictionaries in internal memory
 - may be even faster than AVL-trees
 - first analyze their performance in internal memory, and then (for B-trees) in external memory

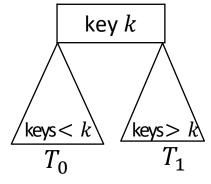
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External Memory

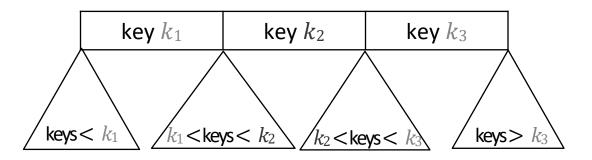
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2-4 Trees Motivation

Binary Search tree supports efficient search with special key ordering

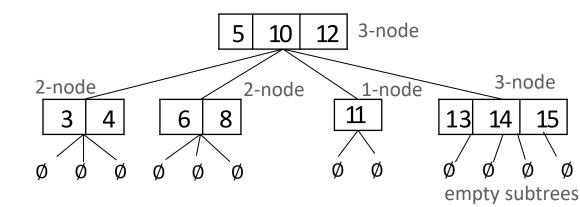


- Need nodes that store more than one key
 - how to support efficient search?

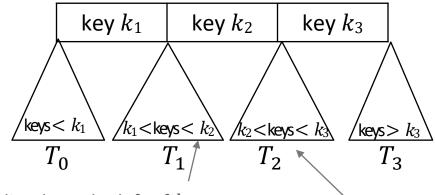


Need more properties to ensure tree is balanced and *insert, delete* are efficient

2-4 Trees



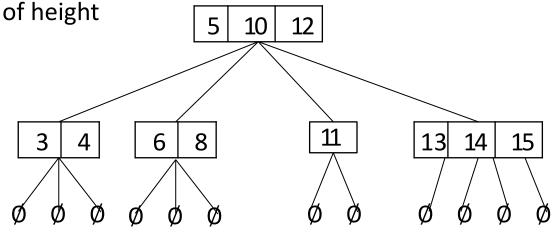
- Structural properties
 - Every node is either
 - 1-node: one KVP and two subtrees (possibly empty), or
 - 2-node: *two KVPs* and *three subtrees* (possibly empty), or
 - 3-node: three KVPs and four subtrees (possibly empty)
 - allowing 3 types of nodes simplifies insertion/deletion
 - All empty subtrees are at the same level
 - necessary for ensuring height is logarithmic in the number of KVP stored
- Order property: keys at any node are between the keys in the subtrees



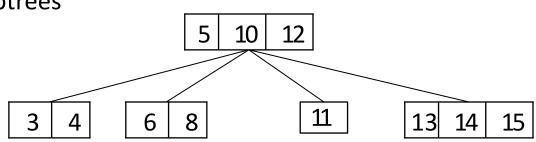
subtree immediately to the left of k_2 subtree immediately to the right of k_2

2-4 Tree Example

- Empty subtrees are not part of height computation
 - height = 1



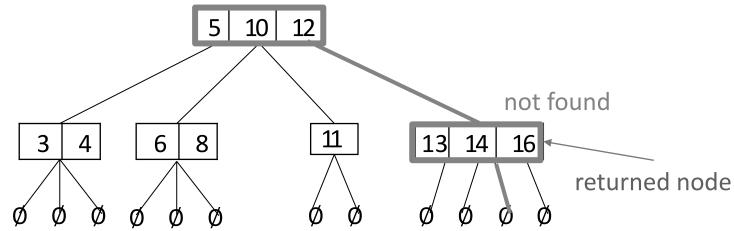
Often do not show empty subtrees



2-4 Tree: Search Example

Search

- Similar to search in BST
- Search(k) compares key k to k₁, k₂, k₃, and either finds k among k₁, k₂, k₃ or figures out which subtree to recurse into
- if key is not in tree, search returns parent of empty tree where search stops
 - key can be inserted at that node
- Search(15)

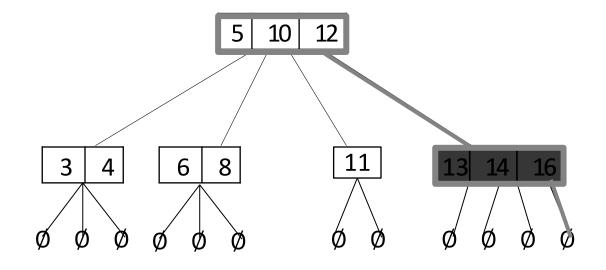


2-4 Tree operations

24TreeSearch $(k, v \leftarrow root, p \leftarrow empty subtree)$ if v represents empty subtree return "not found, would be in p" let $T_0, k_1, \dots, k_d, T_d$ be keys and subtrees at v, in order if $k \ge k_1$ $i \leftarrow maximal index such that <math>k_i \le k$ if $k_i = k$ return "at *i*th key in v" else 24TreeSearch (k, T_i, v) else 24TreeSearch (k, T_0, v)

