The A-tree: An Index Structure for High-Dimensional Spaces Using Relative Approximation

Yasushi Sakurai† Masatoshi Yoshikawa§ Shunsuke Uemura§ Haruhiko Kojima†

† NTT Cyber Solutions Laboratories
sakurai@marsh.hil.ntt.co.jp,
kojima@aether.hil.ntt.co.jp

§ Graduate School of Information Science
Nara Institute of Science and Technology
{*yosikawa, uemura*}*@is.aist-nara.ac.jp*

Abstract

We propose a novel index structure, A-tree (Approximation tree), for similarity search of high-dimensional data. The basic idea of the A-tree is the introduction of Virtual Bounding Rectangles (VBRs), which contain and approximate MBRs and data objects. VBRs can be represented rather compactly, and thus affect the tree configuration both quantitatively and qualitatively. Firstly, since tree nodes can install large number of entries of VBRs, fanout of nodes becomes large, thus leads to fast search. More importantly, we have a free hand in arranging MBRs and VBRs in tree nodes. In the A-trees, nodes contain entries of an MBR and its children VBRs. Therefore, by fetching a node of an A-tree, we can obtain the information of exact position of a parent MBR and approximate position of its children. We have performed experiments using both synthetic and real data sets. For the real data sets, the A-tree outperforms the SR-tree and the VA-File in all range of dimensionality up to 64 dimension, which is the highest dimension in our experiments. The A-tree achieves 77.3% (77.7%, resp.) savings in page accesses compared to the SR-tree (the VA-File, resp.) for 64-dimensional real data.

Proceedings of the 26th VLDB Conference, Cairo, Egypt, 2000.

1 Introduction

1.1 Data Retrieval in High-Dimensional Space

Fast content-based retrieval is a core function to provide high-quality human interface for large-scale multimedia databases. In content-based retrieval, usually, feature vectors extracted from multimedia data are used as keys. For instance, the features extracted from images include color, texture, structure and so on. In the balance of the reduction of computational cost and the raise of object recognition ratio, feature vectors of which dimensionality is ten or tens are used in many recognition methods[12][13] or systems[17]. Since retrieving high-dimensional feature vectors incurs high cost for large data sets, new spatial indices and search methods that offer efficient data retrieval are required. Various spatial indices[16][6] have been proposed so far. This paper introduces a new index structure, named A-tree (Approximation tree), that offers remarkably higher search performance than existing indices.

1.2 Related Work

The conventional approach to supporting similarity search in high-dimensional vector space can be broadly classified into two categories. The first approach is using data-partitioning index trees. Neighbor vectors are covered by MBRs (Minimum Bounding Rectangles) or MBSs (Minimum Bounding Spheres), which are organized in a hierarchical tree structure. Many index trees have been proposed so far. They include the R-tree[8], the R*-tree[2], the Hilbert R-tree[10] and the SS-tree[19]. Also, nearest neighbor search methods using such indices have been proposed[14][9]. Two recently proposed indices, the X-tree[5] and the SR-tree[11], are reported to offer good performance. The X-tree[5] introduces the notion of supernode, and outperforms the R*-tree. The SR-tree[11] has a unique feature in that it uses both MBRs and MBSs, and is

reported to outperform both the R*-tree and the SS-tree. The second approach is the use of approximation files. Among others, the VA-File (Vector Approximation File)[18] is a simple yet powerful scheme. The VA-File divides the data space into cells and allocates a bit-string to each cell. The vectors inside a cell are approximated by the cell, and the VA-File itself is simply an array of these geometric approximations. For search, the entire VA-File is scanned to select candidate vectors. Those candidates are then verified by visiting the vector files. In [18], Weber et al. have reported that the VA-File outperforms both the R*-tree and the X-tree when the dimensionality is high ($\geq$ around 6.) To sum up, among access methods for high-dimensional vector space search, the SR-tree and the VA-File are two methods which are not reported to be outperformed by other methods[1] .

In the field of spatial search for high-dimensional data, the well-known problem, the "curse of dimensionality" looms large before us. Of late, search methods which present an approximate answer [1] [7], have been proposed to avoid the influence of the problem. Although these works are useful, the goal of our work to overcome the problem by providing a search method which gives an exact answer.

1.3 The Introduction of the A-tree

In this paper, we propose a new index structure, the A-tree. The introduction of the A-tree is motivated by the comparison and analysis of the SR-tree and the VA-File. Since no result on the comparison between these two access methods is available, we first performed experiments comparing the two access methods. Based on the experiments, we have developed a new tree index structure, A-tree, and search and update algorithms. The basic idea of the A-tree is the introduction of Virtual Bounding Rectangles (VBRs), which contain and approximate MBRs and data objects, respectively. VBRs can be represented rather compactly, and thus affect the tree configuration both quantitatively and qualitatively. Firstly, since tree nodes can install large number of entries of VBRs, fanout of nodes becomes large, thus leads to fast search. More importantly, we have a free hand in arranging MBRs and VBRs in tree nodes. In the A-trees, nodes contain entries of an MBR and its children VBRs. Therefore, by fetching a node of an A-tree, we can obtain the information of exact position of a parent MBR and approximate position of its children.

We evaluate the performance of the A-tree using both synthetic and real data. The results demonstrate the effectiveness of the A-tree in high-dimension search. The mechanism of the A-tree is remarkably successful, especially for non-uniformly distributed data sets such as real data sets. For both real data sets and synthetic clustered data sets, the A-tree outperforms the SR-tree and the VA-File in all dimensionality ranges up to 64 dimensions, the highest dimension examined in our experiments. The A-tree achieves 77.3 % (77.7 %, resp.) savings in page access compared to the SR-tree (the VA-File, resp.) for real data with 64-dimensions. As far as we know, 64 is the highest dimension of real data used for performance evaluation in high-dimensional access methods with the only exception of 100-dimensional EigenFace data used in [19].

The remainder of this paper is organized as follows. In Section 2, the summary of the comparison and analysis of the SR-tree and the VA-File is given. Based on the summary, the motivation and design principles of the A-tree are presented. Section 3 describes the definitions and algorithms of the A-tree. Section 4 presents the results of a performance evaluation of the A-tree and conventional access methods. Finally, Section 5 concludes the paper.

2 Motivation: An Introduction of Approximation Mechanism in Tree Structure

In this section, we summarize the result of performance evaluation of the SR-tree and the VA-File. Based on the summary, we present the design philosophy of the A-tree, and shows the uniqueness of the A-tree among the proposed indices for high-dimensional data.

