Hierarchical Subspace Sampling: A Unified Framework for High Dimensional Data Reduction, Selectivity Estimation and Nearest Neighbor Search

Charu C. Aggarwal
IBM T. J. Watson Research Center
Yorktown Heights, NY 10598
charu@us.ibm.com

ABSTRACT

With the increased abilities for automated data collection made possible by modern technology, the typical sizes of data collections have continued to grow in recent years. In such cases, it may be desirable to store the data in a reduced format in order to improve the storage, transfer time, and processing requirements on the data. One of the challenges of designing effective data compression techniques is to be able to preserve the ability to use the reduced format directly for a wide range of database and data mining applications. In this paper, we propose the novel idea of hierarchical subspace sampling in order to create a reduced representation of the data. The method is naturally able to estimate the local implicit dimensionalities of each point very effectively, and thereby create a variable dimensionality reduced representation of the data. Such a technique has the advantage that it is very adaptive about adjusting its representation depending upon the behavior of the immediate locality of a data point. An interesting property of the subspace sampling technique is that unlike all other data reduction techniques, the overall efficiency of compression *improves* with increasing database size. This is a highly desirable property for any data reduction system since the problem itself is motivated by the large size of data sets. Because of its sampling approach, the procedure is extremely fast and scales linearly both with data set size and dimensionality. Furthermore, the subspace sampling technique is able to reveal important local subspace characteristics of high dimensional data which can be harnessed for effective solutions to problems such as selectivity estimation and approximate nearest neighbor search.

1. INTRODUCTION

In recent years, the advances in hardware technology have made it possible to collect large amounts of data in many applications. Such data sets are often very high dimensional. Examples of such domains include supermarket data, multimedia data and telecommunication applications. This often results in massive data tables whose sizes are of the order of tera-bytes. In such cases, it is desirable to reduce the data in order to save on critical system resources such as storage space and transfer time of large files. In addition, many database applications can be implemented more efficiently on reduced representations of the data.

A well known technique for dimensionality reduction is the method of Singular Value Decomposition [9, 15] (SVD), which projects the data into a lower dimensional subspace. The idea is to transform the data into a new orthonormal coordinate system in which the second order correlations are eliminated. In typical applications, the resulting axis-system has the property that the variance of the data along many of the new dimensions is very small [15]. These dimensions can then be eliminated, a process resulting in a compact representation of the data with some loss of representational accuracy. However, the dimensionality reduction technique does not provide hard bounds on the deviation of a record from its true value, and is prohibitively expensive for increasing data dimensionality. Even though a variety of other compression techniques [4, 12, 19] provide such guarantees, dimensionality reduction methods are more popular because of their use of multidimensional representations for the compressed format. Such representations allow the use of database applications such as indexing directly on the reduced representation without a first phase of reconstruction. On the other hand, the multidimensional representation is also a constraint which reduces the effectiveness of the reduction process. This inflexibility also makes it difficult for standard dimensionality reduction techniques to provide worst-case guarantees of the reduction loss of each record. Furthermore, the high computational requirements of the dimensionality reduction method reduce the applicability of the approach for large and high dimensional databases.

Recent research has shown that even though the implicit dimensionality of a given data set may be quite high, particular subsets of it may show data dependencies which lead to much lower implicit dimensionality [2, 7]. An effective data compression system would try to optimize the representation of a record depending upon the distribution of the data in its locality. Clearly, it is a non-trivial task to find a representation in which each point adjusts its storage

requirements naturally to the corresponding local implicit dimensionality. Since the issue of data reduction is most relevant in the context of large data sets, it is also necessary for the computational and representational requirements of such approaches to scale efficiently with increasing data size. Unfortunately, the techniques in [2, 7] are orders of magnitude slower than even the standard dimensionality reduction techniques, and are inflexible in determining the dimensionality of data representation. Therefore these methods are restricted in applicability to specific problems such as indexing.

In recent years, random projection [1, 14] has been used as an efficient alternative for dimensionality reduction of high dimensional data sets. These techniques typically use spherically symmetric projections, in which arbitrary directions from the data space are sampled repeatedly in order to create a new axis system for data representation. While random projection is a much more efficient process than methods such as SVD, its average reduction quality is a little less effective. In this paper, we investigate the use of subspace sampling approaches in which the subspaces picked are determined by the (local) properties of the particular data set at hand. The use of a locality sensitive random sampling approach results in a system which is *both more effective and efficient* than SVD, while providing worst case bounds on the error loss of each record. The locality sensitive sampling method uses a hierarchical subspace sampling approach in which the storage requirement of each data point is influenced by the corresponding local implicit dimensionality. This variation from the global approach of standard dimensionality reduction methods has the interesting property that local implicit dimensionalities can be estimated more robustly for larger data sets. *As a result, the effectiveness of reduction improves with increasing database size.* We note that this is a unique feature over any known dimensionality reduction technique. It is also especially important in the context of larger data sets which are the motivating factor for the dimensionality reduction problem.

In addition, we will show that the local characteristics of the data revealed by the hierarchical subspace sampling technique can be effectively leveraged for innovative solutions to problems such as selectivity estimation and nearest neighbor indexing. The selectivity estimation problem is motivated by the time-consuming nature of the query resolution problem in very large databases. In such cases, it may be desirable to estimate the sizes of the query responses, rather than resolve the query itself. Typical approaches to the selectivity estimation problem such as histograms work well in low dimensionality, but degrade rapidly with increasing dimensionality because of dependencies among attributes [8, 10, 18]. In this paper, we will show that the local characteristics of the data revealed by the subspace sampling technique can be utilized in order to improve the effectiveness of the selectivity estimation procedure. We will also demonstrate similar results for the approximate nearest neighbor search problem.