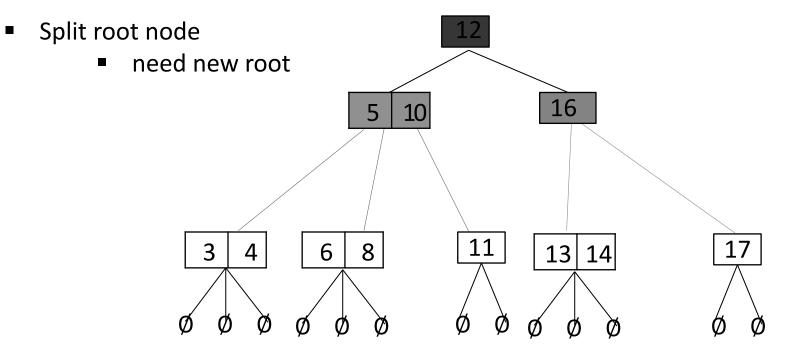
Example: 2-4 tree Insert

- Example: 24TreeInsert(17)
 - first step is 24TreeSearch(17)

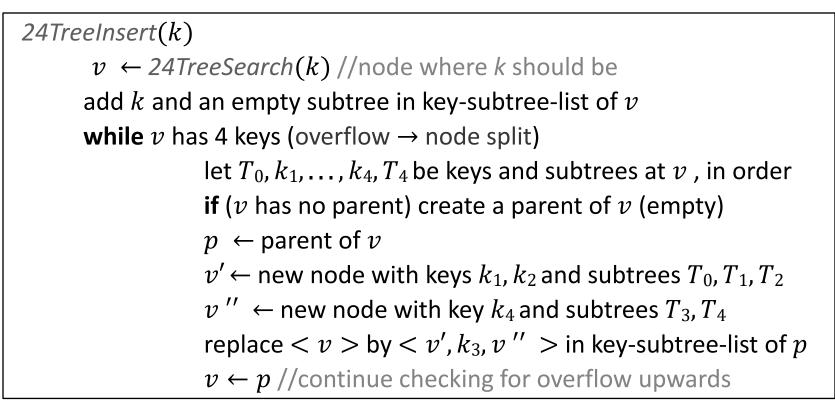


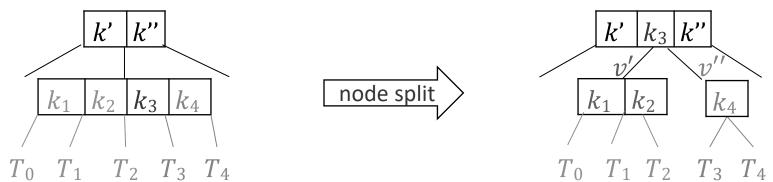
Example: 2-4 tree Insert

Example: 24TreeInsert(17)



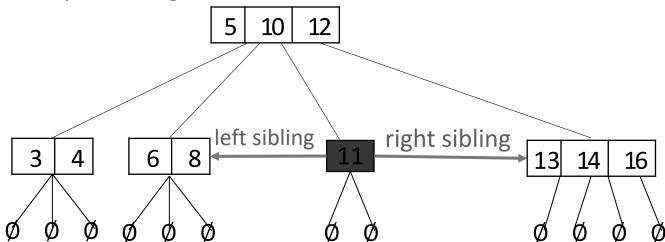
2-4 Tree Insert Pseudocode



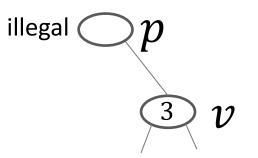


2-4 Tree: Left and Right Sibling

- Left sibling of a node is a subtree tree of the parent node which is immediately to the left
- Right sibling of a node is a subtree tree of the parent node which is immediately to the right