2.1 Properties of the SR-tree and the VA-File

We have performed extensive experiments to analyze the SR-tree and the VA-File. The details of the experiments are described in [15]. The result revealed that both indices have their own drawbacks. The evaluation result can be summarized as follows:

(1) For non-uniformly distributed data such as real data and synthetic clustered data, the SR-tree offers better performance than the VA-File. Since the tree structure changes flexibly according to the distribution of data sets, the SR-tree exhibits higher search performance for non-uniformly distribute data sets. In the VA-File, vector data are approximated based on absolute positions. Since the approximation of absolute vector positions is independent of data distribution, a large number of dense data tend to be approximated by same value. Hence, the absolute approximation leads to large approximation errors for skew data. Thus, the VA-File is not effective for non-uniformly distributed data which are commonly found in real applications.

(2) However, in the SR-tree, like many other indices in the R-tree family, the size of entries in a node

[1] Recently, Berchtold et al. have reported that the IQ-tree outperforms the VA-File in the range of dimensionality up to 16 [4].

is directly proportional to dimensionality. Hence, as dimensionality increases, the fanout of nodes becomes small. This causes the increase of backtracks of non-leaf nodes; thus degrades search performance.

(3) Increasing node page size leads to the increase of fanout. With real data, the SR-tree provides the lowest search cost at one page per node, and the structures for larger node size require higher cost. However, larger fanout contributes to the reduction of the number of node accesses.

(4) In the SR-tree, as dimensionality increases, the frequency of the usage of MBSs decreases since MBSs occupy much larger volume than MBRs. Hence the contribution of MBSs in node pruning is small in high-dimensional spaces.

2.2 The Design Philosophy of the A-tree

By analyzing the experimental results, we have developed a new index data structure, A-tree, which is based on the following design philosophy:

- **Tree Structure:** From the evaluation result (1), we adopt a tree index.
- **Relative Approximation:** To overcome the problem of tree indices identified in the evaluation result (2), we introduced a new notion, relative approximation, which is a simple yet powerful approximation method utilizing the hierarchy of tree indices. In relative approximation, bounding regions or data points are approximated by their relative positions in terms of parent's bounding region. Relative approximation has the following benefits:
  - Unlike the absolute approximation in the VA-File, approximation values of the relative approximation change in accordance with the data distribution. By this flexibility, the approximation error in the relative approximation is considerably smaller than that of the VA-File. This feature is especially effective for non-uniformly distributed vectors, commonly found in real applications.
  - Since approximation values can be compactly represented, the size of entries in an index node becomes small, which implies larger fanout. This leads to the reduction of the number of node accesses as shown in evaluation result (3).
  - Compact representation of approximated bounding regions allows wider design options of tree configuration freed from traditional tree indices. More concretely, each index node of the A-tree contains representation of i) exact position of a bounding region B; and ii) relative approximation of B's children. Therefore, by fetching a node of an A-tree, we can obtain the (partial) information on bounding regions in two generations. This configuration is also useful for efficient handling of update operations.

  As a negative side, approximation error may cause the degradation of the power of pruning subtrees in searching. From the performance evaluation presented in Section 4, we have confirmed the benefits of relative approximation well compensate the approximation error.
- **Partial Usage of MBSs:** Since the SR-tree is one of the best indices among the tree indices proposed so far, the SR-tree is used as a start point in the design of the A-tree. However, as shown in the evaluation result (4), the effect of MBSs is limited in search of high dimensional data. Hence, MBSs are not stored in the A-tree, but the centroid of data objects in a subtree is used only for insertion and deletion.

In all, the A-tree is a new index which applied the notion of the relative approximation to the hierarchical structure of the SR-tree. However, this application is not simple; the configuration of the A-tree is unique in that 1) each node contains an MBR and representation of relative approximation of its children; and 2) centroid of data objects are used only for update.

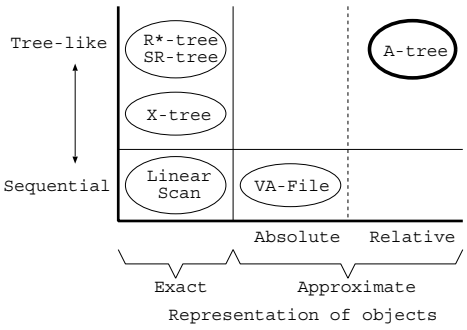


Figure 1: Classification of spatial access methods.

2.3 Classification of Indices

Figure 1 shows a classification of spatial access methods from two viewpoints: representation of spatial objects and index structure. Conventional spatial access methods can be roughly classified into the following three categories: (1) linear scan; (2) the VA-File, a sequential file of absolute approximation of feature vectors; and (3) R-tree family which has tree structures. R-tree family can be further classified into "pure" tree-structured indices such as the R*-tree and the SR-tree, and "hybrid" of tree and sequential structure such as

the X-tree, which, with the notion of supernode, shows stronger property of sequential scan as dimensionality increases. The A-tree does not belong to any of these categories and is unique in that i) the A-tree is a tree-structured index; and ii) the representation of MBRs and data objects is based on approximation relative to their parent MBRs.

3 The Data Structure and Algorithms of the A-tree

In this section, we first give the definitions of **VBR (Virtual Bounding Rectangle)**, which is representation of relative approximation of an MBR or a data object in the A-tree. Then we describe the structure of the A-tree. Also, algorithms for searching and updating are presented. The nearest neighbor search algorithm is guaranteed to return exact answers, that is, the A-tree finds the desired objects without omission.

3.1 Virtual Bounding Rectangle

A VBR is a rectangle that contain and approximate an MBR or a data object. In the A-tree, children MBRs and data objects are approximated as VBRs by the relative position in terms of their parent MBR.

A rectangle A in n-dimensional space is represented by the two endpoints $\boldsymbol{a}$ and $\boldsymbol{a'}$ of its major diagonal: $A = (\boldsymbol{a}, \boldsymbol{a'})$, where $\boldsymbol{a} = [a_1, a_2, \ldots, a_n]$, $\boldsymbol{a'} = [a'_1, a'_2, \ldots, a'_n]$, and $a_i \leq a'_i$ for $i \in \{1, 2, \ldots, n\}$. Let $B = (\boldsymbol{b}, \boldsymbol{b'})$ ($\boldsymbol{b} = [b_1, b_2, \ldots, b_n]$, $\boldsymbol{b'} = [b'_1, b'_2, \ldots, b'_n]$) be a rectangle contained in A. Hence, $a_i \leq b_i \leq b'_i \leq a'_i$ $(i = 1, 2, \ldots, n)$ holds. The basic idea of relative approximation is to quantize the start value b_i and the end value b'_i of the interval (b_i, b'_i) relatively to the interval (a_i, a'_i). The quantization functions for the start and end values are similar but slightly different.

