ABSTRACT: A B-tree is compact if it is minimal in number of nodes, hence has optimal space utilization, among equally capacious B-trees of the same order. The space utilization of compact B-trees is analyzed and is compared with that of noncompact B-trees and of (node)-visit-optimal B-trees, which minimize the expected number of nodes visited per key access. Compact B-trees can be as much as a factor of 2.5 more space-efficient than visit-optimal B-trees; and the node-visit cost of a compact tree is never more than 1 + the node-visit cost of an optimal tree. The utility of initializing a B-tree to be compact (which initialization can be done in time linear in the number of keys if the keys are pre-sorted) is demonstrated by comparing the space utilization of a compact tree that has been augmented by random insertions with that of a tree that has been grown entirely by random insertions. Even after increasing the number of keys by a modest amount, the effects of compact initialization are still felt. Once the tree has grown so large that these effects are no longer discernible, the tree can be expeditiously compacted in place using an algorithm presented here; and the benefits of compactness resume.

Time- and Space-Optimality in B-Trees*

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1. Introduction

The B-tree data structure of Bayer and McCreight [1; 36.2.4] is an effective method of organizing an external file when the operations of searching, insertion and deletion must be supported since these operations on B-trees require time at most logarithmic in the size of the file. This logarithmic performance is achievable [6] because the B-tree definition is underconstrained: one file has numerous legal B-tree representations. Specifically, a finite rooted tree must satisfy two conditions to be a B-tree of order $M$:

(1.1) each internal node must have at least $\lceil M/2 \rceil$ descendants (except the root which can have as few as two), and at most $M$ descendants,

(1.2) all root-to-leaf paths must be of equal length.

To illustrate that these conditions do not constrain B-trees to a unique structure, let $T^M_k$ denote the set of all order $M$ B-trees with a capacity of $k$ keys. Then $T^3_{15}$ contains ten (structurally) distinct B-trees of order 3 [also called 2,3-trees] each capable of containing fifteen keys. Figure 1 exhibits these ten trees.

The first purpose of this paper is to characterize the optimally space efficient trees in the forest $T^M_k$. Space will be measured by the total number of internal nodes. (The leaves may be ignored since all trees in $T^M_k$ have $k+1$ leaves.) Our use of the number of internal nodes as a cost measure for externally stored B-trees is motivated by the usual policy of allocating for each node a fixed-size block of storage (page, track, etc.) capable of holding the maximum of $M$ descendant pointers and $M-1$ keys. Should a node actually have fewer than the maximum
Figure 1: The ten structurally distinct B-trees of $T_{15}^3$. 
descendants and keys, then the remaining space is unused, and therefore, wasted. Thus, for a given number of keys, fewer internal nodes implies a greater average number of keys per node and hence less wasted space. Table 1 illustrates this point for the trees of $T^3_{15}$.

A second purpose of this paper is to measure the time performance of space-minimal trees and the space utilization of time-efficient trees in $T^M_k$. Time costs are measured by the expected root-to-key path length for equally likely keys. This measure was used in [4] where it was called "node-visit-cost." It is motivated by the fact that external reference to a node usually requires an expensive disk fetch. Thus, a smaller number of nodes visited to reference an arbitrarily selected key, implies a smaller expected searching time. See Table 1 for the node-visit-costs of elements $T^3_{15}$.

<table>
<thead>
<tr>
<th>Tree from Figure 1</th>
<th>Time Cost (node-visit)</th>
<th>Space Cost (internal nodes)</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>3.27</td>
<td>15</td>
</tr>
<tr>
<td>b</td>
<td>2.60</td>
<td>9</td>
</tr>
<tr>
<td>c</td>
<td>2.60</td>
<td>9</td>
</tr>
<tr>
<td>d</td>
<td>2.53</td>
<td>10</td>
</tr>
<tr>
<td>e</td>
<td>2.53</td>
<td>10</td>
</tr>
<tr>
<td>f</td>
<td>2.47</td>
<td>11</td>
</tr>
<tr>
<td>g</td>
<td>2.47</td>
<td>11</td>
</tr>
<tr>
<td>h</td>
<td>2.47</td>
<td>11</td>
</tr>
<tr>
<td>i</td>
<td>2.47</td>
<td>11</td>
</tr>
<tr>
<td>j</td>
<td>2.40</td>
<td>12</td>
</tr>
</tbody>
</table>

Table 1: Comparison of Time and Space costs for trees of Figure 1.
It is evident from Table 1 that in \( T^3_{15} \) no single 15 key tree minimizes both space and time costs, although for other numbers of keys it does occasionally happen. In general, as Table 1 suggests, there is a trade-off between time and space. Our study of this trade-off will indicate that

\[(1.3) \text{ space-optimal trees are nearly time-optimal, but time-optimal trees are nearly space-pessimal.} \]

Thus, the trade-off is strongly biased in favor of space-minimizing B-trees. This observation is important because a "heuristic" has, we are told, gained reasonably wide acceptance among B-tree users\(^\dagger\) as a means of constructing "better" B-trees: keep the nodes near the root filled, "... thereby increasing the branching degree of the nodes near the root, where a high branching degree is most beneficial" [2, p.13]. In light of (1.3) this "heuristic" is of dubious merit if not wrong, since keeping nodes near the root filled reduces space efficiency.

Although any element of \( T^M_k \) might be created during the dynamic operation of the B-tree algorithms, we can arrange matters so that the more efficient trees are more likely to be chosen. This is accomplished by acknowledging certain pragmatic considerations in the use of B-trees. For example, very large B-trees are often quite stable, tending to change only by a small percentage each day. Furthermore, B-tree files are periodically "backed-up" for error recovery or archival purposes. These two considerations suggest that if the tree were compactified, i.e. made space-minimal, during a daily "back-up" operation then the

\(^\dagger\) Private communication.
benefits indicated by (1.3) would be realized at the beginning of each
day. As the tree is modified the magnitude of the benefits would diminish
as the insertions and deletions cause it to depart further and further
from its compact profile. But by our assumption of only modest modifi-
cations in a given day, this decay would not be rapid.