In order to facilitate further development of the ideas, we will introduce additional notations and definitions. We assume that the data set is denoted by $\mathcal{D}$. The number of points in the data set is denoted by N and the dimensionality by d. The full dimensional data space is denoted by $\mathcal{U}$. We define the l-dimensional hyperplane $\mathcal{H}(\overline{y}, \mathcal{E})$ by an anchor $\overline{y}$ and a mutually orthogonal set of vectors $\mathcal{E} = \{\overline{e}_1 \ldots \overline{e}_l\}$. The hyperplane passes through $\overline{y}$, and the vectors in $\mathcal{E}$ form the basis system for its subspace. The projection of a point $\overline{x}$ onto this hyperplane is denoted by $\mathcal{P}(\overline{x}, \overline{y}, \mathcal{E})$ and is the closest approximation of $\overline{x}$, which lies on this hyperplane. In order to find the value of $\mathcal{P}(\overline{x}, \overline{y}, \mathcal{E})$, we use $\overline{y}$ as the reference point[1] for the computation. Specifically, we determine the projections of $\overline{x} - \overline{y}$ onto the $\{\overline{e_1} \ldots \overline{e_l}\}$. Then, we translate the resulting point by the reference point $\overline{y}$. Therefore, we have:

$$\mathcal{P}(\overline{x}, \overline{y}, \mathcal{E}) = \overline{y} + \sum_{i=1}^{l} [(\overline{x} - \overline{y}) \cdot \overline{e_i}] \, \overline{e_i} \tag{1}$$

We have illustrated a pictorial representation of $\overline{x'} = \mathcal{P}(\overline{x}, \overline{y}, \mathcal{E})$ in Figure 1. We note that $\overline{x'}$ can be represented in the orthonormal axis system for $\mathcal{E}$ with the use of only l cooordinates $((\overline{x} - \overline{y}) \cdot \overline{e_1} \ldots (\overline{x} - \overline{y}) \cdot \overline{e_l}))$. This incurs the additional overhead of maintaining $\overline{y}$ and $\mathcal{E}$. This is however a constant storage overhead, which can be amortized over the large number of points stored on this hyperplane. The error of approximating $\overline{x}$ with $\mathcal{P}(\overline{x}, \overline{y}, \mathcal{E})$ is given by the euclidean distance between $\overline{x}$ and $\mathcal{P}(\overline{x}, \overline{y}, \mathcal{E})$ and is denoted by $\Delta(\overline{x}, \overline{y}, \mathcal{E})$. The lossy reduction system discussed in this paper will determine locality specific hyperplanes, so that for each data record, this value is less than a pre-specified tolerance ϵ. In other words, for each data point $\overline{x}$ projected into a hyperplane denoted by $(\overline{y}, \mathcal{E})$, we have $\Delta(\overline{x}, \overline{y}, \mathcal{E}) \leq \epsilon$.

This paper is organized as follows. In the next section, we will introduce the hierarchical subspace sampling technique and discuss some of its properties. In section 3, we will discuss how the data is stored in compressed form using the hierarchically sampled subspaces. Section 4 will discuss the application to the nearest neighbor search and selectivity estimation problems. The empirical results are discussed in section 5. Finally, we present the conclusions and summary in section 6.

1.1 Contributions of this paper

This paper introduces an effective and linearly scalable subspace sampling approach to the problem of data reduction. This technique uses a hierarchical partitioning approach in conjunction with a subspace sampling procedure which is sensitive to the data set at hand. The dual nature of this hierarchical partitioning and subspace sampling approach makes the reduction process very effective. While the subspace sampling approach provides a much more compact representation than traditional dimensionality reduction techniques, it also provides hard bounds on the error of the approximation. An interesting and surprising property of the subspace sampling technique is that the compression factor actually *improves* with increasing database size. This is different from most other dimensionality reduction techniques in which the compression ratio is largely unaffected by database size. This behavior with increasing database size is especially significant, since the data reduction problem is motivated by the large size of data sets. The use of a sampling approach also results in a computationally efficient

[1] We always choose a point on the hyperplane as the reference point.

implementation which is almost linearly scalable both with data set size and dimensionality. In addition, the locality specific multi-dimensional representation makes the reduced data friendly to use in database applications such as nearest neighbor search and selectivity estimation. In fact, the subspace sampling method reveals important local characteristics of the data which can be used for effective solutions to these problems. We note that traditional methods for selectivity estimation such as histograms do not provide accurate results for even ten dimensional applications [10], whereas our empirical results indicated that the subspace sampling technique provides accurate results on color-histogram data sets of dimensionality larger than fifty. We will also show that the partitioning created by the hierarchical subspace method can be used for effective nearest neighbor search in a way which is significantly more effective than currently used dimensionality reduction techniques.

2. HIERARCHICAL SUBSPACE SAMPLING

The method of random projections [1, 14] has recently been recognized as an efficient and scalable alternative to dimensionality reduction. These techniques sample[2] spherically symmetric random directions on which the data is projected. Such methods may often require an unnecessarily higher dimensionality to represent the data, since they do not utilize the properties of the particular data set at hand. In order to intuitively understand this point, we will illustrate with the use of 1-dimensional projections of 2-dimensional data. Consider the data set illustrated in Figure 2 in which we have illustrated two kinds of projections. In Figure 2(a), the data *space* is sampled in order to find a 1-dimensional line along which the projection is performed. In data space sampling, random projections are chosen in a spherically symmetric fashion [1, 14] irrespective of the data distribution. The reduced data in this 1-dimensional representation is simply the projection of the data points onto the line, as illustrated in lower diagram of Figure 2(a). Though repeated applications of subspace sampling [1, 14] provide bounds on data reduction quality, it is clear from the above illustration that such a projection may often turn out to be blind to the basic patterns in the data. In the second case of Figure 2(b), we have sampled the *points* in order to create a random projection. The sampled subspace is defined as the $(l-1)$-dimensional hyperplane containing l randomly chosen points from the data. In this case, the chosen subspace is naturally biased by the original data distribution. For example, in Figure 2(b), the 1-dimensional line obtained by sampling two points picks up the directions of greater variance more effectively than the space-sampled random projection of Figure 2(a). For this reason, the quality of the reduction for Figure 2(b) is significantly better than that in Figure 2(a).

