CS 240 – Data Structures and Data Management

Module 11: External Memory

A. Hunt   O. Veksler

Based on lecture notes by many previous cs240 instructors

David R. Cheriton School of Computer Science, University of Waterloo

Winter 2023

version 2023–03–30 09:53

Outline

11. External Memory
    - Motivation
    - Stream-based algorithms
    - External sorting
    - External Dictionaries
    - 2-4 Trees
    - *a*-*b*-Trees
    - B-Trees

Outline

11 External Memory
- Motivation
- Stream-based algorithms
- External sorting
- External Dictionaries
- 2-4 Trees
- *a*-*b*-Trees
- B-Trees

Different levels of memory

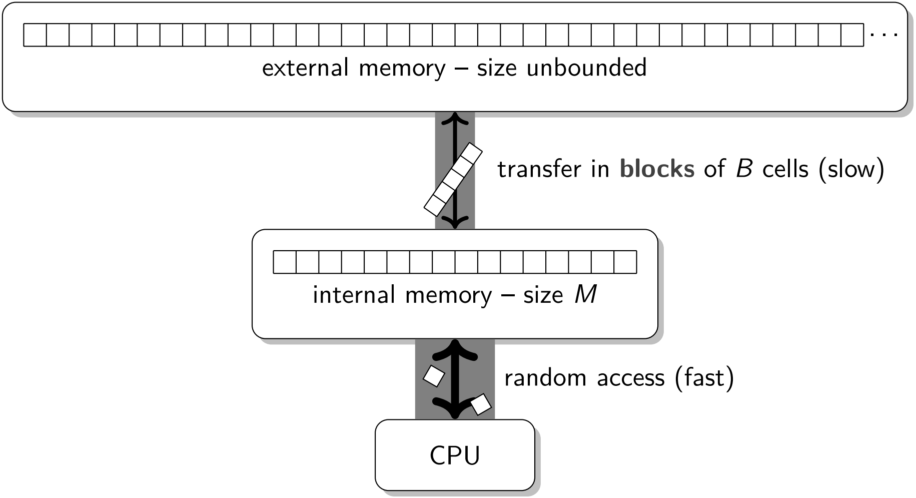
Current architectures:

- registers (very fast, very small)
- cache L1, L2 (still fast, less small)
- main memory
- disk or cloud (slow, very large)

General question: how to adapt our algorithms to take the memory hierarchy into account, avoiding transfers as much as possible?

Observation: Accessing a single location in *external memory* (e.g. hard disk) automatically loads a whole **block** (or "page").

The External-Memory Model (EMM)

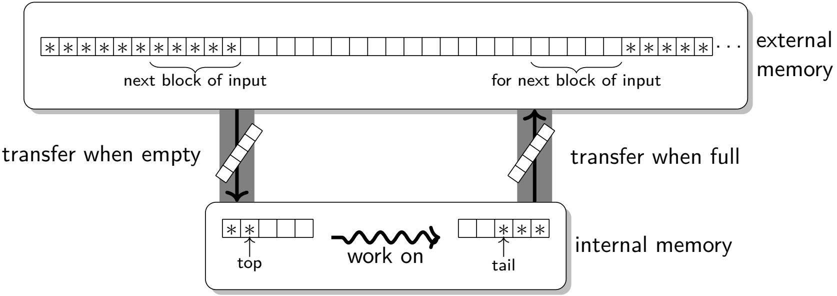


New objective: revisit all algorithms/data structures with the objective of minimizing **block transfers** ("probes", "disk transfers", "page loads")

Outline

Streams and external memory

If input and output are handled via streams, then we automatically use $\Theta(\frac{n}{B})$ block transfers.



So can do the following with $\Theta(\frac{n}{B})$ block transfers:

- Pattern matching: Karp-Rabin, Knuth-Morris-Pratt, Boyer-Moore (This assumes that pattern P fits into internal memory.)
- Text compression: Huffman, run-length encoding, Lempel-Ziv-Welch

Outline

Sorting in external memory

Recall: The sorting problem:
Given an array A of n numbers, put them into sorted order.