To implement this approach we present a linear time (in the size
of the file) in-place compactification algorithm. Also, we give an
analysis of the expected departure from optimal performance of a compact
tree as a function of the number of random insertions into that compact
tree. From the analysis and a few statistics about the use of a
B-tree, one can easily compute the benefits of the "compactify during
back-up" approach.

We shall use the following agenda:

Section 2 - characterization of space- and time-minimal B-trees;
Section 3 - analysis of time/space trade-offs;
Section 4 - analysis of "rate of decay" of a compact tree under
random insertions;
Section 5 - in place-compactification algorithm;
Section 6 - summary and discussion.
2. Characterizations of Space- and Time-Minimal B-trees

Given the use of B-trees as search trees, one can identify at least three natural measures of the efficiency of a B-tree, namely, the expected number of nodes visited per access, the expected number of key-comparisons per access, and the space requirements of the tree. The node-visit cost of B-trees is studied at some length in [4], where the visit-optimal B-trees are characterized. The comparison cost of 2,3-trees is studied in [5], where the comparison-optimal trees are characterized and are compared with their visit-optimal forest mates. This section is devoted to studying the space cost of B-trees and to reviewing the results from [4] on the time cost of B-trees.

An order \( M \) B-tree (\( M \geq 3 \), an integer) is a finite, rooted tree satisfying (1.1) and 1.2). The maximum degree of a node is \( M \); we will denote the minimum degree by \( m = \lceil M \div 2 \rceil \). The root of a B-tree is said to be at level 0 of the tree, and, in general, the sons of a level \( l \) node are said to reside at level \( l+1 \). The (common) level of the tree's leaves is the depth of the tree. (Recall from the introduction that the number of leaves equals the key capacity plus one.)

An order \( M \) B-tree is used as a search tree by loading its nonleaf nodes with keys from a totally ordered set in such a way that (a) each \( s \)-son node contains \( s-1 \) keys; and (b) if the \( s \)-son node \( N \) contains keys

\[ k_1 < k_2 < \ldots < k_{s-1} \]

then

\[ (\text{all keys in subtree } l \text{ of } N) < k_1, \]
\[ k_{s-1} < (\text{all keys in subtree } s \text{ of } N), \]
\[ k_{i-1} < (\text{all keys in subtree } i \text{ of } N) < k_i \]
for $1 < i < s$. Knuth [3, §6.2.4] describes in some detail procedures for accessing, inserting, and deleting keys in an order $M$ B-tree in time bounded above by a small multiple of $\log_m$ (number of keys in $T$).

Two descriptors of B-trees will facilitate the following exposition. The profile of a depth $d$ B-tree $T \in T^M_k$ is a length $d+1$ integer sequence

$$\Pi(T) = v_0, v_1, \ldots, v_d$$

where each $v_l$ is the number of nodes at level $l$ of $T$. Thus, $v_0 = 1$ and $v_d = k+1$. The detailed profile of $T$ is the length $d$ sequence of integer $(M-1)$-tuples

$$\Delta(T) = \langle \sigma_0^2, 0, \ldots, 0, \sigma_0^M, \ldots, \langle \sigma_{d-1}^2, \sigma_{d-1}^3, \ldots, \sigma_{d-1}^M \rangle \rangle$$

where each $\sigma_l^s$ is the number of $s$-son nodes at level $l$ of $T$. Note that if $l > 1$, all $\sigma_l^s = 0$ for $s < m$. These notions and the notation for them originate in [4].

We now define precisely the costs to be studied. For an order $M$ B-tree $T$ with profile

$$\Pi(T) = v_0, \ldots, v_d$$

the node-number cost of $T$ is

$$\text{NNCOST}(T) = \sum_{i < d} v_i$$

(2.1)

This is clearly the "space" cost referred to informally. We measure space efficiency by the node-utilization

$$\text{NU}(T) = (v_d-1) / ((M-1) \text{NNCOST}(T))$$

(2.2)

The node-utilization, $NU$, which never exceeds 1, gives the expected proportion of a node that contains keys. From the definition it is clear that a space-minimal tree $T$ may not have $\text{NU}(T) = 1$ since some space may
be wasted simply to honor the "equal path length" condition (1.2) on B-trees.

Next we define the "time" cost measure to be used. The node-
visit cost of a B-tree $T$ in $T^M_k$ with detailed profile $\Delta(T) = \langle \sigma_0^2, \ldots, \sigma_0^M, \ldots, \sigma_{d-1}^2, \ldots, \sigma_{d-1}^M \rangle$ is

$$NVCOST(T) = \left( \sum_{0 \leq i < d} \sum_{2 \leq s \leq M} (i+1)(s-1)\sigma_i^s \right) \div k. \quad (2.3)$$

Clearly,

$$NVCOST(T) = \text{(expected number of nodes visited when accessing a key in } T).$$

Although the presented definition of node-visit cost is intuitively appealing, we prefer the following less perspicuous but more useful definition.

**Proposition 2.1 [4]:** The node-visit-cost of the B-tree $T$ with profile $\Pi(T) = \nu_0, \ldots, \nu_d$ is precisely

$$NVCOST(T) = (d\nu_d - \sum_{i < d} \nu_i) \div (\nu_d - 1).$$

Having completed the definitions, we are now ready to characterize the space- and time-minimal trees. It will be convenient for comparison purposes to characterize the space- and time-maximal trees as well. These trees will be referred to by the names:

- compact - node-number cost minimal,
- sparse - node-number cost maximal,
- bushy - node-visit cost minimal [4],
- scrawny - node-visit cost maximal [4].
Theorem 2.2: An order $M$ B-tree $T$ with profile $\Pi(T) = v_0', \ldots, v_d'$ minimizes NNCOST over all elements of $T_k^M$ if and only if
for $0 \leq \ell < d$, $v_{\ell} = \lceil \frac{v_{\ell+1}}{M} \rceil$; $T$ maximizes NNCOST over all elements of $T_k^M$ if and only if for $0 \leq \ell < d$, $v_{\ell} = \max(1, \lceil \frac{v_{\ell+1}}{m} \rceil)$.