While it is intuitively clear that point sampling is more effective than space sampling for variance preservation, the advantages are limited when the data distribution varies considerably with locality. For example, in Figure 3(a), even the optimal 1-dimensional random projection cannot represent all points without losing a substantial amount of variance of the data. In Figures 3(b) and (c), we have used the random projection technique *locally* in conjunction with data partitioning. In this technique, each data point is projected on the closest of a number of point sampled hyperplanes. It is clear that in the latter cases, the projections of the data points onto the lines are the best approximations. This is because each subspace is optimized to a locally sampled set of points. It is also interesting to see that even though the data is 2-dimensional, it can be (approximately) represented by projections along 1-dimensional lines. This is because the local implicit dimensionality of each data point is only one, once that data has been partitioned appropriately. We also note that there may be some differences in the quality of the final reduction (such as those in Figures 3(b) and (c)) depending upon the subspaces which get sampled, but the final representation always loses less information than a global approach with the same number of samples. This follows from the straightforward observation that when the k hyperplanes $\mathcal{S}_1 \ldots \mathcal{S}_k$ are sampled, the distance of the data point $\overline{x} \in \mathcal{D}$ to the closest of $\mathcal{S}_1 \ldots \mathcal{S}_k$ is always at most the distance loss of $\overline{x}$ when only one of these hyperplanes (say $\mathcal{S}_i$) is chosen for reduction of each data point in $\mathcal{D}$.

On the other hand, the improvements of the localized subspace sampling technique come at the additional storage costs of the different hyperplanes. This limits the number of hyperplanes which can be retained from the sampling process, and requires us to make judicious choices in picking these hyperplanes. A second important issue is that even the implicit dimensionalities of the different data localities may be different. Therefore, we need a mechanism by which the sampling process is able to effectively choose hyperplanes of the lowest possible dimensionality for each data locality. This is an issue which we will discuss after developing some additional notational machinery:

DEFINITION 2.1. *Let $P = (\overline{x_1} \ldots \overline{x_{l+1}})$ be a set of $(l+1)$ linearly independent points. The representative hyperplane $\mathcal{R}(P)$ of P is defined as the l-dimensional hyperplane which passes through each of these $(l+1)$ points.*

The hyperplane $R(P)$ can also be represented with the use of any point $\overline{y}$ on the hyperplane, and an orthonormal set of vectors $\mathcal{E} = \{\overline{e_1} \ldots \overline{e_l}\}$, which lie on the hyperplane. We shall call $(\overline{y}, \mathcal{E})$ the *axis* representation of the hyperplane, whereas the set P is referred to as the *point* representation. Thus, $\mathcal{R}(P)$ (point representation) is the same as $\mathcal{H}(\overline{y}, \mathcal{E})$ (axis representation). We note that there can be infinitely many point or axis representations of the same hyperplane. The axis representation is more useful for performing distance computations of the hyperplane from individual points in the database, whereas the point representation has advantages in storage efficiency in the context of a hierarchical arrangement of subspaces. We will discuss this issue in a later section.

2.1 The Subspace Tree

In this section, we will introduce the subspace tree, which is a conceptual organization of subspaces used in the data reduction process. This conceptual organization imposes a hierarchical arrangement of the subspaces of different dimensionalities. The hierarchical organization is also useful in de-

[2]The hyperplanes are repeatedly sampled, and the best alternative is picked in order to determine the final representation.