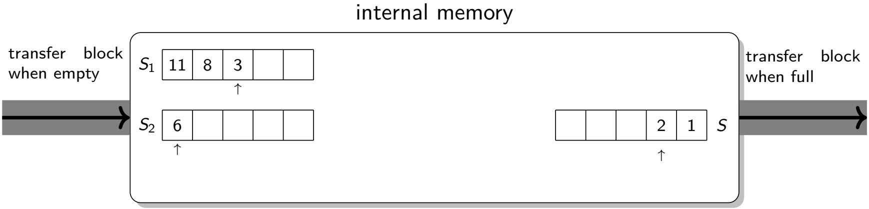
Now assume n is huge and A is stored in blocks in external memory.

- Heapsort was optimal in time and space in RAM model
- But: Heapsort accesses A at indices that are far apart
  $\rightsquigarrow$ typically one block transfer per array access
  $\rightsquigarrow$ typically $\Theta(n \log n)$ block transfers.
  Can we do better?
- Mergesort adapts well to external memory. Recall algorithm:
  - Split input in half
  - Sort each half recursively $\rightarrow$ two sorted parts
  - Merge sorted parts.

  Key idea: Merge can be done with streams.

Merge

Merge(S_1, S_2, S)
S_1, S_2: input streams have items in sorted order, S: output stream
while S_1 or S_2 is not empty **do**
  if (S_1 is empty) $S.append(S_2.pop())$
  else if (S_2 is empty) $S.append(S_1.pop())$
  else if ($S_1.top() < S_2.top()$) $S.append(S_1.pop())$
  else $S.append(S_2.pop())$



Here $B = 5$

Mergesort in external memory

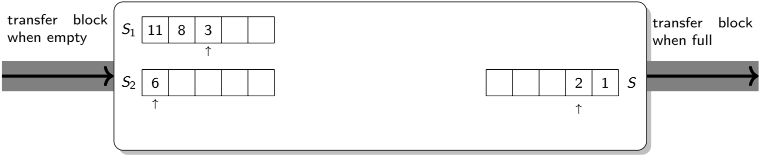
- *Merge* uses streams S_1, S_2, S.
  $\Rightarrow$ Each block in the stream only transferred once.
- So *Merge* takes $\Theta(\frac{n}{B})$ block-transfers.
- Recall: Mergesort uses $\lceil \log_2 n \rceil$ rounds of merging.

$\Rightarrow$ Mergesort uses $O(\frac{n}{B} \cdot \log_2 n)$ block-transfers.

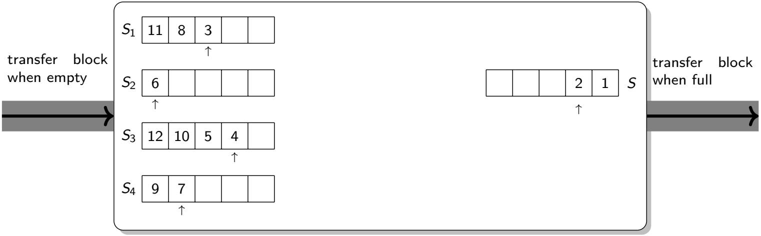
Not bad, but we can do better.

Towards d-way Mergesort

Observe: We had space left in internal memory during *merge*.



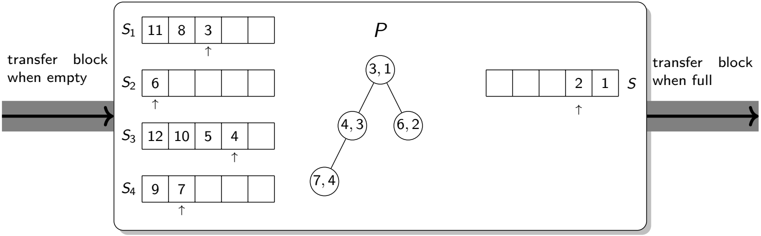
- We use only three blocks, but typically $M \gg 3B$.
- **Idea**: We could merge d parts at once.
- Here $d \approx \frac{M}{B} - 1$ so that $d+1$ blocks fit into internal memory.



d-way merge

d-way-merge$(S_1, \ldots, S_d, S)$
$S_1, \ldots, S_d$: input streams have items in sorted order, S: output stream