Proof: To minimize (resp. maximize) NNCOST($T$) it is necessary to minimize (resp. maximize) $\sum_{\ell < d} v_{\ell}$ of $T$, which is equivalent, in turn, to maximizing (resp. minimizing) the branching ratios of $T$'s nodes. The indicated profiles accomplish the desired shaping. $\square$

Corollary 2.3: If $\Pi(T) = v_0', \ldots, v_d'$ is the profile of a compact B-tree then $d = \lceil \log_M v_d \rceil$; if it is the profile of a sparse B-tree then $d = \lceil \log_m (v_d' \div 2) \rceil + 1$.

Thus, compact B-trees are as "shallow" as possible for their size while the sparse B-trees are as "deep" as possible for their size. (For sparse B-trees, the maximum depth is not $\lceil \log_m v_d \rceil$ as might be expected, because the root is allowed to be binary.)

Using Proposition 2.1, among other facts about node-visit costs, the following computationally attractive characterization of visit-optimal and pessimal B-trees was established.

Theorem 2.4 [4]: The order $M$ B-tree $T$ with profile $\Pi(T) = v_0', \ldots, v_d'$ has minimal NVCOST over all trees in $T_k^M$ if and only if $d = \lceil \log_M v_d \rceil$ and
$v_{\ell} = \min(M, \lceil \frac{v_{\ell+1}}{m} \rceil)$ for $0 \leq \ell < d$; $T$ has maximal NVCOST over all trees in $T_k^M$ if and only if
$d = \lceil \log_m (v_d' \div 2) \rceil + 1$, $v_0 = 1$, $v_1 = 2$ and $v_{\ell} = \max(m, \lceil \frac{v_{\ell+1}}{M} \rceil)$.

Notice that both bushy and compact B-trees have a lot of $M$-ary nodes; but bushy trees have these nodes concentrated as close to the root as
possible while compact trees have them concentrated as close to the leaves as possible. This difference is restated in the following less constructive but no less illuminating characterization of bushy B-trees, whose proof is direct from Proposition 2.1 and Theorem 2.4.

Proposition 2.5: The B-tree $T$ in $T^M_k$ has minimal NVCOST over the class if and only if $T$ is minimal in depth and, for that depth, maximal in number of nonleaf nodes.

Scrawny trees also have their M-ary nodes concentrated near the leaves, but unlike compact trees, they must have maximal depth. Sparse trees have their "fullest" nodes as near the root as possible, but as the following easily proved proposition indicates, they are so rare that it is difficult to say where they are concentrated.

Proposition 2.6: Let $T$ be a maximal NNCOST B-tree in $T^M_k$.
If $M$ is even, then $T$ has no M-ary nodes. If $M$ is odd, then $T$ has at most one M-ary node per level.

This classification is summarized in Table 2.

<table>
<thead>
<tr>
<th></th>
<th>minimum depth</th>
<th>maximum depth</th>
</tr>
</thead>
<tbody>
<tr>
<td>root</td>
<td>bushy</td>
<td>sparse</td>
</tr>
<tr>
<td>fullest nodes near to leaves</td>
<td>compact</td>
<td>scrawny</td>
</tr>
</tbody>
</table>

Table 2: Characteristics of the optimal and pessimal B-trees.

Our main interest, of course, is in the space- and time-minimal trees. Occasionally, the depth requirement is so restrictive that the two notions actually coincide.
Fact 2.7: For all sufficiently large k, there is a B-tree in \( T^M_k \) that is both visit-optimal and space-optimal precisely when 
\[ M^d - M < k+1 \leq M^d. \] "Sufficiently large" here means \( k+1 \geq 4M \) when

\( M \) is even, and \( k+1 \geq 4M\left(1+\frac{2}{M-2}\right) \) when \( M \) is odd.

Proof: By direct calculation using the profile-oriented characterization of the two notions of optimality. \( \Box \)

Thus, the two notions of optimality coincide very infrequently.

The major thrust of the next section is to determine how much they differ the rest of the time.
3. Space and Time Comparisons

In this section we establish time and space bounds on the advantage derivative from the use of optimal B-trees -- both bushy and compact. First we set forth the obvious limits within which the space utilization of B-trees can vary.

Proposition 3.1: As \( k \to \infty \),

(a) for space-optimal order \( M \) B-trees,
\[
\text{NU}(T) \sim 1;
\]

(b) for space-pessimal \( k \)-key order \( M \) B-trees,
\[
\text{NU}(T) \sim \frac{m-1}{M-1};
\]

(c) for "random*" \( k \)-key order \( M \) B-trees, and fixed, large \( M \),
\[
\text{NU}(T) \sim \log_2 e 2 \approx .69.
\]

Proof: (a,b) by direct calculation from (2.2), (c) see [7]. \( \square \)

Proposition 3.2: Let \( T_o \), \( T_p \) and \( T_r \) be respectively, space-optimal, space-pessimal and "random" (in Yao's sense) trees from \( T_k^M \). Then asymptotically (as \( k \to \infty \)),

(a) for \( M \) even,
\[
\text{NU}(T_o) \sim (2 + \frac{2}{M-2}) \cdot \text{NU}(T_p);
\]

(b) for \( M \) odd,
\[
\text{NU}(T_o) \sim 2 \cdot \text{NU}(T_p);
\]

(c) for large fixed \( M \),
\[
\text{NU}(T_o) \sim 1.45 \cdot \text{NU}(T_r).
\]

Hence the space-optimal trees use their nodes between 2 (at odd \( M \)) and 3 (at \( M = 4 \)) times more efficiently as do their space-pessimal forest-mates.

For the sake of completeness it should be noted that these asymptotics take

*We use the word "random" here in the same sense as Yao [7]: the tree is grown from the empty tree by a sequence of \( k \) insertions, with each insertion equally likely to fall between any pair of the already-inserted keys or to either side of these keys.
hold at rather modest values of $k$, as Table 3 indicates.