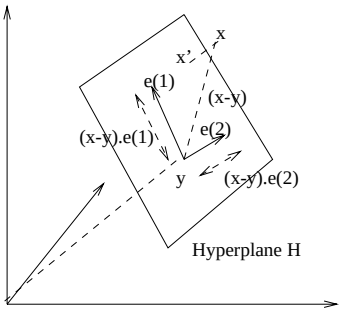


Figure 1: Pictorial Representation of Approximation

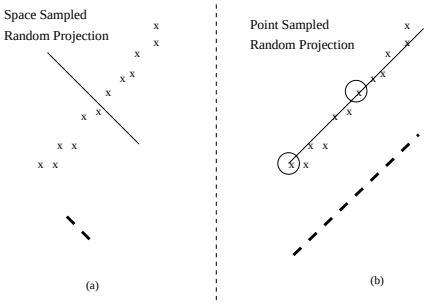


Figure 2: Comparing Point Sampled and Space Sampled Random Projections

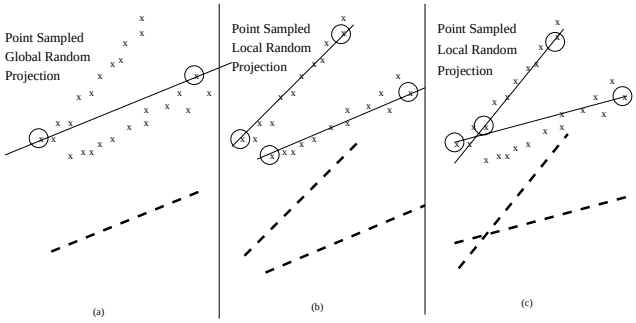


Figure 3: Effects of Data Locality on Subspace Sampling

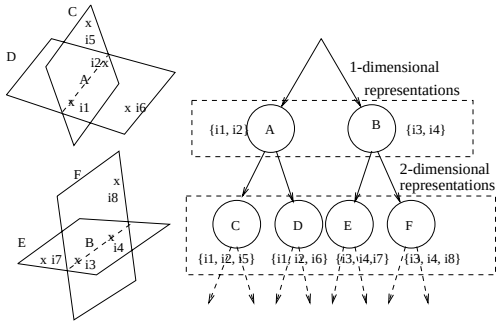


Figure 4: Illustration of the Sampling Procedure

veloping variable dimensionality representations of the data. Each node in the subspace tree corresponds to a hyperplane along with its representative set which is drawn from the database $\mathcal{D}$. The nodes at level-m in the subspace tree correspond[3] to m-dimensional subspaces. The root node corresponds to the null subspace. Thus, the dimensionality of the hyperplane for any node in the tree is determined by its depth. The subspace at a node is hierarchically related to that of its immediate parent. Each subspace other than the null subspace at the root is a 1-dimensional extension of its parent hyperplane. This 1-dimensional extension is obtained by adding a sampled data point to the representative set of the parent hyperplane. In order to elucidate the concept of a subspace tree, we will use an example. In Figure 4, we have illustrated a hierarchically arranged set of subspaces. The figure contains a two-level tree structure which corresponds to 1- and 2-dimensional subspaces. For each level-1 node in the tree, we store two points which correspond to the 1-dimensional line for that node. For each lower level node, we store an additional data point which increases the dimensionality of its parent subspace by 1. Therefore, for a level-m node the representative set is of cardinality $(m+1)$. For example, in the case of Figure 4, the node A in the subspace tree (with representative set $\{i_1, i_2\}$) corresponds to the 1-dimensional line defined by $\{i_1, i_2\}$. This node is extended to a 2-dimensional hyperplane is two possible ways corresponding to the nodes C and D. In each case, an extra point needs to be added to the representative set for creating the 1-dimensional extension. In order to extend to the 2-dimensional hyperplane for node C, we use the point i_5, whereas in order to extend to the hyperplane for node D, we use the point i_6. Note from Figure 4(a) that the intersection of the 2-dimensional hyperplanes C and D is the 1-dimensional line A. The subspace tree is formally defined as follows:

[3]We assume that level 0 corresponds to the root.

DEFINITION 2.2. *The subspace tree is a hierarchical arrangement of subspaces with the following properties: (1) Nodes at level-m correspond to m-dimensional hyperplanes (2) Nodes at level-$(m+1)$ correspond to hyperplanes which are 1-dimensional extensions of their parent hyperplanes at level-m (3) The point representative set of a level-$(m+1)$ node is obtained by adding a sampled data point to the representative set of its m-dimensional parent subspace.*

Once a subspace tree has been constructed, each data point $\overline{x}$ is assigned to a node in this tree, so that the distance of the corresponding hyperplane from $\overline{x}$ is less than the compression tolerance ϵ. The data point $\overline{x}$ is represented in terms of its coordinates on the hyperplane to which it is assigned. Thus, the amount of space needed to represent $\overline{x}$ depends only on the dimensionality of the corresponding hyperplane rather than the dimensionality of $\mathcal{D}$. Since higher levels of the tree require lower storage overhead, it is desirable to assign $\overline{x}$ to as high a level of the tree as possible. We note the following:

OBSERVATION 2.1. *Let S be a set of representative points, and let $\overline{w}$ be a data point which extends the dimensionality of the corresponding hyperplane to that of its child. Let $(\overline{y_1}, \mathcal{E}_1)$*

Algorithm *SampleSubspaceTree(CompressionTolerance: ϵ, MaximumTreeDegree: k_{max}, Database: $\mathcal{D}$, Node Limit: L)*
begin
  Sample $k_{max} * sampfactor$ pairs from $\mathcal{D}$ to create 1-dim. point representative hyperplanes (lines) denoted by $\mathcal{S}$;
  $\mathcal{S} = SampleBestHyperplanes(\mathcal{S}, k_{max})$;
  { Let $S_1 \ldots S_{k_{max}}$ denote the hyperplanes in $\mathcal{S}$ }
  $(\mathcal{T}(S_1), \ldots \mathcal{T}(S_{k_{max}}), \mathcal{Q}(S_1), \ldots \mathcal{Q}(S_{k_{max}})) = AssignData(\mathcal{D}, \mathcal{S})$;
  { Remove nodes with fewer than *min-thresh* points }
  $\mathcal{S} = RemoveNodes(S_1 \ldots S_{k_{max}}, min\text{-}thresh)$;
  { $\mathcal{L}_m$ is the set of level-m nodes }
  $\mathcal{L}_1 = \mathcal{S}$; { Each hyperplane (line) in $\mathcal{S}$ is child of *Root* };
  $m = 1$;
  while ($\mathcal{L}_m \neq \{\}$) and
    (less than L nodes have been generated) **do**
  begin
    for each level-m node $R \in \mathcal{L}_m$ **do**
    begin
      Sample $k_{max} * sampfactor$ points from $\mathcal{T}(R)$;
      Extend node R by each of these $k_{max} * sampfactor$ points (in turn) to create $k_{max} * sampfactor$ $(m+1)$-dimensional hyperplanes $\mathcal{S}$;
      $\mathcal{S} = SampleBestHyperplanes(\mathcal{S}, k_{max})$;
      $(\mathcal{T}(S_1), \ldots \mathcal{T}(S_{k_{max}}), \mathcal{Q}(S_1), \ldots \mathcal{Q}(S_{k_{max}})) = AssignData(\mathcal{T}(R), \mathcal{S})$;
      $\mathcal{S} = RemoveNodes(S_1 \ldots S_{k_{max}}, min\text{-}thresh)$;
      $\mathcal{L}_{m+1} = \mathcal{L}_{m+1} \cup \mathcal{S}$;
    end; $m = m + 1$;
  end;
  Perform final post-processing phase of reassignment of database $\mathcal{D}$ to nodes in subspace tree;
end

Figure 5: Subspace Tree Construction

and $(\overline{y_2}, \mathcal{E}_2)$ be the axis representations of S and $S \cup \{\overline{w}\}$ respectively. Then, for any data point $\overline{z}$, it must be true that $||\overline{z} - \mathcal{P}(\overline{z}, \overline{y_2}, \mathcal{E}_2)|| \leq ||\overline{z} - \mathcal{P}(\overline{z}, \overline{y_1}, \mathcal{E}_1)||$.