We will define the quantization functions more specifically. Let q (≥ 1) be an integer. The quantization function Q_s for start values is defined as follows:

$$Q_s(b_i) = a_i + \frac{(a'_i - a_i)h_s(b_i)}{q}$$

where

$$h_s(b_i) = \begin{cases} q-1 & (\text{if } b_i = a'_i) \\ \left\lfloor (\frac{b_i - a_i}{a'_i - a_i}) \cdot q \right\rfloor & (\text{otherwise}) \end{cases}$$

Similarly, the quantization function Q_e for end values is defined as follows:

$$Q_e(b'_i) = a_i + \frac{(a'_i - a_i)h_e(b'_i)}{q}$$

where

$$h_e(b'_i) = \begin{cases} 1 & (\text{if } b'_i = a_i) \\ \left\lceil (\frac{b'_i - a_i}{a'_i - a_i}) \cdot q \right\rceil & (\text{otherwise}) \end{cases}$$

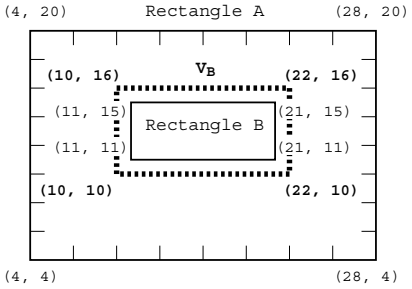


Figure 2: An example of spatial representation using VBR.

Note that $h_s(b_i) \in \{0, 1, \ldots, q-1\}$, and $h_e(b'_i) \in \{1, 2, \ldots, q\}$. Also, it is easy to verify that the following property holds:

$$a_i \leq Q_s(b_i) \leq b_i \leq b'_i \leq Q_e(b'_i) \leq a'_i \qquad (1)$$

The **virtual bounding rectangle** (**VBR** for short) of B (in A with radix q) is the rectangle

$$V_B = (\boldsymbol{v}, \boldsymbol{v'})$$

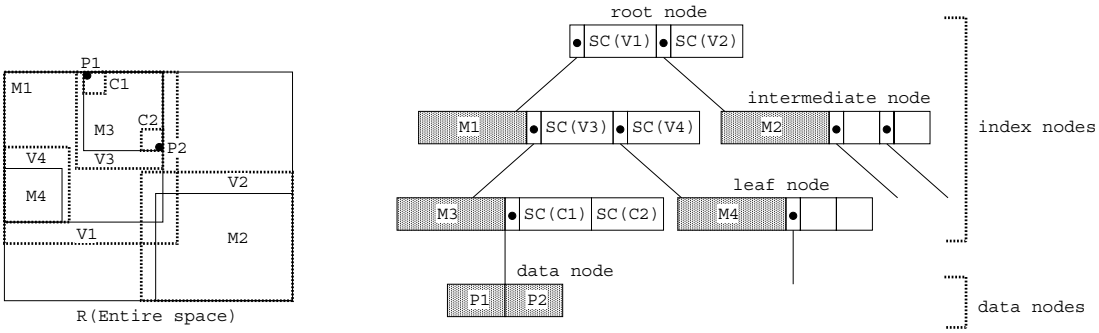
where

$$\boldsymbol{v} = (Q_s(b_1), Q_s(b_2), \ldots, Q_s(b_n))$$
$$\boldsymbol{v'} = (Q_e(b'_1), Q_e(b'_2), \ldots, Q_e(b'_n))$$

From the property (1), B is contained in V_B, and V_B is contained in A. Let C be a data object contained in a rectangle A. Since a data object can be regarded as a special rectangle of which two diagonal endpoints coincide, the VBR of C (in A with radix q) can be similarly defined. Figure 2 shows an example of VBR. In this figure, V_B is the VBR of B in A with radix 8.

The VBR V_B of B (in A with radix q) can be represented by $2n$ integers $h_s(b_i)$, $h_e(b'_i)$ $(i = 1, 2, \ldots, n)$. Since the number of possible values of $h_s(b_i)$ is q, $h_s(b_i)$ can be represented by a binary code of length l ($= \lceil \log_2 q \rceil$). The same discussion applies to $h_e(b'_i)$. More specifically, we define the binary representation of $h_s(b_i)$ be $[h_s(b_i)]_2$. Also, the binary representation of $h_e(b'_i)$ be $[h_e(b'_i) - 1]_2$. Here, $[x]_2$ is the binary number of an integer x. We call the binary code of length $2nl$, which are obtained by concatenating these $2n$ binary codes of length l, as the **subspace code** of V_B (in A with radix q). For a data object C, the VBR V_C of C (in A with radix q) can be represented by n integers $h_s(b_i)$ $(i = 1, 2, \ldots, n)$. Hence, the subspace code of V_C (in A with radix q) is of length nl. For example, for the V_B in Figure 2, $h_s(b_1) = 2$, $h_e(b'_1) = 6$, $h_s(b_2) = 3$, and $h_e(b'_2) = 6$. Hence, 010101011101, which is the concatenation of four binary codes $[2]_2$, $[6-1]_2$, $[3]_2$, $[6-1]_2$ of length 3 ($= \lceil \log_2 8 \rceil$), is the subspace code of V_B in A with radix 8. The subspace code of a VBR V is denoted by $sc(V)$.

Obviously, there is a tradeoff between the length of subspace code and the approximation error. We will discuss this tradeoff in Section 4.



(a)VBR and MBR (b)Tree structure

Figure 3: The A-tree structure.

3.2 Index Structure

Besides MBRs and data objects, subspace code of VBRs are included in the structure of the A-tree. Figure 3 shows an example of this structure. In Figure 3(a), the rectangle R represents the entire space. $M1$ and $M2$ represent rectangles in R. $M1$ is the MBR of $M3$ and $M4$. $M3$ is the MBR of data objects P_1 and P_2. In this structure, $V1$, $V2$, $V3$ and $V4$ are the VBR of $M1$ in R, the VBR of $M2$ in R, the VBR of $M3$ in $M1$, and the VBR of $M4$ in $M1$, respectively. Also, $C1$ and $C2$ are the VBRs of $P1$ and $P2$ in $M3$, respectively.