 $P \leftarrow$ empty *min-oriented* priority queue
 for $i \leftarrow 1$ to d **do** $P.$*insert*$(\,(S_i.$*top*$(), i)\,)$
   // each item in P keeps track of its input-steam
 while P is not empty **do**
  $(x, i) \leftarrow P.$*deleteMin*$()$
  $S.$*append*$(S_i.$*pop*$())$
  if S_i is not empty **do** $P.$*insert*$(\,(S_i.$*top*$(), i)\,)$



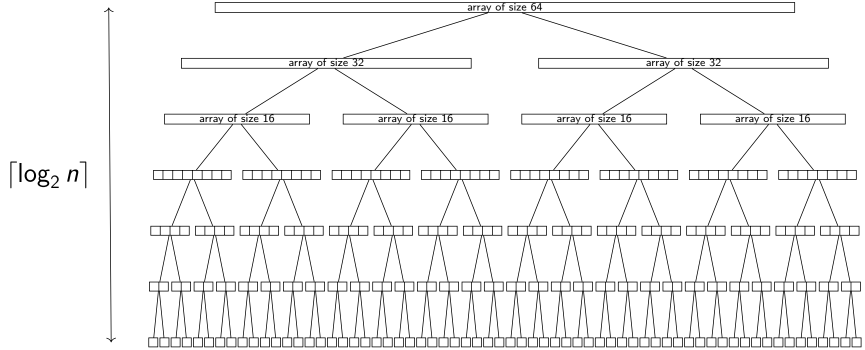
d-way merge

- We use a *min-oriented* priority queue P to find the next item to add to the output.
  - This is irrelevant for the number of block transfers.
  - But there is no space-overhead needed for a priority queue. (Recall: heaps are typically implemented as arrays.)
  - And with this the run-time (in RAM-model) is $O(n \log d)$.
- The items in P store not only the next key but also the index of the stream that contained the item.
  - With this, can efficiently find the stream to reload from.
- We assume d is such that $d + 1$ blocks and P fit into main memory.
- The number of *block transfers* then is again $O(\frac{n}{B})$.

How does *d-way merge* help to improve external sorting?

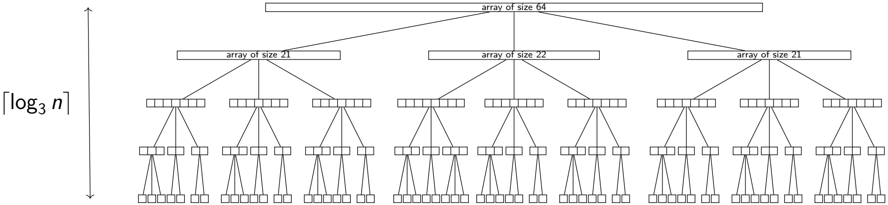
Towards d-way Mergesort

Recall: Mergesort uses $\lceil \log_2 n \rceil$ rounds of splitting-and-merging.



Towards d-way Mergesort

Observe: If we split and merge d-ways, there are fewer rounds.



- Number of rounds is now $\lceil \log_d n \rceil$
- We choose d such that each round uses $\Theta(\frac{n}{B})$ block transfers. (Then the number of block transfers is $\Theta(\log_d n \cdot \frac{n}{B})$.)
- Two further improvements:
  - Proceed bottom-up (while-loops) rather than top-down (recursions).
  - Save more rounds by starting immediately with runs of length M.

d-way 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	43	2	17	6	46	23	20	1	24	7	18	47	26	16	48	50

Internal ($M = 8$):

1. Create $\frac{n}{M}$ sorted runs of length M. $\Theta(\frac{n}{B})$ **block transfers**
2. Merge the first $d \approx \frac{M}{B} - 1$ sorted runs using *d-Way-Merge*
3. Keep merging the next runs to reduce # runs by factor of d $\rightsquigarrow$ one round of merging. $\Theta(\frac{n}{B})$ **block transfers**
4. Keep doing rounds until only one run is left

d-way mergesort

- We have $\log_d(\frac{n}{M})$ **rounds** of merging:
  - $\frac{n}{M}$ runs after initialization
  - $\frac{n}{M}/d$ runs after one round.
  - $\frac{n}{M}/d^k$ runs after k rounds $\Rightarrow k \leq \log_d(\frac{n}{M})$.
- We have $O(\frac{n}{B})$ block-transfers per round.
- $d \approx \frac{M}{B} - 1$.