<table>
<thead>
<tr>
<th>$B$-tree</th>
<th>Optimal profile $\Pi(T)$</th>
<th>Pessimal profile $\Pi(T)$</th>
<th>Pessimal $\text{NNCOST}$</th>
<th>Optimal $\text{NNCOST}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M=3$, $k=127$</td>
<td>1, 2, 5, 15, 43, 128</td>
<td>1, 2, 4, 8, 16, 32, 64, 128</td>
<td>127466 &gt; 1.9</td>
<td></td>
</tr>
<tr>
<td>$M=4$, $k=15$</td>
<td>1, 4, 16</td>
<td>1, 2, 4, 8, 16</td>
<td>3</td>
<td></td>
</tr>
</tbody>
</table>

Table 3

One might argue, with some justification, that the bounds of Proposition 3.2 are only of academic value in that the pessimal trees are arbores non gratae in the context of large trees and, hopefully, will never occur. (One should note, however, that these trees are very often minimal in number of comparisons per expected access [5].) In light of this criticism, we investigate also the disparities in space utilization between compact and bushy trees. We find these disparities to be only marginally less than the ones just exhibited.

**Theorem 3.3:** Let $T^b$ be a space-pessimal element of all visit-optimal (i.e. bushy) trees in $T^M_k$ and $T^c$ a compact tree in $T^M_k$. Then asymptotically (as $k \to \infty$),

(a) for $M$ even,

$$
\text{NU}(T^c) \sim (2 + \frac{2}{M-2} - \frac{M^2}{(M-2)\log M}) \cdot \text{NU}(T^b);
$$

(b) for $M$ odd,

$$
\text{NU}(T^c) \sim (2 + M^{1-\mu} - 2^{1+\mu} (M+1)^{-\mu}) \cdot \text{NU}(T^b);
$$

where

$$
\mu = \frac{\log M}{\log(\frac{2M}{M+1})}.
$$

Hence, the space optimal trees use their nodes between $\frac{5}{6}$ (at $M = 3$) and $2\frac{1}{2}$ (at $M = 4$) times as efficiently as do their visit-optimal forestmates.

**Proof:** Let $T^b$ be a visit-optimal $n$-leaf order $M$ $B$-tree with profile
\( v_0, v_1, \ldots, v_{d-1}, v_d = n. \)

By Theorem 2.4, \( n \) lies in the range
\[
M^{d-1} + 1 \leq n \leq M^d. \tag{3.1}
\]

We shall compute \( NU(T_b) \) by using Lemma A in the Appendix to compute the number \( \sum_{i < d} v_i \) of nonleaf nodes of \( T_b \).

(a) Say first that \( M \) is even. Let
\[
\ell = \log_2 n + (1 - \log_2 M)d.
\]

By Lemma A, those levels of \( T_b \) numbered less than \( \ell \) contribute
\[
\frac{M^{\ell-1}}{M-1}
\]
nonleaf nodes, and those levels of \( T_b \) numbered \( \ell \) to \( d-1 \) contribute
\[
\sum_{1 \leq i \leq d-\ell} \left[ n \div m^i \right] = \frac{2n}{M-2} \left( 1 - \left( \frac{2}{M} \right)^{d-\ell} \right) + \alpha \ell
\]
nonleaf nodes, where \( 0 \leq \alpha \leq 1 \). Now, since \( n \) lies in the range (3.1), the ratio of the number of nonleaf nodes of \( T_b \) to \( n \), hence to the number of keys in \( T_b \), is maximized (thus minimizing \( NU(T_b) \)) when \( n = M^{d-1} + 1 \). In this case, we find that \( T_b \) has
\[
\left( \frac{2}{M-2} - \frac{M^2}{(M-1)(M-2)} \right) \log M + o(n) \tag{3.2}
\]
onleaf nodes. One now invokes Proposition 3.1 and Definition (2.1) to complete the proof for the case of even \( M \).

(b) When \( M \) is odd, one proceeds via a similar chain of reasoning, except that one must now be satisfied with asymptotic inequalities. Let
\[
\ell = (\log_2 n + (1 - \log_2 (M+1))d)/\log_2 \left( \frac{2M}{M+1} \right).
\]

By Lemma A, the number of nonleaf nodes of \( T_b \) residing on levels 0
through \( \ell - 1 \) is given by

\[
\frac{M^{\ell - 1}}{M^{\ell - 1}}
\]

and the number residing on level \( \ell \) through \( d - 1 \) is

\[
\sum_{1 \leq i \leq d - \ell} \left\lfloor \frac{n}{m^i} \right\rfloor = \frac{2n}{M^{\ell - 1}} \left( 1 - \left( \frac{2}{M + 1} \right)^{d - \ell} \right) + \alpha \ell
\]

for some \( 0 \leq \alpha \leq 1 \). Now as in the case of even \( M \), one verifies easily that \( \text{NU}(T_d) \) is minimized when \( n = M^{d - 1} + 1 \). In this case we find that \( T_d \) has at least

\[
\frac{n}{M^{\ell - 1}} \left( 2 + M^{-\mu} - 2 \left( \frac{2}{M + 1} \right)^{\mu} \right) + o(n)
\]

nonleaf nodes, where

\[
\mu = \left\lfloor \frac{\log M}{\log \left( \frac{2M}{M + 1} \right)} \right\rfloor
\]

Once again, we invoke Definition (2.1) and Proposition 3.1 to derive the desired ratio and complete the proof of the theorem. \( \Box \)

From Theorem 3.3 the reader can easily compute the node utilization cost of bushy trees for comparison with Proposition 3.1. However, the resulting equations are not likely to be perspicuous. Therefore, we will illustrate some sample trees that may be more enlightening.