As shown in Figure 3(b), A-trees consist of index nodes and data nodes. Index nodes other than the root in A-trees contain exactly one MBR, say M, and subspace codes of VBRs of MBRs in children nodes. M is the MBR of MBRs (or data objects) contained in children nodes. In the root node, no MBR is contained; instead, the entire data space is assumed. When creating A-trees, subspace codes of children VBRs in a node can be calculated from the information of their parent MBR in the same node and the children MBRs (or data objects). In case of the root node, subspace codes of children VBRs are calculated from the information of the entire data space and the children MBRs. Inversely, when searching data objects, the absolute positions of children VBRs of a node can be calculated from the parent MBR and subspace codes of those VBRs stored in the node. Therefore, a node in A-trees contains partial information of MBRs in two consecutive generations; namely the exact position of an MBR and approximate positions of its children MBRs. The search algorithm of the A-tree effectively uses these VBRs for node pruning.

In A-trees, index nodes are classified into leaf nodes, intermediate nodes and the root node. The configuration of each type of nodes is described below:

1. Data nodes:

   A data node has a list of entries (P_1, o_1), (P_2, o_2), ..., (P_m, o_m), where P_i $(i = 1, 2, \ldots, m)$ is the spatial vector of a data object, and o_i $(i = 1, 2, \ldots, m)$ is the pointer to the data object description record. The number of entries in a leaf, m, is bounded by predefined minimum and maximum.

2. Leaf nodes:

   There is a one-to-one correspondence between data nodes and leaf nodes. The leaf node corresponding to a data node $N((P_1, o_1), (P_2, o_2), \ldots, (P_m, o_m))$ has i) a rectangle M, which is the MBR of $P_1, P_2, \ldots, P_m$. ii) a pointer to N; and iii) a list of entries $sc(V_1), sc(V_2), \ldots, sc(V_m)$, where V_i is the VBR of P_i in M $(i = 1, 2, \ldots, m.)$

3. Intermediate nodes:

   An intermediate node, which is an index nodes other than the root node and leaf nodes, contains i) a rectangle M, which is the MBR of children nodes' MBRs. ii) a list of entries, each of which is a quadruplet $(ptr, sc(V), \omega, P_{centroid})$, where ptr is the pointer to a child node C, V is the VBR of the MBR contained in C, ω is the number of all data objects contained in the subtree rooted by C, and $P_{centroid}$ is the centroid of the data objects in the subtree.

   As explained in Section 2.2, in the A-trees, MBS radius is not stored in non-leaf nodes. ω and $P_{centroid}$ is used only for the insertion or deletion of data objects. Since the search algorithm uses only M, ptr and $sc(V)$, the data of ptr and $sc(V)$ is clustered together in the implementation. This method of implementation allows larger fanout of ptrs and faster access to the necessary data in searching.

4. The root node:

   The root node has entries of the form: $(ptr, sc(V), \omega, P_{centroid})$, where ptr is the pointer to a child node C, V is the VBR of the MBR

contained in C, ω is the number of all data objects contained in the subtree rooted by C, and $P_{centroid}$ is the centroid of the data objects in the subtree.

3.3 Full Utilization

For data-partitioning index trees, the number of entries is less than the maximum number of entry slots in most of the nodes.[2] That is, there are many empty slots in index nodes. We present a new technique, **full utilization**, which fully uses all disk pages in an A-tree structure. With this technique, blank disk space is equitably distributed among all entries in a node. The distributed space is then unevenly assigned to each dimension in an entry. The amount of assigned space in an entry depends on the edge length of the parent MBR. Dimensions along which the MBR has longer edge have higher priority and a large number of bits are assigned to the dimensions. This assignment reduces the approximation error.

Let e_{max} be the maximum number of entry slots in a node. A node has available space of size $l \cdot n \cdot e_{max}$ for entire entry slots, where l is the length of subspace code and n is the dimension of the space. In the full utilization, this space is evenly shared by entries. Hence, if e is the number of stored entries in a node, each entry is assigned a space of the length:

$$L_{entry} = \frac{l \cdot n \cdot e_{max}}{e}$$

Note that the code of length L_{entry} is equitably assigned to each entry. If E_i is the edge length of a parent MBR on the i-th dimension ($i = 1, \ldots, n$), the code length for approximating the i-th position coordinate in an entry is determined as:

$$L_i = \log_2 \left(E_i \cdot \sqrt[n]{\frac{2^{L_{entry}}}{\prod_{j=1}^{n} E_j}} \right)$$

Code length is calculated in every accessed node for the search and the updating of an A-tree with full utilization.

3.4 Searching

Figure 4 shows the k-nearest neighbor search algorithm for the A-tree, which is an improvement on the algorithm in [9]. In the algorithm of [9], which uses traditional tree structures, `MINDIST` (i.e. minimum distance) between MBRs in a node and a given query point are calculated and kept in a priority queue. The priority queue is sorted in the ascending order of `MINDIST`. Nodes are visited from the top of the queue until the queue becomes empty. Also, a list is maintained to keep k-nearest objects found during the execution of the algorithm. The priority queue is pruned

[2] The exception is the Hilbert R-tree [10]; this method can utilize about 100 % page space.

```
Procedure search(point query, integer k)
 1. enqueue(a_pointer_to_the_root, 0);
 2. for i = 1 to k,
              NNOL[i] := (node: dummy, dist: ∞);
 3. for i = 1 to k, NNVL[i] := ∞;
 4. while emptyQueue() = false do
 5.   N := dequeue();
 6.   if N is a data node then
 7.     for each entry ∈ N do
 8.       if DIST(query, entry.vector) ≤
                                NNOL[k].dist then
 9.         NNOL[k].node := entry.oid;
10.         NNOL[k].dist :=
                        DIST(query, entry.vector);
11.         sort NNOL by dist;
12.         pruneQueue(NNOL[k].dist);
13.       endif
14.     enddo
15.   else      // N is an index node
16.     for each entry ∈ N do
17.       vbr := decode(N.MBR, entry.sc(VBR));
18.       if MINDIST(query, vbr) ≤ NNOL[k].dist
           and MINDIST(query, vbr) ≤ NNVL[k]
           then
19.         enqueue(entry.ptr, MINDIST(query, vbr));
20.         if N is a leaf node and
             MAXDIST(query, vbr) ≤ NNVL[k] then
21.           NNVL[k] := MAXDIST(query, vbr);
22.           sort NNVL;
23.           pruneQueue(NNVL[k]);
24.         endif
25.       endif
26.     enddo
27.   endif
28. enddo
29. output(NNOL);    // output the result
```

Figure 4: k-nearest neighbor search algorithm.

by eliminating nodes whose distance to the query is longer than that of the k-th nearest neighbor object in the list.