$\Rightarrow$ Total # block transfers is proportional to

$$\log_d(\tfrac{n}{M}) \cdot \tfrac{n}{B} \in O\big(\log_{M/B}(\tfrac{n}{M}) \cdot \tfrac{n}{B}\big)$$

One can prove lower bounds in the external memory model:

We ***require*** $\Omega\big(\log_{M/B}(\frac{n}{M}) \cdot \frac{n}{B}\big)$ *block transfers in any comparison-based sorting algorithm.*

(The proof is beyond the scope of the course.)

- d-way mergesort is optimal (up to constant factors)!

Outline

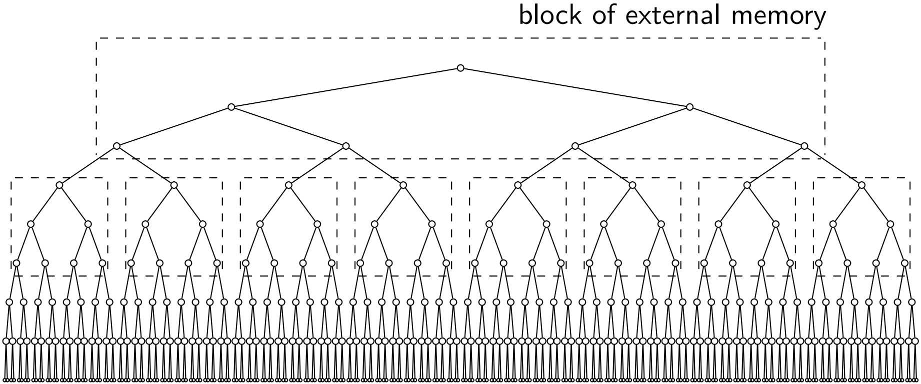
Dictionaries in external memory

Recall: Dictionaries store n KVPs and support *search*, *insert* and *delete*.

- **Recall:** AVL-trees were optimal in time and space in RAM model
- $\Theta(\log n)$ run-time $\Rightarrow$ $O(\log n)$ block transfers per operation
- But: Inserts happen at varying locations of the tree.
  $\rightsquigarrow$ nearby nodes are unlikely to be on the same block
  $\rightsquigarrow$ typically $\Theta(\log n)$ block transfers per operation
- We would like to have *fewer* block transfers.

Better solution: design a tree-structure that *guarantees* that many nodes on search-paths are within one block.

Idealized structure



Idea: Store subtrees in one block of memory.

- If block can hold subtree of size $b-1$, then block covers height $\log b$

$\Rightarrow$ Search-path hits $\frac{\Theta(\log n)}{\log b}$ blocks $\Rightarrow \Theta(\log_b n)$ block-transfers

- Block acts as one node of a *multiway-tree* ($b-1$ KVPs, b subtrees)

Towards B-trees

- **Idea:** Define *multiway-tree*
  - One node stores many KVPs
  - Always true: $b-1$ KVPs $\Leftrightarrow$ b subtrees
- To allow *insert*/*delete*, we permit varying numbers of KVPs in nodes
- This gives much smaller height than for AVL-trees
  $\Rightarrow$ fewer block transfers
- Study first one special case: *2-4-trees*
  - Also useful for dictionaries in internal memory
  - May be faster than AVL-trees even in internal memory

Outline

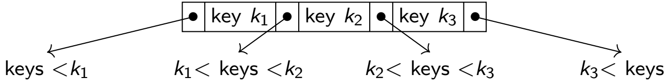
2-4 Trees

Structural property: 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).

Order property: The keys at a node are between the keys in the subtrees.

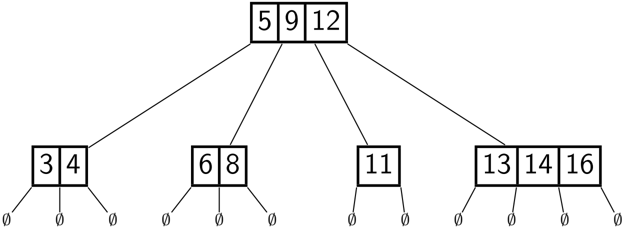
- With this, search is much like in binary search trees.



Another structural property: All empty subtrees are at the same level.