For \( M = 3 \), the most benign of the orders since its bushy trees waste the least space, we have a bushy \( 3^{12} \)-key tree with profile

\[
\Pi(T_d) = 1, 3, 9, 27, 81, 243, 729, 2187, 6561, 19683, 59049, 132860, 265721, 531442
\]

and

\[
\text{NU}(T_d) = .545455.
\]
The compact tree with $3^{12}$-key capacity has profile

$$\Pi(T_c) = 1, 2, 4, 10, 28, 82, 244, 730, 2188, 6562, 19684, 59050, 177148, 531442$$

and

$$NU(T_c) = .99995.$$ 

Thus, there is a premium of 1.8332 which is rather close to the asymptotic value of $\frac{5}{6}$. 

For $M = 4$, the most malevolent of orders: a visit-optimal B-tree with $4^{10}$ keys has the profile

$$\Pi(T_b) = 1, 4, 16, 64, 256, 1024, 4096, 16384, 65536, 262144, 524288, 1048577,$$

and

$$NU(T_b) = .4000002.$$ 

The compact tree of order 4 has profile

$$\Pi(T_c) = 1, 2, 5, 17, 65, 257, 1025, 4097, 16385, 65537, 262145, 1048577$$

and

$$NU(T_c) = .99997.$$ 

The ratio is thus 2.4999 which approaches the asymptotic value of 2.5.

Although our comparison results have emphasized the cases most favorable to space minimality, Table 4 illustrates that the situation arises throughout $T_k^M$. 

<table>
<thead>
<tr>
<th>order</th>
<th>leaves</th>
<th>premium as $d \to \infty$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M = 3$</td>
<td>$3^{d-1}+1$</td>
<td>$\frac{5}{6}$</td>
</tr>
<tr>
<td></td>
<td>$4 \cdot 3^{d-2}$</td>
<td>$\frac{3}{4}$</td>
</tr>
<tr>
<td></td>
<td>$2 \cdot 3^{d-1}$</td>
<td>$\frac{1}{2}$</td>
</tr>
<tr>
<td>$M = 4$</td>
<td>$4^{d-1}+1$</td>
<td>$\frac{2}{2}$</td>
</tr>
<tr>
<td></td>
<td>$2 \cdot 4^{d-1}$</td>
<td>$2$</td>
</tr>
<tr>
<td></td>
<td>$3 \cdot 4^{d-1}$</td>
<td>$\frac{5}{6}$</td>
</tr>
</tbody>
</table>

Table 4

To complete the comparison, we next consider the node-visit cost of bushy and compact trees.

**Proposition 3.4:** Let $T_b$ be a bushy order $M$ B-tree and let $T_c$ be a compact order $M$ B-tree each with $n$ leaves. As $n \to \infty$,

\[
\text{NVCOST}(T_b) \asymp \left\lceil \log_{3} n \right\rceil - \frac{2}{M-2} + \frac{M^2}{(M-1)(M-2)} - \log M,
\]

\[
\text{NVCOST}(T_c) \sim \left\lceil \log_{3} n \right\rceil - \frac{1}{M-1}.
\]

In particular, independent of $M$, as $n \to \infty$,

\[
\text{NVCOST}(T_c) - \text{NVCOST}(T_b) \ll 1.
\]

**Proof:** The bound on NVCOST($T_b$) is immediate by Proposition 2.1 and the derivation, in the proof of Theorem 3.3, of the expression (3.2) for the number of nonleaf nodes in an even order B-tree. The expression for NVCOST($T_c$) follows directly from Propositions 2.1 and 2.4.

Both visit-optimal and space-optimal B-trees have minimum depth for a given number of keys (Corollary 2.3 and Theorem 2.4, respectively); however, given this depth, the visit-optimal trees are maximal in the number of nonleaf nodes (Propositions 2.1, 2.5) while the space-optimal trees are minimal in number of nonleaf nodes (Definition 2.1). What
has emerged in this section is that, notwithstanding their minimal
depths, visit-optimal trees can be very wasteful of space (Theorem 3.3);
indeed, as the maximum branching, or order, of the trees grows without
bound, visit-optimal trees can waste space with a profligacy approxima-
ting that of space-pessimal trees (Proposition 3.2 and Theorem 3.3). In
sharp contrast, notwithstanding their node-visit pessimality given their
depths (Corollary 2.3), space-optimal trees have virtually the same
NVCOST as do visit-optimal trees (Proposition 3.4): depth is the prime
determinant of NVCOST, with the number of nonleaf nodes playing only a
secondary role.

The moral of the tale seems, thus, to be that compact B-trees are
the preferred ones when one is initially loading a large data base into
a B-tree. But how long will the tree remain compact?
4. The Persistence of Compactness

The three notions of optimality that have been studied in [4,5] and the present paper are static notions, and fragile ones at that: insertion or deletion in an optimal B-tree is likely to destroy its optimality. One can easily verify that space-optimal B-trees are statistically more fragile for insertions than are visit-optimal B-trees, which in turn are more fragile for deletions. (This is due to the space-optimal trees' preference for dense nodes at high-numbered levels and the visit-optimal trees' preference for sparse nodes at those levels.) It is the purpose of this section to quantify this statistical fragility of space-optimal trees.

The major conclusion of the section will be that compact B-trees are always desirable when one initializes a data base (this follows from the previous section); they are reasonable to maintain for a stable data base (say one with no more than a 10% insertion rate between "backup" reorganizations); but they are too fragile to use directly with a volatile data base.

Since the analysis we present here is only suggestive and not definitive, we shall content ourselves with an analysis under simplified conditions. Specifically, we shall consider only order 3 B-trees (i.e. 2,3-trees), and we shall carry out only a "first-order" analysis (in the sense of Yao [7]) of these trees.

(4.1) Define the real-valued function ENU with domain \( \mathbb{N} \times \mathbb{N} \) (\( \mathbb{N} \) denotes the positive integers) as follows: for \( n_0 < n \), \( ENU(n, n_0) \) is the expected NU of an \( n \)-leaf 2,3-tree that is obtained from a space-optimal \( n_0 \)-leaf 2,3-tree by a sequence of \( n - n_0 \) "random" insertions. Here as in [7] an insertion into a \( k \)-key 2,3-tree is termed "random" if it is equally likely to fall in any of the \( k + 1 \) intervals defined by the order on the keys.
The competition for our compact-initialized B-trees are the purely random B-trees studied by Yao.