In the priority queue of the search algorithm of the A-tree, pairs of a pointer to a node and a distance are kept. The queue is sorted in the ascending order of the distance. Since the sort of queue incurs high CPU cost if a substantial amount of data is stored in the queue, the search algorithm performs filtering using two nearest neighbor lists. One is the usual nearest neighbor list created using the algorithm of [9]. Candidate data objects and their distance from the query point are stored in this list. It is called the **NNOL** (Nearest Neighbor Object List) in this paper. The other list stores the maximum distance from the query point to VBRs of data objects, and is called the **NNVL** (Nearest Neighbor VBR List.)

In Procedure *search* (see Figure 4), as an initialization, the pair of a pointer to the root and 0 is stored in the priority queue (step 1). In step 5, the function `dequeue()` dequeues the pair from the top of the pri-

ority queue, extracts a pointer to a node from the pair, traverses the extracted pointer, and fetch a node. If a fetched node is an index node, the positions of VBRs are calculated from the MBR of the node and the subspace codes for all entries by the function `decode()` (step 17). If the distance between *query* and a VBR is less than or equal to the k-th distance in NNOL (and the k-th distance in NNVL), the function `enqueue()` inserts the pair of the pointer to the corresponding child node and the distance into the queue, then sort the queue in the ascending order of the distance. (steps 18 and 19). In steps 20 to 24, `MAXDIST`(*query*, *vbr*), the maximum distance from *query* to each VBR, is calculated. Moreover, if the distance is less than or equal to the k-th distance in NNVL, NNVL is updated and the function `pruneQueue()` is executed. This function reduces the queue size by eliminating pairs in the queue whose distance to *query* is longer than the argument.

If the extracted node is a data node, data objects in the node are examined (steps 6 and 7). If the distance between *query* and the data object is less than or equal to the k-th nearest neighbor object found so far, the data object together with its distance is stored in NNOL as a nearest neighbor candidate (steps 8, 9, 10), and NNOL is sorted (step 11). Furthermore, queue filtering is performed using NNOL (step 12).

We explain the search algorithm using Figure 3(a) as an example. First, VBRs $V1$ and $V2$ are calculated from the position coordinates of R, $sc(V1)$ and $sc(V2)$. If the distance from the query point to $V1$ is less or equal to the distance to the k-th nearest neighbor, the node which contains $M1$ is fetched, then VBRs $V3$ and $V4$ are calculated from $M1$, $sc(V3)$ and $sc(V4)$. Similarly, the calculated VBRs are compared to the k-th nearest neighbor. If $V3$ is not subject to pruning, the node which contains $M3$ is fetched, then the VBRs $C1$ and $C2$ are calculated from $M3$, $sc(C1)$ and $sc(C2)$, and the calculated VBRs are compared to the k-th nearest neighbor. Moreover, `MAXDIST` from the query point to $C1$ and to $C2$ are stored in NNVL. If $C1$ is not subject to pruning, $P1$ is accessed.

3.5 Updating

The update algorithm of the A-tree is based on that of the SR-tree. Starting from data object insertion or deletion, it propagates upward while adjusting MBRs and centroids in non-leaf nodes. The difference between the A-tree and the SR-tree is that the A-tree algorithm needs to calculate and update the codes of VBRs. Concretely, the A-tree structure is updated as follows:

(1) Let N be a data node, and M be the MBR of N. Then, M is stored in the parent node of N. If a data object insertion or deletion occurs in N, adjust M and the centroid of all data objects contained in N.

(2) If M is unchanged, calculate the code of the VBR that approximates the inserted object from M, and update. Otherwise, update the codes of all VBRs stored in the parent node of N.

(3) Let N be an index node, and M be the MBR of N. If a data object insertion or deletion occurs in the subtree whose top node is N, update the centroid of all data objects contained in the subtree, which is stored in the parent node of N. Moreover, if the insertion or deletion causes a change in a child MBR, adjust M.

(4) If M is unchanged, calculate the code of the VBR that approximates the updated child MBR from M, and update. Otherwise, update the codes of all VBRs stored in the parent node of N.

On structures with full utilization, code length for approximating MBRs or data objects in each node varies according to circumstances. Therefore, if the MBR or the number of entries in a node is changed, the codes for all entries in the node must be calculated. Concretely, the A-tree with full utilization performs (2') and (4') instead of (2) and (4):

(2') If M and the number of entries in N are unchanged, calculate the code of the VBR that approximates the inserted object, and update. Otherwise, calculate the code length assigned to each dimension for approximating all data objects from M and the number of entries, and update the codes of all VBRs stored in the parent node of N.

(4') If M and the number of entries in N are unchanged, calculate the code of the VBR that approximates the updated child MBR, and update. Otherwise, calculate the code length assigned to each dimension for approximating all children MBRs, and update the codes of all VBRs stored in the parent node of N.

4 Performance Test

To verify the effectiveness of the A-tree, we implemented the algorithm and compared our proposed method with the VA-File and the SR-tree. The experiments used three data sets:

(1) Uniformly distributed data sets
Random point sets uniformly distributed in the range [0.1) in each dimension.

(2) Real data sets
Feature vectors of Hue histograms extracted from color images.

(3) Cluster data sets
For cluster data sets, the number of clusters is 100 in each data set and the center of cluster is

Table 1: Maximum number of entry slots in SR-trees.

Dimensionality	4	8	16	24	32
Non-leaf	73	39	20	13	10
Leaf	227	120	62	41	31
Dimensionality	40	48	56	64	
Non-leaf	8	7	6	5	
Leaf	25	21	18	15	

Table 2: Maximum number of entry slots in A-trees.

Dimensionality	4	8	16	24	32
Root	818	511	292	204	157
Intermediate	812	503	283	195	147
Leaf	2706	1342	660	433	319
Dimensionality	40	48	56	64	
Root	127	107	93	81	
Intermediate	117	97	82	71	
Leaf	251	205	173	149	

distributed uniformly in the range [0.10). In addition, as the number of objects is N, $N/100$ objects are gathered according to Gaussian distribution around the center of cluster.