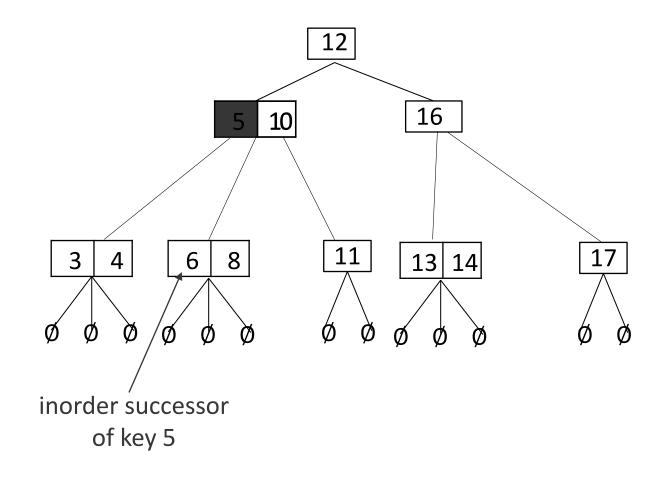


 Any node (except the root) must have a left or a right sibling (or both)



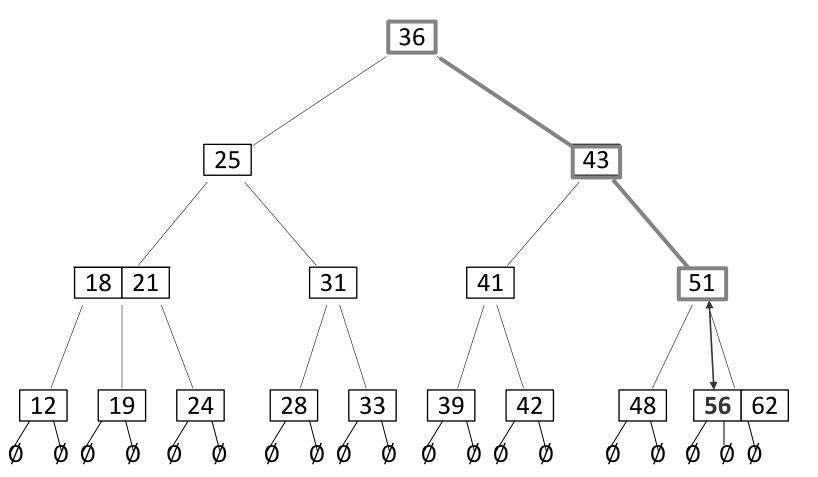
2-4 Tree: Inorder Successor

 Inorder successor of key k stored in node v is the smallest key in the subtree of v "immediately to the right" of k



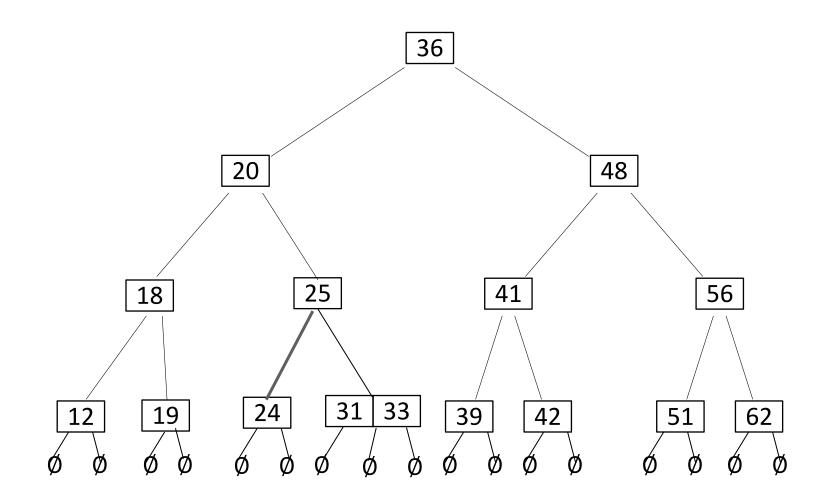
2-4 Tree Delete

- Example: *delete*(51)
- Search for key to delete
 - can delete keys only from a node with empty subtrees
 - replace key with in-order successor



2-4 Tree Delete

- Example: delete(28)
 - transfer from a rich sibling
 - together with a subtree



2-4 Tree Delete Summary

- If key not at a node with empty subtrees, swap with inorder successor
- Delete key and one empty subtree from node
- If underflow
 - If there is a sibling with more than one key, transfer
 - no further underflows caused
 - do not forget to transfer a subtree as well
 - convention: if two siblings have more than one key, transfer with the right sibling
 - If all siblings have only one key, merge
 - there must be at least one sibling, unless root
 - if root, delete
 - convention: if both siblings have only one key, merge with the right sibling
 - merge may cause underflow at the parent node, continue to the parent and fix it, if necessary