**Proposition 4.1** [7]: As \( n \to \infty \), \( 0.64 \leq \text{ENU}(n,1) \leq 0.72 \).

To evaluate the effect of compact initialization, we contrast Proposition 4.1 with the following.

**Theorem 4.2**: For \( 0 < \alpha \leq 1 \), as \( n \to \infty \), \( \frac{21}{18-4\alpha} \leq \text{ENU}(n,\alpha n) \leq \frac{14}{9-2\alpha} \).

Theorem 4.2 dictates, and Table 5 illustrates for various values of \( \alpha \), the range in which the expected node utilization will fall in the presence of random insertions.

<table>
<thead>
<tr>
<th>% random increase</th>
<th>( \alpha )</th>
<th>expected node utilization ( n \to \infty )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1%</td>
<td>( \frac{100}{101} )</td>
<td>( 0.74 \leq \text{ENU}(n,\alpha n) \leq 0.98 )</td>
</tr>
<tr>
<td>2.5%</td>
<td>( \frac{40}{41} )</td>
<td>( 0.72 \leq \text{ENU}(n,\alpha n) \leq 0.96 )</td>
</tr>
<tr>
<td>5%</td>
<td>( \frac{20}{21} )</td>
<td>( 0.69 \leq \text{ENU}(n,\alpha n) \leq 0.92 )</td>
</tr>
<tr>
<td>10%</td>
<td>( \frac{10}{11} )</td>
<td>( 0.66 \leq \text{ENU}(n,\alpha n) \leq 0.88 )</td>
</tr>
</tbody>
</table>

Table 5

Thus even after moderate growth of the data base, the expected benefits of compact initialization are still discernible.

The remainder of this section is devoted to proving Theorem 4.2.

**Proof**: The proof follows the strategy of Yao's proof of his Theorem 2.6 [7], the first-order version of Proposition 4.1.

**Lemma 4.3** [7]: If the 2,3-tree \( T \) has profile

\[ \Pi(T) = v_0,v_1,\ldots,v_{d-1},v_d \]

then the number of nonleaf nodes of \( T \) satisfies
\[ \frac{3}{2^{v_{d-1}}} - \frac{1}{2} \leq \text{NNCOST}(T) \leq 2^{v_{d-1}} - 1. \]

Define the following quantities:

For \( i = 1, 2 \), let

\[ A_i(n, n_0) = \text{def} \quad \text{the expected number of \((i+1)\)-son nodes at level} \quad d-1 \text{ of the tree constructed from an } n_0 \text{-leaf space-optimal tree via a sequence of } n-n_0 \text{ random insertions.} \]

Let \( N^*(n, n_0) = \text{def} \quad \text{the expected NNCOST of the tree just described.} \]

**Lemma 4.4 [7]:** Letting \( A(n, n_0) = A_1(n, n_0) + A_2(n, n_0) \),

\[ \frac{3}{2} A(n, n_0) - \frac{1}{2} \leq N^*(n, n_0) \leq 2A(n, n_0) - 1. \]

**Proof:** Lemma 4.3. \( \square \)

**Lemma 4.5:** For \( 0 < \alpha < 1 \), as \( n \to \infty \),

\[ A_1(n, an) = \frac{2}{7} n(1 - \alpha^7) + o(1); \]

and \( A_2(n, an) = n\left(\frac{1}{7} + \frac{4}{21} \alpha^7\right) + o(1) \).

**Proof:** Yao, in his Lemma 2.6 [7], shows that when \( n > an \),

\[ A_1(n, an) = (1 - \frac{6}{n}) A_1(n, 1, an) + 2. \]

Since the \( an \)-leaf tree we start with is space-optimal, we have the initial condition \( A_1(an, an) \leq 2 \). We find, therefore, as \( n \) grows without bound,

\[ A_1(n, an) = 2 \sum_{6 \leq i \leq n-an} \sum_{0 \leq k \leq 5} (1 - \frac{i}{n-k}) + o(1). \]

This simple form is found by just expanding the recurrence and noting the resulting cancellations. This sum is easily seen to evaluate to

\[ A_1(n, an) = 2n^{-6} \sum_{6 \leq i \leq n-an} (n-i)^6 + o(1), \]

whence the asserted value of \( A_1 \). The value of \( A_2(n, an) \) now follows directly from the obvious equation \( 2A_1(n, an) + 3A_2(n, an) = n \). \( \square \)

Lemmas 4.4 and 4.5 combine to yield
Lemma 4.6: For 0 < α ≤ 1, as $n \to \infty$, $n \left( \frac{9}{14} - \frac{1}{7^\alpha} \right) \leq N^*(n, an) \leq n \left( \frac{6}{7} - \frac{4}{21^\alpha} \right)$.

The theorem is now immediate by definition of ENU. □

Thus, if a compact tree grows (by random insertions) by less than 2½ %, the expectation of its space utilization is strictly greater than that for randomly grown trees. In order to use compact trees for these stable files, we present in the next section an \textit{in situ} compactification algorithm that can be used as a "back-up" procedure for essentially no additional cost over the naive "back-up" operation.
5. Algorithms

The import of Section 3 is that compact B-trees minimize space and nearly minimize time. The import of Section 4 is to quantify the robustness of compact B-trees in the presence of insertions. An obvious way to apply these results in practice would be (1) to initialize a B-tree to compact form, (2) to monitor the NVCOST and NU functions as the file is modified, and (3) when NU begins to stray too far from unity, to recompact the entire file. An alternative approach would be to dispense with the monitoring operation and simply recompact during routine "back-up" of the file. This latter approach depends on the (likely) condition that large data bases do not grow so rapidly that recompactification would be required more often than the frequency of the "back-up" operation.