- This is important to ensure small height.

2-4 Tree example

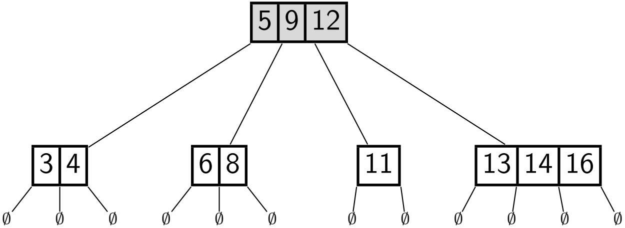


- Empty trees do not count towards height
  - This tree has height 1
- Easy to show: Height is in $O(\log n)$, where $n = \#$ KVPs.
  - Layer i has at least 2^i nodes for $i = 0, \dots, h$
  - Each node has at least one KVP.

2-4 Tree Operations

- Search is similar to BST:
  - Compare search-key to keys at node
  - If not found, recurse in appropriate subtree

Example: *search*(15) *not found*



2-4 Tree operations

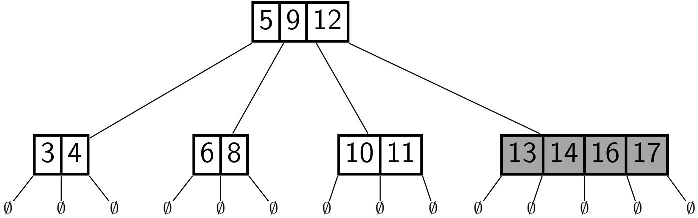
24Tree::search$(k, v \leftarrow \text{root}, p \leftarrow \texttt{NIL})$
k: key to search, v: node where we search, p: parent of v

if v represents empty subtree
    return "not found, would be in p"
Let $\langle T_0, k_1, \ldots, k_d, T_d \rangle$ be key-subtree list at v
if $k \geq k_1$
    $i \leftarrow$ maximal index such that $k_i \leq k$
    if $k_i = k$
        return KVP at k_i
    else *24Tree::search*(k, T_i, v)
else *24Tree::search*(k, T_0, v)

Insertion in a 2-4 tree

Example: *insert*(17)

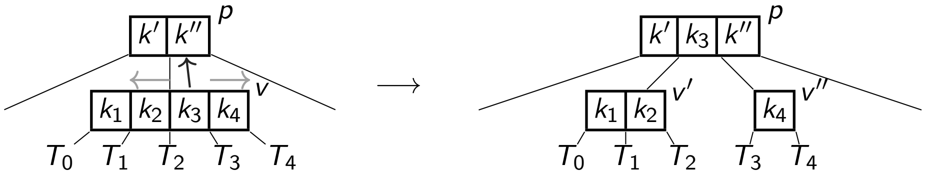
- Do *24Tree::search* and add key and empty subtree at leaf.
- If the leaf had room then we are done.
- Else **overflow**: More keys/subtrees than permitted.
- Resolve overflow by **node splitting**.



2-4 Tree operations

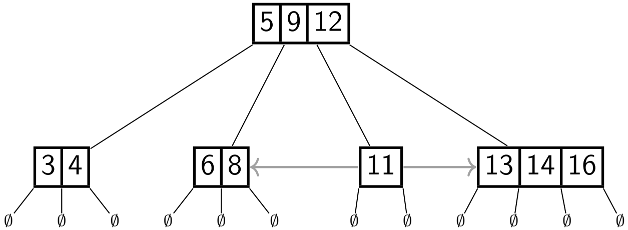
24Tree::insert(k)

$v \leftarrow$ *24Tree::search*(k) // leaf where k should be
Add k and an empty subtree in key-subtree-list of v
while v has 4 keys (**overflow** $\rightsquigarrow$ **node split**)
    Let $\langle T_0, k_1, \ldots, k_4, T_4 \rangle$ be key-subtree list at v
    if (v has no parent) create a parent of v without KVPs
    $p \leftarrow$ parent of v
    $v' \leftarrow$ new node with keys k_1, k_2 and subtrees T_0, T_1, T_2
    $v'' \leftarrow$ new node with key k_4 and subtrees T_3, T_4
    Replace $\langle v \rangle$ by $\langle v', k_3, v'' \rangle$ in key-subtree-list of p
    $v \leftarrow p$