Deletion from a 2-4 Tree

24TreeDelete(k) $w \leftarrow 24 TreeSearch(k) //node containing k$ if w is not a node with only leaf children $v \leftarrow$ leaf containing predecessor or successor k' of k replace k by k' in w delete k' and an empty subtree in key-subtree-list of vwhile v has 0 keys // underflow if v is the root, delete it and break $p \leftarrow \text{parent of } v$ if v has sibling u with 2 or more keys // transfer/rotate let *u* be that sibling if u is a right sibling // say p contains $\langle v, k, u \rangle$ replace key k in p by $u.k_1$ remove $\langle u, T_0, u, k_1 \rangle$ from u and append $\langle k, u, T_0 \rangle$ to v else // symmetrical procedure if u is a left sibling else // merge/repeat if v has a right sibling $v' \leftarrow$ new node with list $(v, T_0, k, u, T_0, u, k_1, u, T_1)$ replace $\langle v, k, u \rangle$ by $\langle v \rangle$ in p $v \leftarrow p$ else ... // symmetrically with left sibling

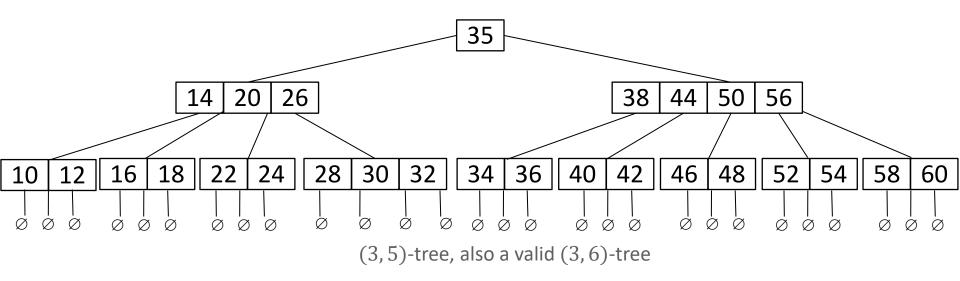
Outline

External Memory

- Motivation
- External sorting
- External Dictionaries
 - 2-4 Trees
 - (*a*, *b*)-Trees
 - B-Trees

(*a*, *b*)-Trees

- 2-4 Tree is a specific type of (a, b)-tree
- (a, b)-tree satisfies
 - each node has at least a subtrees, unless it is the root
 - root must have at least 2 subtrees
 - each node has at most b subtrees
 - if node has k subtrees, then it stores k 1 key-value pairs (KVPs)
 - all empty subtrees are at the same level
 - keys in the node are between keys in the corresponding subtrees



(*a*, *b*)-Trees: Root

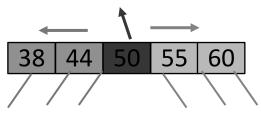
- Why special condition for the root?
- Needed for (a,b)-trees storing very few KVP
- (3,5) tree storing only 1 KVP



- Could not build it if forced the root to have at least 3 children
 - remember # keys at any node is one less than number of subtrees

(*a*, *b*)-Trees

- If $a \leq \lfloor b/2 \rfloor$, then *search*, *insert*, *delete* work just like for 2-4 trees
 - straightforward redefinition of underflow and overflow
- For example, for (3,5)-tree
 - at least 3 children, at most 5
 - each node is at least a 2-node, at most a 4-node
 - during insert, overflow if get a 5-node



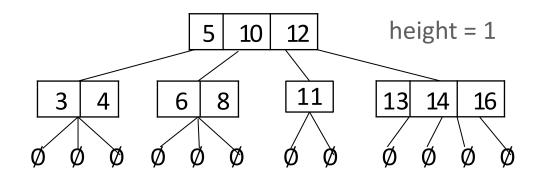
split results in 2-nodes, and 2-nodes are smallest allowed nodes



- If $a > \lfloor b/2 \rfloor$, for example (4,5)-tree, cannot split like before
 - equal (best possible) split results in two 2 nodes, which is not allowed