In our evaluation, the dimensionality for synthetic and real data is varied from 4 to 64. The size of all data sets is 100,000. The page size is 8KB. For the A-tree and the SR-tree, one node occupies one page (i.e. 8KB) because both indices give the best search performance under this configuration. In assessing search performance, the page access number and CPU-time were measured by the average of 1,000 queries. Query points were generated randomly and independently of data points in indices. 20-nearest neighbor queries are used. CPU-time was measured on a SUN UltraSPARC-II 296MHz. The search performance of the SR-tree was measured using the algorithm presented in [9], which outperforms the branch-and-bound R-tree traversal algorithm [14] as shown in [3]. As for insertion, the average cost for 1,000 insertions was measured; 1,000 objects not included in the indices were inserted into the data sets. The maximum number of entry slots in SR-trees is shown in Table 1. For the A-tree, the most superior structure from among five variants, $l = 4$, $l = 6$, $l = 8$, $l = 10$ and $l = 12$, was chosen. The maximum number of entry slots in A-trees of code length $l = 6$, is shown in Table 2 as an example.

4.1 Search Performance

Figure 5 shows a comparison of the A-tree with the VA-File and the SR-tree. The comparison used code lengths of $l(\in \{4, 6, 8, 10, 12\})$ of the A-tree because these values yield the best search performance for the different levels of dimensionality. The optimum code length for uniformly distributed data sets was $l = 12$ for 4 dimensions, and $l = 4$ for dimensions from 8 to 64. For real data sets, the code lengths selected were $l = 12$ for 4 dimensions, $l = 8$ for 8 dimensions, $l = 6$ for dimensions from 16 to 64. Also, for clustered data sets, the optimum code length was $l = 12$ for 4 dimensions, $l = 6$ for dimensions from 8 to 64. For the comparison shown in Figure 5, we selected the best code length for each dimension. Also, for the VA-File, the most superior approximation file from among three variants, $l = 4$, $l = 6$ and $l = 8$, was chosen according to [18].

As shown in Figure 5, in all data sets ranging in dimensionality from 4 to 64, the effectiveness of the A-tree is obvious. The A-tree is almost equal to the VA-File with uniform data sets, and greatly outperforms the other structures for non-uniformly distributed data sets such as real data sets. The A-tree is extremely effective for non-uniformly distributed data sets in particular. For example, the A-tree needs 77.3 % (77.7 %) fewer accesses than the SR-tree (the VA-File) for real data sets with 64 dimensions.

Figure 6 shows the effectiveness of full utilization. Although both A-trees have the same organization, their coding differs. Since full utilization distributes blank disk space among all entries in a node for coding, the approximation errors of VBRs are reduced. Accordingly, this technique decreases the search cost of the A-tree.

The experimental results in the rest of the paper are based on real data sets.

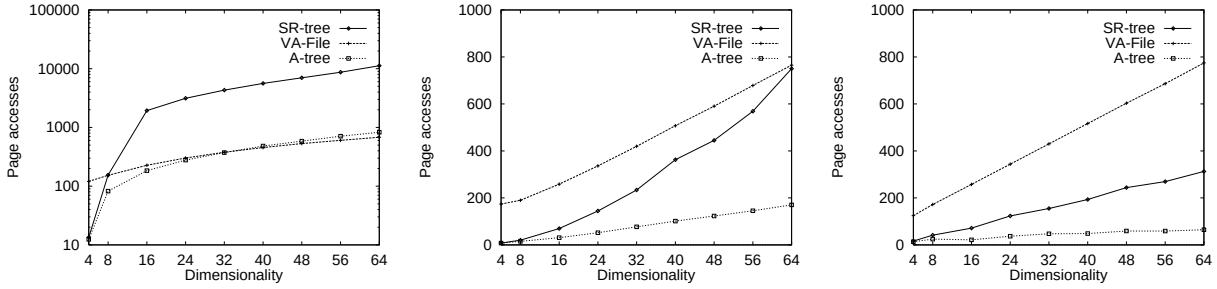
4.2 Superiority of the A-tree

4.2.1 Comparison of the A-tree with the SR-tree

Figure 7 shows the number of page accesses to index nodes of the A-tree and non-leaf nodes of the SR-tree. Also, Figure 8 shows the page accesses to data nodes of the A-tree and leaf nodes of the SR-tree. As shown in these figures, the A-tree requires remarkably fewer accesses to both index nodes and data nodes compared with the SR-tree. Moreover, the difference between the two curves increases with dimensionality. Confirming the position stated in Section 2.1, one of the most significant problems with the SR-tree is its high search cost for non-leaf node accesses because both MBRs and MBSs are stored in non-leaf nodes. Since the A-tree is based on relative approximation, the cost of storing VBRs is small. This property leads to higher performance.

4.2.2 Approximation Error with Variable Length Code

VBRs include approximation error which could degenerates the search performance of the A-tree. There is a tradeoff between approximation error and the length of subspace code. We measured the approximation



(a)Uniformly distributed data sets (b)Real data sets (c)Clustered data sets

Figure 5: Number of page accesses versus dimensionality.

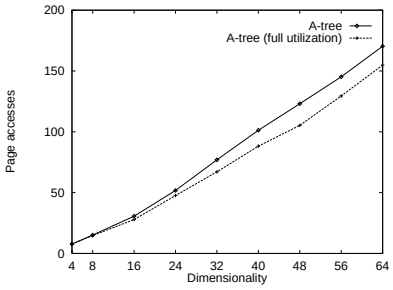


Figure 6: Number of page accesses for the structure with full utilization.

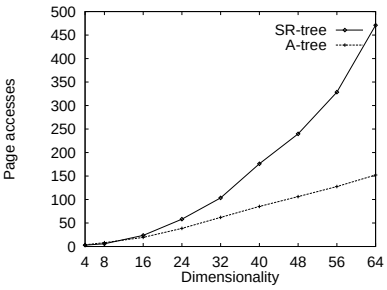


Figure 7: Number of page accesses to index nodes of the A-tree and non-leaf nodes of the SR-tree.

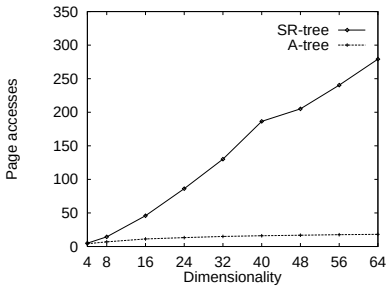


Figure 8: Number of page accesses to data nodes of the A-tree and leaf nodes of the SR-tree.

error of the distance between query points and visited VBRs in the root and intermediate nodes during search. Figure 9 plots the error of MBR approximation against dimensionality for different code lengths. Note the logarithmic scale of the vertical axis in this figure. We defined the approximation error ϵ of the distance as follows:

$$\epsilon = (1 - r) \cdot 100, \quad r = \frac{1}{S} \sum_{i=1}^{S} \frac{\|\boldsymbol{p}, V_i\|}{\|\boldsymbol{p}, M_i\|}$$

where $\boldsymbol{p}$ is a query point and S is the number of visited VBRs in the root and intermediate nodes during search. V_i are the visited VBRs, and $\|\boldsymbol{p}, V_i\|$ is the distance between $\boldsymbol{p}$ and V_i. M_i are the MBR corresponding to V_i. ϵ was measured by the average of 1,000 queries.