Towards 2-4 Tree Deletion

- For deletion, we symmetrically will have to handle **underflow** (too few keys/subtrees)
- Crucial ingredient for this: **immediate sibling**

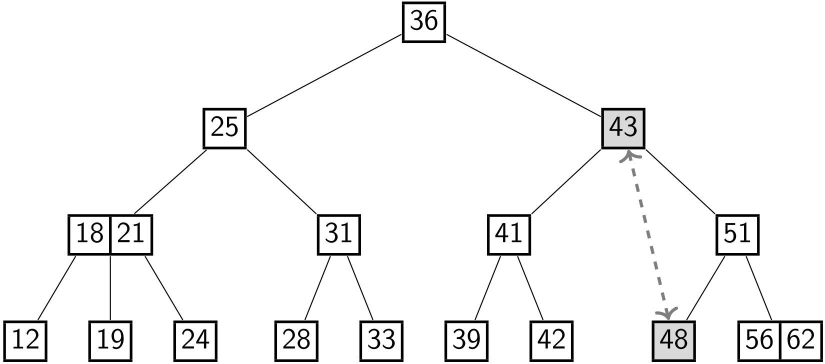


- **Observe:** Any node except the root has an immediate sibling.

2-4 Tree Deletion

Example:

- *24Tree::search*, then trade with successor if KVP is not at a leaf.
- If underflow:
  - If immediate sibling has extras, **rotate/transfer**
  - Else **node merge** (this affects the parent!)



Deletion from a 2-4 Tree

24Tree::delete(k)

$v \leftarrow$ *24Tree::search*(k) // node containing k
if v is not leaf
    swap k with its successor k' and v with leaf containing k'
delete k and one empty subtree in v
while v has 0 keys (**underflow**)
    if parent p of v is NIL, delete v and **break**
    if v has immediate sibling u with 2 or more keys (**transfer/rotate**)
        transfer the key of u that is nearest to v to p
        transfer the key of p between u and v to v
        transfer the subtree of u that is nearest to v to v
        break
    else (**merge & repeat**)
        $u \leftarrow$ immediate sibling of v
        transfer the key of p between u and v to u
        transfer the subtree of v to u
        delete node v and set $v \leftarrow p$

2-4 Tree summary

- A 2-4 tree has height $O(\log n)$
  - In internal memory, all operations have run-time $O(\log n)$.
  - This is no better than AVL-trees in theory.
    (Though 2-4-trees are faster than AVL-trees in practice, especially when converted to binary search trees called *red-black trees*. No details.)
- A 2-4 tree has height $\Omega(\log n)$
  - Level i contains at most 4^i nodes
  - Each node contains at most 3 KVPs
- So not significantly better than AVL-trees w.r.t. block transfers.
- But we can generalize the concept to decrease the height.

Outline

a-b-Trees

A 2-4 tree is an a-b-tree for $a = 2$ and $b = 4$.

An a-b-**tree** satisfies:

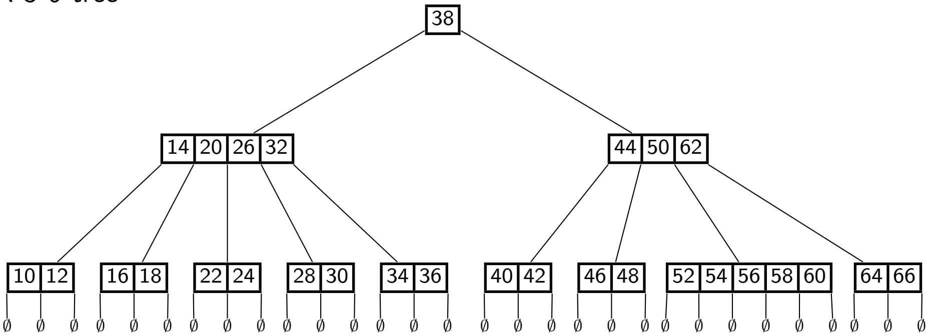
- Each node has at least a subtrees, unless it is the root.
  The root has at least 2 subtrees.
- Each node has at most b subtrees.
- A node has d subtrees $\Leftrightarrow$ it stores $d-1$ KVPs
- Empty subtrees are at the same level.
- The keys in the node are between the keys in the corresponding subtrees.