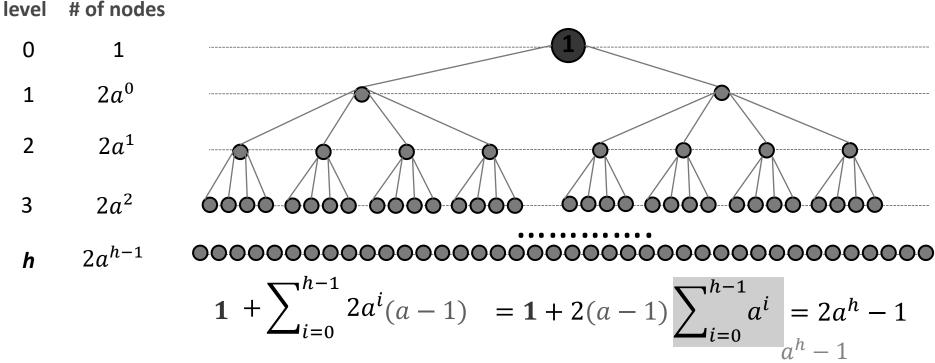
Height of (a, b)-tree

Height = number of levels **not** counting empty subtrees



Height of (a, b)-tree

- Consider (a,b)-tree with smallest number of KVP and of height h
 - red node (the root) has 1 KVP, blue nodes have (a 1) KVP



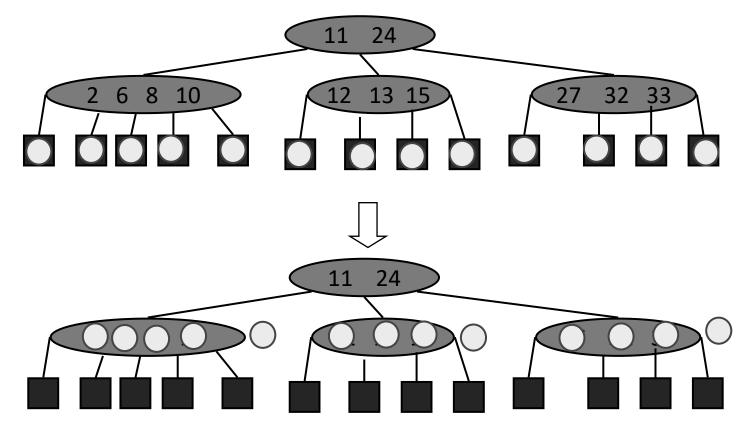
• Let n the number of KVP in any (a, b)-tree of height h

$$n \ge 2a^h - 1$$
 and, therefore, $\log_a \frac{n+1}{2} \ge h$

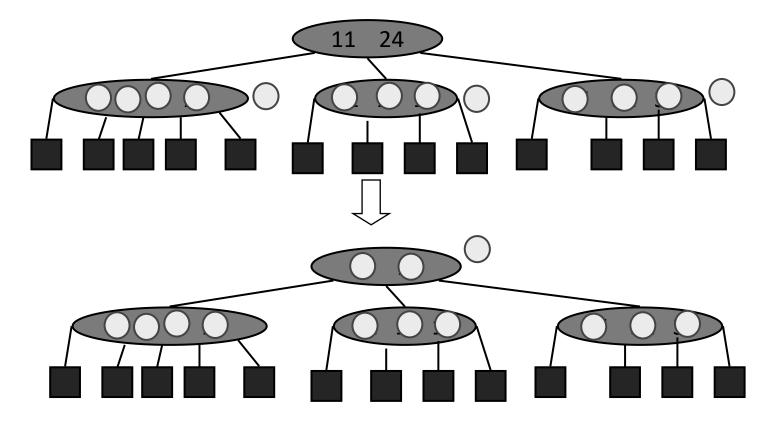
• Height of tree with n KVPs is $O(\log_a n)$

Useful Fact about (*a*, *b*)-trees

- number of of KVP = number of empty subtrees − 1 in any (*a*, *b*)-tree
 - **Proof:** Put one stone on each empty subtree and pass the stones up the tree. Each node keeps 1 stone per KVP, and passes the rest to its parent. Since for each node, #KVP = # children 1, each node will pass only 1 stone to its parent. This process stops at the root, and the root will pass 1 stone outside the tree. At the end, each KVP has 1 stone, and 1 stone is outside the tree.