Figure 9 shows that the approximation errors versus dimensionality for the A-trees with $l = 4$, $l = 6$ and $l = 8$. In the structures with $l = 4$, $l = 6$ and $l = 8$, the distance decreases by about 10 %, 2 % and 0.7 %, respectively. The approximation error decreases significantly as the length of the code increases. However, on the other hand, longer codes cause smaller fanout of nodes, thus could degenerate search performance. Hence, there is an optimum code length in terms of search performance. As described in Section 4.1, in our experimental setting, the optimum code length changes from $l = 4$ to 12 depending on the dimensionality and distribution of data sets. In A-trees with optimum code length, the effect of reducing the entry size outweighs the influence of VBR error; consequently, fewer node accesses are required.

4.2.3 Comparison of the A-tree with the VA-File

This section explains why the A-tree is superior to the VA-File. Although both the A-tree and the VA-File employ a common idea of approximating position coordinates, their data structures and algorithms are completely different. In the A-tree, the approximation is calculated in terms of a parent MBR. Therefore, as the level of nodes goes down to the leaves, smaller VBRs are used for approximation. This property is in clear contrast to the approximation computed by the entire space in the VA-File. The difference of data structures causes the difference in accuracy of data object approximation. Figure 10 shows the average edge length of VBRs for data objects. In the VA-File, the edge of each cell occupies the interval 2^{-l}. When compared with the VA-File, the A-tree provides high accuracy for VBRs as shown in the figure. Consequently, fewer data object accesses are required and the search cost is reduced. Figure 11 gives the number of object accesses as a function of dimensionality. As expected, the difference in data object access number between the A-tree and the VA-File is significant.

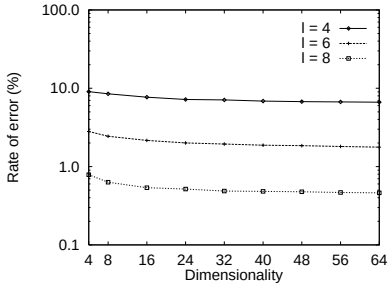


Figure 9: Approximation error in the distance between query points and VBRs in root and intermediate nodes.

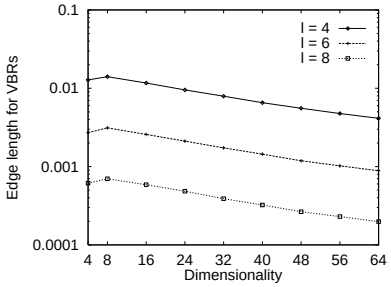


Figure 10: Edge length of VBRs in leaf nodes.

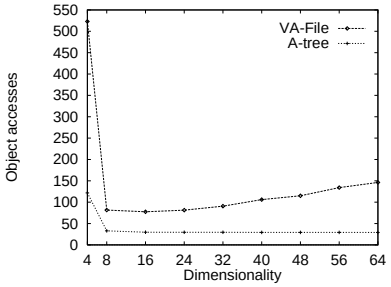


Figure 11: Number of object accesses versus dimensionality.

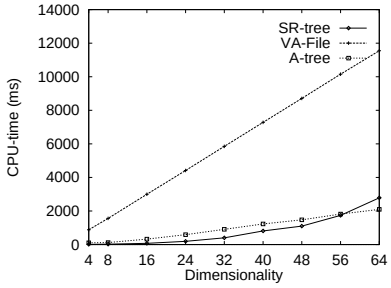


Figure 12: CPU time for search.

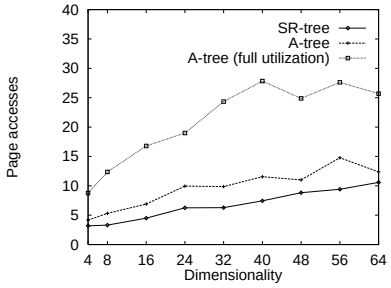


Figure 13: Page accesses for insertion.

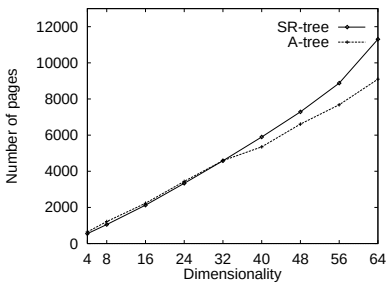


Figure 14: Storage cost.

4.3 Evaluation of CPU-time

Figure 12 shows the CPU-time measured for the VA-File, the SR-tree, and the A-tree. CPU-time was measured using the same conditions used in Figure 5(b). The figure indicates that the A-tree is superior in terms of CPU-time. For 64 dimensions, the performance of the A-tree is almost equal to that of the SR-tree, and it outperforms the VA-File by 81.8 %.

Since the VA-File must calculate the approximated position coordinates for all objects, its CPU-time is much higher than the A-tree as shown in Figure 12. On the other hand, although the A-tree needs to calculate VBRs, the CPU-time of the A-tree is lower than that of the VA-File for the following reason. Since the number of node accesses is extremely low, calculation and comparison of the distances from the query point are reduced. Therefore, the A-tree requires less CPU time even though it must calculate VBRs. In addition, the search algorithm filters the queue using two nearest neighbor lists in order to lower CPU cost. This filtering lowers queue length and provides a valuable contribution to the reduction in CPU-time. As a result, the A-tree provides reasonable CPU cost.

4.4 Insertion Cost

Figure 13 compares the A-tree with the SR-tree in terms of insertion cost under the same conditions as used in Figure 5(b). Insertion cost was measured as the average cost of inserting 1,000 randomly-selected objects. Random objects were used because inserted objects are usually unpredictable in practical situations.

Since the A-tree must access VBRs in addition to MBRs and data objects to maintain the structure, the A-tree incurs larger insertion cost than the SR-tree. However, the increase in cost for the A-tree without full utilization is modest. On the other hand, the A-tree with full utilization considerably increases insertion cost. Since full utilization provides lower search cost, this method is suitable for static data set.