Requirement: $a \leq \lceil b/2 \rceil = \lfloor (b+1)/2 \rfloor$.

search, *insert*, *delete* then work just like for 2-4 trees, after re-defining underflow/overflow to consider the above constraints.

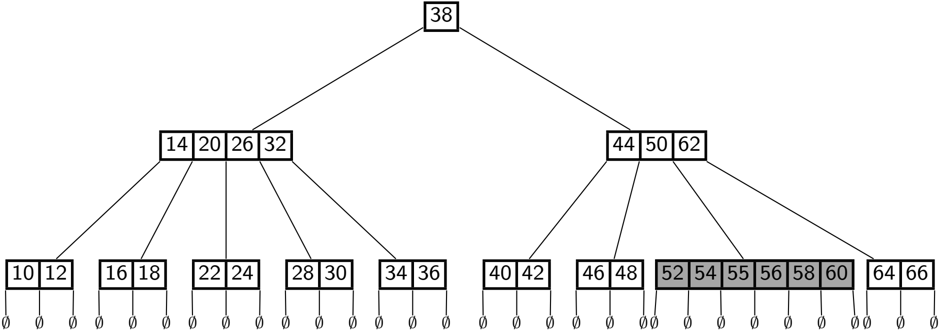
a-b-tree example

A 3-6-tree



a-b-tree insertion

insert(55):

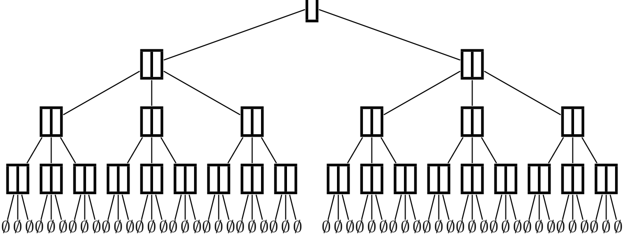


- Overflow now means b keys (and $b + 1$ subtrees)
- Node split $\Rightarrow$ new nodes have $\geq \lfloor (b-1)/2 \rfloor$ keys
- Since we required $a \leq \lfloor (b+1)/2 \rfloor$, this is $\geq a-1$ keys as required.

Height of an a-b-tree

Recall: $n =$ numbers of KVPs (*not* the number of nodes)
What is smallest possible number of KVPs in an a-b-tree of height-h?

Level	**Nodes**
0	≥ 1
1	≥ 2
2	$\geq 2a$
3	$\geq 2a^2$
$\cdots$	$\cdots$
h	$\geq 2a^{h-1}$



$$\#\text{ nodes} \;\geq\; \underbrace{1}_{\text{root: } \geq 1 \text{ KVP}} + \underbrace{\textstyle\sum_{i=0}^{h-1} 2a^i}_{\text{others: } \geq a-1 \text{ KVPs}}$$

$$n = \#\text{ KVPs} \;\geq\; 1 + (a-1)\sum_{i=0}^{h-1} 2a^i = 1 + 2(a-1)\frac{a^h}{a-1} = 1 + 2a^h$$

Therefore the height of an a-b-tree is $O(\log_a(n)) = O(\log n / \log a)$.

a-b-trees as implementations of dictionaries

Analysis (if entire *a*-*b*-tree is stored in internal memory):

- *search*, *insert*, and *delete* each requires visiting $\Theta(\textit{height})$ nodes
- Height is $O(\log n / \log a)$.
- Recall: $a \leq \lceil b/2 \rceil$ required for *insert* and *delete*

$\Rightarrow$ choose $a = \lceil b/2 \rceil$ to minimize the height.

- Work at node can be done in $O(\log b)$ time.

$$\text{Total cost: } O\left(\frac{\log n}{\log a} \cdot (\log b)\right) = O(\log n \cdot \frac{\log b}{\log b - 1}) = O(\log n)$$

This is still no better than AVL-trees.