The above observation simply states that the distance of the point $\overline{z}$ to a hyperplane $\mathcal{H}(\overline{y_2}, \mathcal{E}_2)$ is lower than the distance to its parent hyperplane $\mathcal{H}(\overline{y_1}, \mathcal{E}_1)$, since the former subsumes the latter. Thus, if the reduced data points are stored in the subspace tree, then as the value of ϵ is reduced, a larger number of points would need to be stored at the lower levels of the tree. Since the storage at lower levels requires a greater number of coordinates for representation, it follows that there is a natural trade-off between the storage requirements and representational accuracy.

2.2 Subspace Tree Construction

In this section, we will show how the subspace tree may be constructed by careful localized sampling of the data points in conjunction with a recursive partitioning of the data. This procedure turns out to be extremely effective in influencing the subspace sampling process so that the resulting subspaces are effectively biased for particular data localities. The input to the subspace sampling algorithm includes the compression tolerance ϵ, and the data set $\mathcal{D}$. The subspace tree is constructed hierarchically in top-down fashion, while also partitioning the data set $\mathcal{D}$ along this hierarchy. The subspace tree construction uses a levelwise algorithm in order to build the tree structure. This is done in order to restrict the number of database passes during the tree construction phase. Each node of the subspace tree corresponds to a hyperplane defined by the sequence of representative points sampled, starting from the root up to that node. Therefore, we will be using the term hyperplane and node interchangeably throughout the discussion of the subspace tree.

At each stage of the algorithm, every node N in the subspace tree has a set of *descendent assignments* $\mathcal{T}(N) \subseteq \mathcal{D}$ from the database $\mathcal{D}$. These are the data points which will be assigned to one of the descendants of node N during the tree construction process. In addition, each node also has a set of *direct assignments* $\mathcal{Q}(N)$, which are data points within the specified tolerance ϵ of the hyperplane corresponding to node N. In each iteration, the descendent assignments $\mathcal{T}(N)$ in each of the nodes at a given level are partitioned further into at most k_{max} children of node N. This partitioning is based on the distance of the data points to the hyperplanes corresponding to the k_{max} children of N. Specifically, each data point is assigned to the hyperplane from which it has the least distance. This results in each point from $\mathcal{T}(N)$ becoming either a direct or descendent assignment of one of these k_{max} children depending upon whether or not it lies within the tolerance factor ϵ of the corresponding hyperplane. This process continues until each data point becomes either the direct assignment of some node or is identified as an outlier. The overall algorithm for subspace tree construction is illustrated in Figure 5.

The subspace tree construction algorithm proceeds in an iterative levelwise fashion. The mth level of the tree is constructed during the mth levelwise phase. The reason for this levelwise approach is that the database operations during the construction of a given level of nodes can be consolidated into a single database pass. The actual construction of the mth level is achieved by sampling one representative point for each of the k_{max} children of the level-$(m-1)$ nodes in order to create the corresponding 1-dimensional extension. However, we also use oversampling in order to improve the quality of the resulting subspaces. The subspace sampling algorithm defines a parameter called *sampfactor*, which is the factor by which we oversample the points at a given node from which the final k_{max} representative extensions are chosen. Thus, a total of $k_{max} * sampfactor$ points are picked for extension of the nodes from level-$(m-1)$ to level-m. Only the first iteration of the algorithm ($m = 1$) is special in which we sample $2 * k_{max} * sampfactor$ points in order to create $k_{max} * sampfactor$ lines. Next, the procedure *SampleBestHyperplanes* picks k_{max} lines out of these $k_{max} * sampfactor$ lines for which the localized projection losses are as low as possible. Details of the *SampleBestHyperplanes* procedure are discussed in subsection 2.3. Once the hyperplanes for the first level nodes have been determined, we assign each point in the database to one of these nodes either as a direct assignment or as a descendent assignment. This is achieved by the procedure *AssignData*, and is discussed in detail in subsection 2.4. We also ensure that those nodes with fewer than *min-thresh* points assigned to them are removed from consideration. These are the outlier nodes which are discarded by the procedure *RemoveNodes*. The assigned points for these nodes are outliers which need to be stored separately by the algorithm. Details of this procedure are discussed in subsection 2.5. As a result, the

final outdegree of the node may be less than k_{max}. The algorithm then proceeds in a levelwise fashion of building level-m of the tree in the same sequence of operations as discussed above for level-1 of the tree. The main difference for $m \geq 2$ is in the methodology for extending the subspaces by a dimensionality of one. In this case, for each node N, we sample $k_{max} * sampfactor$ points from $\mathcal{T}(N)$. The process of sampling the points from $\mathcal{T}(N)$ intentionally biases the children subspaces depending upon the data distribution of $\mathcal{T}(N)$. Further, the purpose of oversampling by a factor of *sampfactor* is to increase the effectiveness of the final children subspaces which are picked. The larger the value of *sampfactor*, the better the sampled subspaces, but the greater the computational requirement. Thus, a total of $k_{max} * sampfactor$ m-dimensional hyperplanes can be generated by combining the representative points from node N with each of these sampled points. In each iteration, the algorithm assigns the data points in a given node N to its closest child. Next, the *SampleBestHyperplanes* procedure picks the k_{max} hyperplanes out of these $k_{max} * sampfactor$ hyperplanes in order to create the most effective partitioning. As in the case of level-1 nodes, the *AssignData* procedure determines the assignments of the data points in the nodes of $\mathcal{T}(N)$ to the respective children. We note that in Figure 5, we have presented the *AssignData* procedure separately for each node for ease in description. In the actual implementation, this procedure is executed simultaneously for all nodes at a given level in one scan. Similarly, the process of picking the best hyperplanes for all nodes at a given level is executed simultaneously in a single scan of the data. We will discuss details of these issues in a later subsection. The process of levelwise tree construction continues until no node in the current level can be extended any further, or the maximum limit L for the number of nodes has been reached. This limit L is governed by the amount of available memory since we would like the subspace tree to be memory-resident for a number of useful applications such as nearest neighbor indexing and selectivity estimation. For our implementation, we used a conservative limit of only $L = 10,000$ nodes, which was well within current main memory limitations for even 1000-dimensional data sets. At the end of the subspace tree construction process, we re-optimized the assignment of each data point $\overline{x}$ by finding the hyperplane at the highest level of the tree for which the distance value was less than ϵ. In many cases, this reduces the data even further by reducing the dimensionality of the representation.