It is, perhaps, worthwhile to emphasize the importance of taking special precautions when initializing B-trees from sorted or "nearly" sorted files. In [4] it was observed that construction of a B-tree by repeated insertion from a sorted file frequently results in a scrawny tree. In fact, if the file has size $2^m$ (for odd $M$), the repeated insertion produces a tree with a binary root whose descendent are both complete $m$-ary trees. This result is both sparse and scrawny and is thus space- and time-pessimal.

The purpose of this section is to address the algorithmic issues involved in initialization, monitoring and compactification. (All complexity bounds are for a uniform cost random-access machine.)

Initialization Algorithm: In [4] a linear-time (in the size of the file) algorithm was presented for constructing a 2,3-tree given a (detailed) profile for the tree and a sorted list of records.* Conversion of that

*This algorithm was used in conjunction with Theorem 2.4 to construct visit-optimal 2,3-trees.
algorithm to operate on B-trees of arbitrary order is a straightforward matter requiring no further discussion. Construction of the proper compact profile can be performed in logarithmic time using the characterization Theorem 2.2. From the profile, a detailed profile can be constructed by observing that at level \( l \) the \( v_l \) vertices must have \( v_{l+1} \) outedges and a vertex containing \( s \) keys has \( s+1 \) outedges. In the absence of any other criterion, we simply distribute the keys "evenly" throughout the \( v_l \) vertices by assigning \( s \) keys to \( r \) of the vertices and \( s+1 \) to the remaining vertices. Thus, \( s = \left\lceil \frac{v_{l+1}}{v_l} \right\rceil - 1 \) and \( r = v_l - v_{l+1} \mod v_l \). Finally, the records can be sorted by any external sorting algorithm.

**Monitoring algorithm:** As insertions and deletions change the structure of the B-tree, the profile and/or detailed profile can be updated easily in time proportional to that of insertion or deletion. For example, if an insertion changes \( t \) internal levels in the tree, then \( t+1 \) entries in the profile and \( 2t \) entries in the detailed profile must be changed. Maintenance of these profiles gives a current description of the structure of the tree.

If, however, only the NU and NVCOST are to be monitored, then these values can be updated in constant time since by Proposition 2.1 and equation (2.1) they both depend on \( k \), the number of keys, the current depth, and \( \sum_{i<d} v_i \), the number of internal nodes. If \( I \) is the current number of internal nodes and an insertion or deletion changes \( t \) internal levels then the number of internal nodes in the new tree is \( I \pm (t-1) \) where the sign depends on whether the operation is an insertion (+) or a deletion (−).

**Compactification Algorithm:** Obviously, compactification can be accomplished simply by using the initializing algorithm with the existing
tree as input. However, this approach requires two copies of the tree to exist simultaneously, and if space were that plentiful, compact trees would have only limited benefit. So we present an in situ compactification scheme that requires at most d free nodes. These d nodes need not all be available when the algorithm starts; it is sufficient, after having compacted n keys, to have freed \( \lceil \log^*_M n \rceil + 1 \) nodes.

In order to simplify the presentation, we give the compactification algorithm only for 2,3-trees, assuming that the generalization to arbitrary M is obvious. The algorithm takes three inputs: a 2,3-tree T, a depth d, and a detailed profile for the desired compact tree. Since 2,3-trees have such simple detailed profiles \( \sigma^2_0, \sigma^3_0, \ldots, \sigma^2_{d-1}, \sigma^3_{d-1} \), it is sufficient to know only one component of each pair. Accordingly, the array variable \( \sigma_3[0:d-1] \) gives the number of ternary nodes at each level of the new compact tree. The output from compact is a reference (i.e. pointer) to the root of the compacted tree.

The details of the tree representation are purposely left obscure except that we follow the initialization algorithm of [4] in assuming that each node has fields: left, key1, middle, key2, right with the obvious meanings. By convention, binary nodes have NIL as values in the last two fields. Also, by convention, the resulting compact tree will have all ternary nodes "left justified" on a level. Clearly, other distributional disciplines can be implemented easily.

The overall structure of the algorithm can be viewed abstractly as a "producer/consumer" solution. That is, two procedures are used: one to fetch keys from the existing tree (producer) and one to construct a compact tree given its keys one-at-a-time (consumer). These two abstract operations
could be implemented by means of recursive co-routines, but such exotic
control structures are unnecessary. Instead, the producer operation is
implemented explicitly by a recursive depth-first traversal procedure
\((dft)\) and at each point where a key is "produced" a nonrecursive sub-
routine \((\text{build})\) is called which implicitly implements the consumer operation.

The only subtlety in this approach is that the \text{build} routine must
keep track of the subtrees currently "under construction." Say that a
subtree is \textit{under construction at level} \(i\) if a subtree rooted at level \(i\)
has at least one but not all of its immediate descendant subtrees comple-
ted. For instance, if the portion of the tree shown in bold in Figure 2
has so far been constructed, then subtrees at levels 1 and 3 are under
construction. In order to keep track of this progress, then, a variable
\(\text{UC}[0:d-1]\) (mnemonic for \text{under construction}) is used to record a reference
to each node under construction. Initially, \text{UC} contains only \text{NIL}'s,
indicating that no nodes are under construction.