Useful Fact about (*a*, *b*)-trees



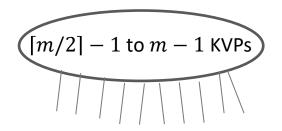
Outline

External Memory

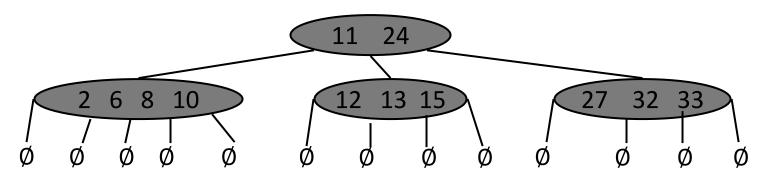
- Motivation
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B-trees

- A B-tree of order m is a $(\lceil m/2 \rceil, m)$ -tree
- 2-4 tree is a B-tree of order 4
 - at least 2, at most 4 subtrees
- Example: B-tree of order 6
 - at least 3, at most 6 subtrees

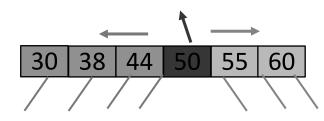


node must be at least 2-node, at most 5-node



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Overflow if get a 6-node



- Underflow if get a 1-node
 - transfer, if have a 3, 4 or 5-node sibling, merge if all siblings are 2-nodes

B-trees in Internal Memory

- A B-tree of order m is a $(\lceil m/2 \rceil, m)$ -tree
 - Sedgewick uses *M* rather than *m*
- Analysis if stored in internal memory
 - each node stores its KVPs in a dictionary that supports O(log m) search, insert, and delete

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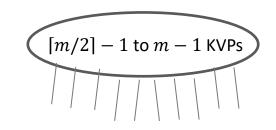
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• *search* require $\Theta(height)$ node operations

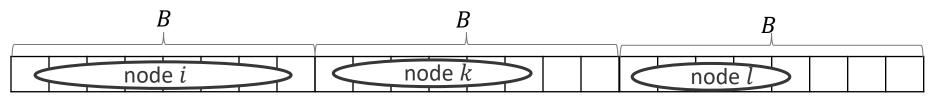
• height is
$$O(\log_a n) = O\left(\frac{\log n}{\log m/2}\right) = O\left(\frac{\log n}{\log m}\right)$$

- each node operation is O(log m) time
- total cost for each *search* $O\left(\frac{\log n}{\log m} \cdot \log m\right) = O(\log n)$
- analysis for *insert* and *delete* is the same
- No better than 2-4-trees or AVL-trees



Dictionaries in External Memory

- Main applications of B-trees is to store dictionaries in external memory
- AVL tree or 2-4 tree, need to load $\Theta(\log n)$ blocks in the worst case
- Instead, use a B-tree of order m
 - *m* is chosen so that an *m*-node fits into a single block
 - typically $m \in \Theta(B)$

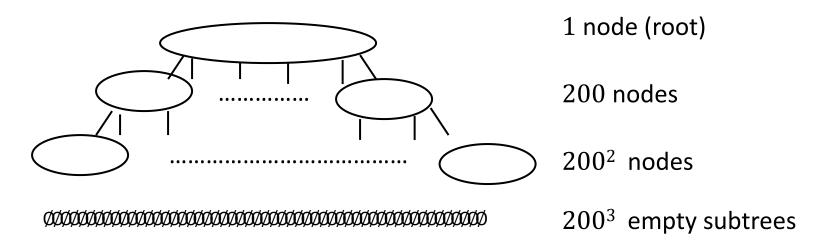


- Node that if *m*-node fills block *B* completely, then blocks are at least half-full
 - since each node is at least an [m/2]-node
 - not much storage wasted
- Each operation can be done with $\Theta(height)$ block transfers
- The height of a B-tree is $\Theta(\log_m n) = \Theta(\log_B n)$

•
$$\Theta(\log_B n) = \Theta\left(\frac{\log n}{\log B}\right)$$

• Large savings of block transfers, $\log B$ factor compared to AVL trees

Example of B-tree usage



- *B*-tree of order 200
 - node fits into one block of external memory
 - *B*-tree of order 200 and height 2 can store up to $200^3 1$ KVPs
 - from the 'useful fact' proven before
 - if store root in internal memory, then only 2 block reads are needed to retrieve any item

B-tree variations

- For practical purposes, some variations are better
 - B-trees with pre-emptive splitting/merging
 - during search for insert, split any node close to overflow
 - during search for delete, merge any node close to underflow
 - can insert/delete at leaf and stop, this halves block transfers
 - B⁺-trees: Only leaves have KVPs, link leaves sequentially
 - interior nodes store duplicates of keys to guide search-path
 - twice as many items
 - larger *m* since interior nodes do not hold values
 - **Cache-oblivious** trees: What if we do not know *B*?
 - build a hierarchy of binary trees
 - each node v in binary tree T "hides" a binary tree T' of size $\Theta(\sqrt{n})$
 - achieves $\Theta(\log_B n)$ block transfers *without* knowing *B*