Each of the procedures *SampleBestHyperplanes* and *AssignData* require the computation of distances of data points $\overline{x}$ to the representative hyperplanes. In order to perform these distance computations, the axis representations of the hyperplanes need to be determined. A hyperplane node N at level-m is only implicitly defined by the $(m+1)$ data points $\{\overline{z_1} \ldots \overline{z_{m+1}}\}$ stored at the nodes along the path from the root to N. The next tricky issue is to compute the axis representation $(\overline{y}, \mathcal{E} = \{\overline{e_1} \ldots \overline{e_m}\})$ of the points $\{\overline{z_1} \ldots \overline{z_{m+1}}\}$ efficiently in a way that can be replicated exactly at the time of data reconstruction. This is especially important, since there can be an infinite number of axis representations of the same hyperplane, but the projection coordinates are computed only with respect to a particular axis-representation. The corresponding representation $(\overline{y}, \mathcal{E} = \{\overline{e_1} \ldots \overline{e_m}\})$ is computed in a procedure which is essentially similar to the Gram-Schmidt orthogonalization process [11].

We first set $\overline{y} = \overline{z_1}$ and $\overline{e_1} = (\overline{z_2} - \overline{z_1})/||\overline{z_2} - \overline{z_1}||$. Next, we iteratively compute $\overline{e_i}$ from $\overline{e_1} \ldots \overline{e_{i-1}}$ as follows:

$$e_i = \frac{\overline{z_{i+1}} - \overline{z_1} - \sum_{j=1}^{i-1} [(\overline{z_{i+1}} - \overline{z_1}) \cdot \overline{e_j}] \overline{e_j}}{||\overline{z_{i+1}} - \overline{z_1} - \sum_{j=1}^{i-1} [(\overline{z_{i+1}} - \overline{z_1}) \cdot \overline{e_j}] \overline{e_j}||} \quad (2)$$

It can be shown that the set $(\overline{y}, \mathcal{E})$ generated by the Equation 2 is an axis representation of the hyperplane defined by the points $\{\overline{z_1} \ldots \overline{z_{m+1}}\}$.

Many axis representations can be generated using Equation 2 for the same hyperplane $\mathcal{R}(\{\overline{z_1} \ldots \overline{z_{m+1}}\})$ depending upon the ordering of $\{\overline{z_1} \ldots \overline{z_{m+1}}\}$. Since we need to convert from point representations to axis representations in a consistent way for both data reduction and reconstruction, this ordering needs to be fixed in advance. For the purpose of this paper, we will assume that the point ordering is always the same as one in which it was sampled during the top-down tree construction process. This leads to representative points sampled at higher levels of the tree to be ordered first, and points at lower levels to be ordered last. The only ambiguity is for the level-1 nodes at which 2 points are stored instead of one. In that case, the record which is lexicographically smaller is ordered earlier. We shall refer to this particular convention for axis representation as the *path-ordered axis representation*.

2.3 Oversampling and Selection of Subspaces

This section describes details of the *SampleBestHyperplanes* subroutine of Figure 5. The first task is to partition the $k_{max} * sampfactor$ hyperplanes into *sampfactor* sets of k_{max} hyperplanes. We will pick one of these partitions depending upon the quality of the assignment of the data points to these hyperplanes. In order to do this, the distance of the data point $\overline{x}$ to each of the $k_{max} * sampfactor$ hyperplanes is determined. For each of the *sampfactor* sets of hyperplanes, we assign the data point $\overline{x}$ to the closest hyperplane from that partition. This results in a total of *sampfactor* possible assignments of the data points. The cost of the assignment is the average distance of the data point to its assigned hyperplane, and is equal to the average distance information lost by the corresponding reduced representation. The lowest cost of these *sampfactor* assignments is determined. The *SampleBestHyperplanes* procedure returns the k_{max} points which can be used to extend the current node to each of the k_{max} children by a dimensionality of one.

2.4 Partitioning the Points

In this section, we will describe the *AssignData* procedure of Figure 5. The procedure *AssignData* partitions the points among the children nodes, and also decides whether the assignment of a data point $\overline{x}$ to a hyperplane is of the descendent or direct type. For each child hyperplane $(\overline{y}, \mathcal{E})$, the distance value $\Delta(\overline{x}, \overline{y}, \mathcal{E})$ is calculated. Next, we check if this value is below the compression tolerance ϵ. If so, then the data point $\overline{x}$ is directly assigned to that node. Otherwise, it is assumed that a higher implicit dimensionality is needed to represent that point and it is considered a descendent assignment. The top-down algorithmic process of subspace tree construction ensures that such a data point

will be a direct assignment for one of the descendants of its current node, unless it is determined to be an outlier.

2.5 Removal of Outlier Nodes

This procedure is denoted by *RemoveNodes* in Figure 5. Many points in any data set may be outliers for which efficient locality specific representations cannot be found. Such points need to be stored separately by the algorithm. In each iteration, we find all nodes in the current level of the tree which have less than *min-thresh* descendent assignments. These nodes and the corresponding points are removed by the algorithm. The corresponding points are stored separately in their full dimensional representation.