\textbf{Algorithm} - input: \(T = \text{a 2,3-tree to be compacted}\)
\(d = \text{depth of the new compact tree}\)
\(\text{sigma3}[0:d-1] = \text{a vector of the number of ternary}\)
\(\text{nodes at each level in the new compact tree}\)
output: \(\text{a reference to the root of the compact tree}\)
function compact(T, d, sigma3);  
  tree T;  integer d;  
  integer array sigma3;  
  begin integer level;  
    ref n,  
    ref array UC[0:d-1];  
  procedure dft(node);  
    ref node;  
  begin  
    if node.left = NIL  
      then (build(node.key1);  
        if node.key2 = NIL  
          then build(node.key2))  
      else (dft(node.left);  
        build(node.key1);  
        dft(node.middle);  
        if node.key2 = NIL  
          then build(node.key2);  
        dft(node.right));  
    free(node)  
  end;  
  procedure build(key);  
    ref integer key;  
  begin  
    comment global var. "level" is set at the  
    level of last key placement; initially, -1;  
    while level ≠ d-1 do  
      (level = level + 1;  
        UC[level] = NIL);  
      desc = NIL;  
    while key ≠ NIL ∧ level ≥ 0 do  
      (if UC[level] = NIL  
        then n = UC[level] + getspace  
        else n = UC[level];  
      cond  
        n.key1 = NIL  
        → (n.left + desc;  
          n.key1 = key;  
          key = NIL)  
        n.key2 = NIL ∧ σma3[level] > 0  
        → (n.middle + desc;  
          n.key2 = key;  
          key = NIL)  
        n.key2 = NIL ∧ σma3[level] = 0  
        → (n.middle + desc;  
          desc + n;  
          level + level - 1)  
        n.key1 = NIL ∧ n.key2 = NIL  
        → (n.right + desc;  
          desc + n;  
          σma3[level] + σma3[level] - 1;  
          level + level - 1))  
    end;  
    comment declaration completed;  
    level = -1;  
    dft(root(T));  
    build();  
    compact = UC[0]  
  end;
To see that the algorithm halts we observe first that the basic control
flow is determined by $\delta t$ and amounts to a simple depth-first traversal of
a 2,3-tree that obviously halts if its subparts do. Secondly, we note that
the two other loops ([29-31] and [33-54] of the build procedure) can not
possibly cycle forever for positive $d$. The [29-31] while-loop always termi-
nates since the initial value of level is always less than or equal to
d-1 upon entry to the loop. The [33-54] loop clearly terminates since in
each clause of the conditional some change is made that effects the dis-
junction controlling the loop.

The tree that results from build, (if it is a tree at all) will evidently
be compact since binary and ternary nodes are built according to the dictates
of the profile. To see that a valid 2,3-tree results from build, say that in
a tree containing keys $k_1 < k_2 < \ldots < k_n$ and leaves $l_1, l_2, \ldots, l_{n+1}$ (numbered
left to right), that the left leaf of $k_i$ is $l_i$. Then build is called $n$ times
by the $\delta t$ routine and on the $i^{th}$ call, build (1) begins by moving to the left
leaf of $k_i$ (2) creates all edges from $l_i$ to the vertex containing $k_i$, (3)
"completes" the vertices between $l_i$ and the vertex containing $k_i$ according as
they are either binary [46-49] or ternary [50-54], and (4) places $k_i$ in the
proper position in the vertex according to whether it is in the first key
position [39-41] or the second key position [42-45]. Thus, the calls
from $\delta t$ complete all portions of the tree except the edges on the right
spine. The dummy call from compact [59] completes this feature and the
algorithm halts.

Evidently, compact operates in linear time on a uniform-cost random-
access machine since it is simply the composition of two depth-first tree
traversals. The total number of tree records that are required in excess of
the number freed is $d$ (i.e. if a compact tree were compacted, $d$ extra cells
would be needed for the algorithm to operate.)
6. Summary and Discussion

In the set $I^M_k$ of all order $M$ B-trees with capacity $k$, we have characterized the space-minimal elements. We have bounded the time performance of these space-minimal B-trees as well as bounding the space utilization of the time-minimal B-trees. The main result of this analysis is that

the space-minimal trees are nearly time-minimal, but
the time-minimal trees are nearly space-maximal.

This bias in favor of using space-minimal trees when possible motivated our analysis of the robustness of space-minimal trees in the presence of random insertions. Though space-minimal B-trees are only modestly robust, pragmatic considerations such as file stability suggest that they could be beneficial with periodic recompaction, e.g. during routine file "back-up." This compactification can be accomplished inexpensively using the linear time algorithm presented here.

Many issues remain to be investigated. For example, are there variants on the B-tree theme that enhance the robustness of space efficient trees? How robust are compact B-trees under "random" insertions? How do variable length keys affect the analysis presented here -- is it better to have smaller nodes when the keys are variable in length? What are the time and space characteristics of random B-trees created by random insertions and deletions?

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APPENDIX A

Lemma A: Let $T$ be a visit optimal $n$-leaf order $M$ B-tree with profile

$$\Pi(T) = \nu_0, \nu_1, \ldots, \nu_d.$$  

If $M$ is even, then

$$\nu_\ell = M^\ell$$

for all

$$\ell \leq \log_2 n + (1 - \log_2 M) d - 1,$$  \hspace{1cm} (A.1)

and

$$\nu_\ell = \left\lfloor n \div m^{d-\ell} \right\rfloor$$

for all

$$\ell \geq \log_2 n + (1 - \log_2 M) d.$$  \hspace{1cm} (A.2)

If $M$ is odd, then

$$\nu_\ell = M^\ell$$

for all

$$\ell \leq (\log_2 n + (1 - \log_2 (M+1))d) / \log_2 \left( \frac{2M}{M+1} \right) + o(1)$$

as $n \to \infty$; and

$$\nu_\ell = \left\lfloor n \div m^{d-\ell} \right\rfloor$$

for all

$$\ell \geq (\log_2 n + (1 - \log_2 (M+1))d) / \log_2 \left( \frac{2M}{M+1} \right).$$

Proof: Assume first that $M$ is even. Inequality (A.1) on $\ell$ yields

$$\ell \cdot \log_2 M \leq \log_2 n - (d-\ell)(\log_2 M-1) - 1$$

so that

$$M^\ell \leq \left\lfloor n \div (M/2)^{d-\ell} \right\rfloor = \left\lfloor n \div m^{d-\ell} \right\rfloor$$

and the lemma follows by Theorem 2.4. By similar calculations, inequality

(A.2) on $\ell$ yields

$$M^\ell \geq \left\lfloor n \div m^{d-\ell} \right\rfloor,$$

so again the lemma follows by Theorem 2.4.

The case of odd $M$ follows by similar reasoning, using the fact that

$m = (M+1)/2$ when $M$ is odd.