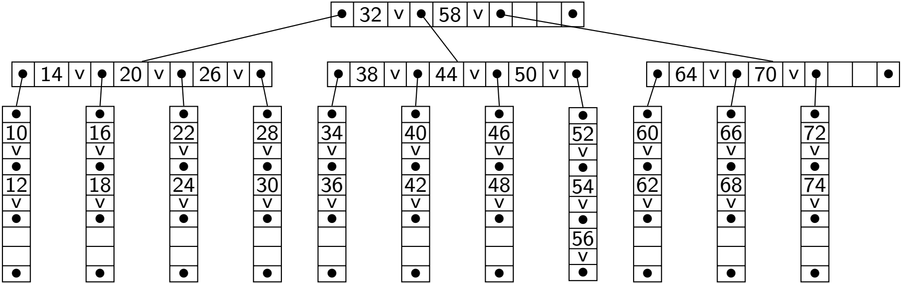
The main motivation for *a*-*b*-trees is *external memory*.

Outline

B-trees

A **B-tree** is an *a*-*b*-tree tailored to the external memory model.

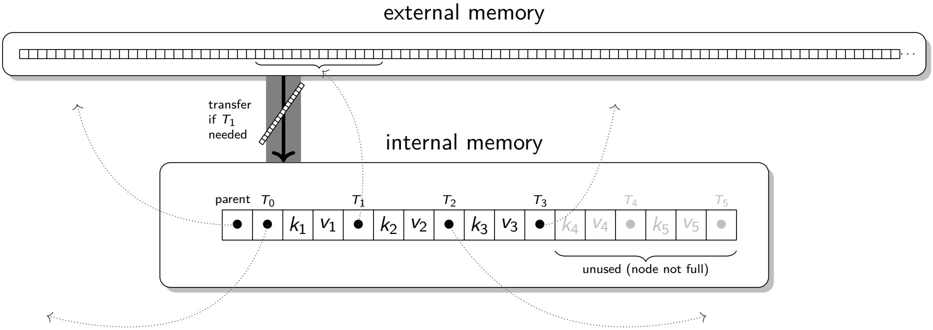
- Every node is one block of memory (of size B).
- b is chosen maximally such that a node with $b-1$ KVPs (hence $b-1$ value-references and b subtree-references) fits into a block.
  b is called the **order** of the B-tree. Typically $b \in \Theta(B)$.
- a is set to be $\lceil b/2 \rceil$ as before.



('v' indicates the value or value-reference associated with the key next to it)

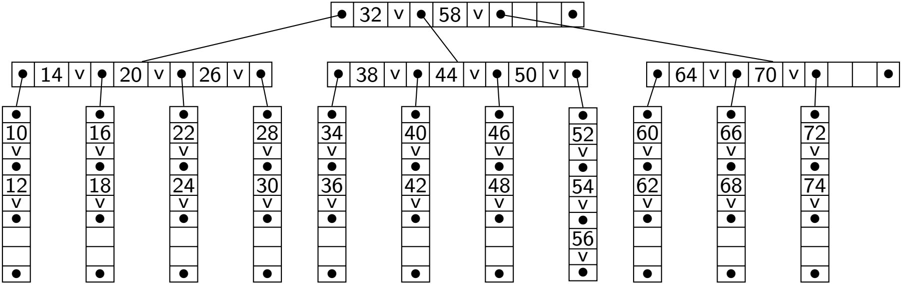
B-tree in external memory

Close-up on one node in one block:



In this example: 17 computer-words fit into one block, so (assuming keys and values fit into computer-words) the B-tree can have order 6.

B-tree analysis



- *search*, *insert*, and *delete* each requires visiting $\Theta(\textit{height})$ nodes
- Work within a node is done in internal memory $\Rightarrow$ no block-transfer.
- The height is $\Theta(\log_a n) = \Theta(\log_B n)$ (presuming $a = \lceil b/2 \rceil \in \Theta(B)$)

So all operations require $\Theta(\log_B n)$ **block transfers**.

B-tree summary

- All operations require $\Theta(\log_B n)$ **block transfers**.
  This is asymptotically optimal.
- In practice, height is a small constant.
  - Say $n = 2^{50}$, and $B = 2^{15}$. So roughly $b = 2^{14}$, $a = 2^{13}$.
  - B-tree of height 4 would have $\geq 1 + 2a^4 > 2^{50}$ KVPs.
  - So height is 3.
- There are some variations that are even better in practice (no details).
- B-trees are hugely important for storing data bases ($\rightsquigarrow$ cs448)