2.6 Disk Sensitive Implementation

Each of the procedures *AssignData* and *SampleBestHyperplanes* require the assignment of the data to nodes at a given level of the tree. In order to improve the I/O efficiency, we process all the nodes at a given level in a single database scan. We maintain an additional vector with one entry for each database record. Each entry in this vector indicates the node to which the corresponding database record is assigned and whether the corresponding record is a descendent or direct assignment. During the database scan, we use the vector to find the hyperplane $(\overline{y}, \mathcal{E})$ for each database record $\overline{x}$. This is then used to calculate the value of $\Delta(\overline{x}, \overline{y}, \mathcal{E})$ for the *AssignData* and *SampleBestHyperplanes* procedure.

3. STORAGE AND RECONSTRUCTION

Since the reduction process stores the reduced data in the context of a hierarchical subspace tree structure, we need to maintain the following two pieces of information:

• **The Subspace Tree:** This is a constant overhead which can be maintained very efficiently with the use of the *point representation*. For each level-1 node we maintain the two points which define the sampled line in lexicographic ordering. For each level-m node, we maintain the additional data point which increases the dimensionality of the corresponding subspace by one. In addition, we need to maintain the identity of the node and its immediate parent, which requires another two integers for each node. Thus, for a subspace tree with β nodes, the storage requirement is of the order of $(\beta \cdot (d+2))$ values. This is almost the best that one could hope to achieve, since at least $\beta \cdot d$ values will always be required in order to store all the β subspaces of a d-dimensional space. In fact if the subspaces were maintained explicitly, then the storage requirement would be $\beta \cdot d \cdot l$ values for an average subspace dimensionality of l. The storage requirement of $\beta \cdot (d+2)$ values requires the storage of only 1 additional vector for each of the β subspaces. The reason for this extraordinarily high storage efficiency is the use of the point representation in which the hyperplane at a given node is not stored explicitly, but is implicitly represented by the points stored along the path from that node to the root. (Therefore, the vector stored at a node is reused for the subspace representation of all descendents of that node.) Our empirical results indicated that the overhead for maintaining the subspace tree is very small compared to the storage requirements of the database itself.

• **The Reduced Database:** For each data point, we need to maintain one integer which indicates the identity of the node for which it is a direct assignment. In addition, we maintain the coordinates of the data point for the axis representation $(\overline{y}, \mathcal{E})$ of this hyperplane in accordance with Equation 1. For the data point $\overline{x}$, these coordinates are given by $(c_1 \ldots c_m) = \{\overline{e_1} \cdot (\overline{x} - \overline{y}) \ldots \overline{e_m} \cdot (\overline{x} - \overline{y})\}$. Thus, only $(m+1)$ values need to be stored for each database point.

3.1 Reconstruction Algorithm

The reconstruction algorithm proceeds in two phases. In the first phase, the (path-ordered) axis representation of the subspace tree is built. In the second phase, this subspace tree is used in order to reconstruct the database.

At first sight, it would seem that the first phase could be time consuming, since for each node in the subspace-tree, we would need to find its d-dimensional axis representation. However, it turns out that because of the use of the path-ordered convention for axis-representations, the first phase can be achieved in a time complexity which requires the computation of only one axis per node. The trick is to construct the axis representations of the nodes in the tree in a top-down fashion. This is because the axis representation $\{\overline{e_1} \ldots \overline{e_i}\}$ of a given node can be computed using the axis representation $\{\overline{e_1} \ldots \overline{e_{i-1}}\}$ of its parent and the point $\overline{z'}$ stored at that node in just the single computation of Equation 2. (For the nodes at level-1, lexicographic ordering of the representative points is assumed.) This automatically results in the path-ordered axis representation of the node.

Once the axis representations of the nodes have been constructed, it is simple to perform the necessary axis transformations which represent the reconstructed database in terms of the original attributes. Recall that for each database point $\overline{x}$, the identity of the corresponding node is also stored along with it. Let $(\overline{y}, \mathcal{E})$ be the corresponding hyperplane and $(c_1 \ldots c_m) = \{\overline{e_1} \cdot (\overline{x} - \overline{y}) \ldots \overline{e_m} \cdot (\overline{x} - \overline{y})\}$ be the coordinates of $\overline{x}$ along this m-dimensional axis representation. Then, as evident from Equation 1, the reconstructed point $\overline{x'}$ is given by:

$$\overline{x'} = \overline{y} + \sum_{i=1}^{m} [c_i]\, \overline{e_i} \tag{3}$$

4. APPLICATIONS

The hierarchical subspace sampling technique exposes the differing implicit dimensionalities in different parts of the data. Traditional indexing structures [6] and selectivity estimation techniques [18] treat all parts of the data in a homogeneous way from the dimensionality perspective. This strategy results in the worst-case behavior of the data to dominate. In this section, we will provide additional insights into how hierarchical subspace sampling techniques can lead to inherently more effective solutions to such problems by using its variable dimensionality local decompositions. The aim of writing this section is to demonstrate that even simple applications of the proposed principles can lead to dramatically improved solutions for difficult high dimensional problems. A detailed treatment of the optimization of these schemes will be discussed in future work.

4.1 Approximate Nearest Neighbor Search

In the approximate nearest neighbor search problem, we would like to find the nearest neighbor to a given target

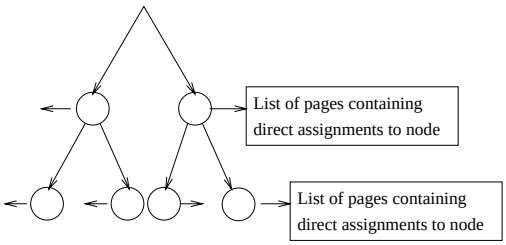


Figure 6: Index built from Subspace Tree

record within the pre-specified error bound of ϵ. Since our compression system provides such a worst-case guarantee, a sequential scan can be used on the reduced representation in order to find the approximate nearest neighbor. In fact, any compression method can provide savings in I/O even with the use of a sequential scan, as long as the reconstruction procedure can recognize individual records as they are generated in main memory. Such a technique works quite effectively, since the I/O requirements are the motivation for index structure construction. However, the subspace tree provides savings even beyond the advantages of lower storage requirements, since it allows us to create an index in which large portions of the *reduced representation* need not even be accessed. The ability to use such query optimization directly on compressed database systems has recently been recognized as a promising approach for optimizing performance in database systems.