4.5 Storage Cost

Figure 14 compares the storage cost of the A-tree to that of the SR-tree under the same conditions as used in Figure 5(b). The A-tree and the SR-tree incur similar storage costs for 4 to 32 dimensions, but the A-tree incurs 19.5 % less cost for 64 dimensions. The storage cost of the A-tree is low even though it includes VBRs. There are two reasons for this. First, VBRs need only small storage volumes. Second, the number of index nodes in the A-tree is extremely small due to its larger fanout.

5 Conclusions

This paper has presented the A-tree (approximation tree) which offers excellent performance in searching

for data in high-dimensional spaces. First, we analyzed the VA-File and the SR-tree, existing structures used for high-dimensional searching, and discussed their problems. Based on this analysis, we developed the A-tree to overcome the problems and so achieve higher search performance.

The A-tree achieves high performance due to its use of relative approximation. Since the A-tree index nodes contain VBRs, whose storage size is low, the volume of entries in the nodes is reduced which yields improved search performance. Although VBRs include approximation error in terms of size, the error is reduced by the mechanism of relative approximation. By using this mechanism, A-tree bests the alternative search methods, the VA-File and the SR-tree.

The mechanism of the A-tree is remarkably efficient, especially for non-uniformly distributed data sets such as real data sets. For non-uniformly distributed data sets, the A-tree outperforms the SR-tree and the VA-File in all dimensions up to 64, which is the highest dimension examined in our experiments. The A-tree requires 77.3 % (77.7 %) fewer page accesses than the SR-tree (the VA-File) for real data with 64-dimensions.

We also present a new technique, full utilization, which fully uses all disk pages in an A-tree structure. This technique provides higher search performance since the approximation errors of VBRs are reduced.

VBRs approximate MBRs and data objects, however, searches yield exact solutions, that is, the A-tree finds the desired objects without omission. The search performance of the A-tree is greatly improved, and its storage cost is low. Thus, this method well supports practical applications.

References

[1] S. Arya, D. M. Mount, N. S. Netanyahu, R. Silverman, and A. Y. Wu. An Optimal Algorithm for Approximate Nearest Neighbor Searching. In *Proc. of ACM-SIAM Symposium on Discrete Algorithms*, pp. 573–582, 1994.

[2] N. Beckmann, H. P. Kriegel, R. Schneider, and B. Seeger. The R*-tree: An Efficient and Robust Access Method for Points and Rectangles. In *Proc. ACM SIGMOD Conf.*, pp. 322–331, Atlantic City, NJ, May 1990.

[3] S. Berchtold, C. Böhm, D. A. Keim, and H.-P. Kriegel. A Cost Model For Nearest Neighbor Search in High-Dimensional Data Space. In *Proc. ACM Symp. on Principles of Database Systems*, pp. 78–86, March 1997.

[4] S. Berchtold, C. Böhm, H. V. Jagadish, H.-P. Kriegel, and J. Sander. Independent Quantization: An Index Compression Technique for High-Dimensional Data Spaces. In *Proc. of IEEE 16th International Conference on Data Engineering*, pp. 577–588, 2000.

[5] S. Berchtold, D. A. Keim, and H.-P. Kriegel. The X-tree: An Index Structure for High-Dimensional Data. In *Proc. of the 22nd International Conference on Very Large Data Bases (VLDB)*, pp. 28–39, Bombay, September 1996.

[6] V. Gaede and O. Günther. Multidimensional Access Methods. *ACM Computing Surveys*, Vol. 30, No. 2, pp. 170–231, June 1998.

[7] A. Gionis, P. Indyk, and R. Motwani. Similarity Search in High Dimensions via Hashing. In *Proc. of the 25th International Conference on Very Large Data Bases (VLDB)*, Edinburgh, Scotland, September 1999.

[8] A. Guttman. R-Trees: A Dynamic Index Structure for Spatial Searching. In *Proc. ACM SIGMOD Conf.*, pp. 47–57, Boston, MA, June 1984. Reprinted in M. Stonebraker, Readings in Database Sys., Morgan Kaufmann, San Mateo, CA, 1988.

[9] G. R. Hjaltason and H. Samet. Ranking in Spatial Databases. In *Proceedings of the 4th Symposium on Spatial Databases*, pp. 83–95, Portland, Maine, August 1995.

[10] I. Kamel and C. Faloutsos. Hilbert R-tree: An Improved R-tree using Fractals. In *Proceedings of the Twentieth International Conference on Very Large Databases*, pp. 500–509, Santiago, Chile, 1994.

[11] N. Katayama and S. Satoh. The SR-tree: An Index Structure for High-Dimensional Nearest Neighbor Queries. In *Proc. ACM SIGMOD International Conference on Management of Data*, pp. 369–380, May 1997.

[12] H. Murase and S. Nayar. Visual Learning and Recognition of 3-D Objects from Appearance. *International Journal of Computer Vision*, Vol. 14, No. 1, pp. 5–24, 1995.

[13] A. Pentland, B. Moghaddam, and T. Starner. View-Based and Modular Eigenspaces for Face Recognition. In *Proc. IEEE Conf. on CVPR*, pp. 84–91, Seattle, Washington, June 1994.

[14] N. Roussopoulos, S. Kelley, and F. Vincent. Nearest Neighbor Queries. In *Proc. ACM SIGMOD International Conference on Management of Data*, pp. 71–79, May 1995.

[15] Y. Sakurai, M. Yoshikawa, S. Uemura, and H. Kojima. The A-tree: An Index Structure for High-Dimensional Spaces Using Relative Approximation. Technical report, Nara Institute of Science and Technology, 2000.

[16] T. K. Sellis, N. Roussopoulos, and C. Faloutsos. Multidimensional Access Methods: Trees Have Grown Everywhere. In *Proc. of the 23rd International Conference on Very Large Data Bases (VLDB)*, pp. 13—14, Athens, August 1997.

[17] H. D. Wactlar, T. Kanade, M. A. Smith, and S. M. Stevens. Intelligent Access to Digital Video: Informedia Project. *IEEE Computer*, Vol. 29, No. 5, pp. 46–52, May 1996.

[18] R. Weber, H.-J. Schek, and S. Blott. A Quantitative Analysis and Performance Study for Similarity-Search Methods in High-Dimensional Spaces. In *Proc. of the 24th International Conference on Very Large Data Bases (VLDB)*, pp. 194–205, New York City, NY, August 1998.

[19] D. A. White and R. Jain. Similarity Indexing with the SS-tree. In *Proc. of IEEE 12th International Conference on Data Engineering*, pp. 516–523, 1996.