The subspace tree imposes a natural partitioning of the data in which similar records occur together in one block. Unlike an index tree in which only leaf nodes contain the individual records, we allow each node in the tree to point to a *list* of pages which contain all the direct assignments to that node. Thus, the internal tree size is only dependent upon the original subspace tree, rather than the restrictions created by the page sizes of individual nodes. Furthermore, the subspace tree construction algorithm imposes a maximum limit L on the number of subspace tree nodes, which is determined by the main memory limitations. Thus, the subspace tree itself is maintained in main memory. On the other hand, the lists of pages pointed to by each node are maintained on the disk. The index structure is illustrated in Figure 6.

The actual nearest neighbor search of the tree uses a branch and bound method on the partitioning created by the direct assignments of data points to nodes. The branch and bound method is a classical technique in combinatorial optimization. It uses an ordered search method on a partitioning of the data in order to avoid searching many of the sets in this partitioning. A global pessimistic bound is maintained which provides an upper bound on the distance of the query point to the nearest neighbor. Pruning is done by finding good *optimistic* bounds (lower bounds) on the distance of a target point to each set in this partition. A set may be pruned when its optimistic bound is higher than the global pessimistic bound. For example, in the case of a query point $\overline{q}$ and subspace $(\overline{y}, \mathcal{E})$, this optimistic bound for any direct assignment of that hyperplane is given by $||\overline{q} - \mathcal{P}(\overline{q}, \overline{y}, \mathcal{E})||$. This is the nearest distance between the query point and the hyperplane, and any point lying on the hyperplane cannot have distance lower than this value. The global pessimistic bound is the nearest distance to any subset of the data accessed so far. However, unlike a traditional branch and bound technique, we cannot prune entire subtrees by using the optimistic bound at the root of the subtree. This is because in traditional index structures, lower level nodes are subsumed by higher level nodes, whereas in the subspace tree structure, the lower level subspaces subsume the higher level subspaces. Therefore, in a traditional index structure, the optimistic distance bounds from the query point to the nodes along a given path increase with the depth of the tree structure, whereas this is the reverse in a subspace tree (see Observation 2.1). Hence, one cannot use the optimistic bounds at the root of a subtree as representative of the optimistic bounds at the lower level nodes. In order to account for this, we treat each node as an independent entity irrespective of the hierarchical relationships between the nodes. Initially the pessimistic bound is set to the closest of all the outlier points and is gradually updated as more and more records are accessed. The nodes in the tree are accessed in increasing order of optimistic distance. When the distance $||\overline{q} - \mathcal{P}(\overline{q}, \overline{y}, \mathcal{E})||$ is larger than the pessimistic bound, all data points assigned to this node can be pruned from consideration. This is because it is certain that all data points which lie on this hyperplane are not as close as the best point found so far. Otherwise, we need to access the records in the list for the node $(\overline{y}, \mathcal{E})$, and calculate their distances to the query point q. This may result in the improvement of the pessimistic bound to the closest record to query point q lying on this hyperplane. The record corresponding to the pessimistic bound at termination is returned as the approximate nearest neighbor. We note that this approximate nearest neighbor is an exact nearest neighbor over the set of reduced data points. However, since each reduced data point may have distance at most ϵ from its original representation, it follows that the final nearest neighbor found lies within the error tolerance of ϵ.

4.2 Selectivity Estimation

The selectivity estimation problem becomes increasingly difficult in high dimensional cases. For the high dimensional case, it has been conjectured [10] that simple random sampling may be the most effective method for selectivity estimation: "We conjecture that sampling will outperform any of these techniques for dimensionality of around 10, but the error will be too large to make the technique practical."

The reason for the (relative) robustness of random sampling in higher dimensionality is that it can model the correlations in multi-dimensional data more accurately than methods such as histograms, since the correlations in the data are also reflected in the sample. On the other hand, the histogram technique is significantly more effective for lower dimensional cases.

The subspace tree procedure naturally reveals those parts of the data which have low implicit dimensionality. Since it is known that different techniques work more effectively in different implicit dimensionalities, this data decomposition naturally suggests an *ensemble-based* approach to the problem. Ensemble based approaches are especially attractive

because of their ability to combine different techniques in a flexible way so that the final solution is significantly more robust than the use of each individual method.

In the ensemble-based approach for selectivity estimation, we use a histogram based technique for all hyperplanes in the subspace tree with dimensionality at most q_{max}, whereas we use random sampling for data points in the higher dimensional components. The histograms for the lower dimensional component are built *directly* on the sampled hyperplanes, and are thus not parallel to the original axis-system. Thus, a separate set of histograms is constructed for each partition of the data in its locally optimized subspace. A wide array of methods are available to construct histograms. This choice is orthogonal to our primary aim of showing the effectiveness of the decomposition and the corresponding ensemble based approach. We will demonstrate that even the use of a simple equi-width grid based histogram for the lower dimensional component of the ensemble is sufficient to outperform existing approaches.

Let n_s be the total number of points with implicit dimensionality larger than q_{max} and n_t be the remaining number of points. We define a fraction r_f known as the *representation factor*, which has the same value but is defined differently for each of the two components of the ensemble:
(1) For the random sampling approach, the representation factor r_f is defined as the fraction of the n_s points (with implicit dimensionality greater than q_{max}) which are sampled.
(2) For the histogram based approach, the representation factor r_f is defined as the number of buckets b used divided by the number n_t of low implicit dimensionality points.

For the histogram based approach, we assume uniform distribution within each bucket and store the number of points and index of each bucket. Empty buckets are not included in this list. The index of a bucket provides its position in the multidimensional grid assuming a unique ordering convention of the grid points. Thus, only two values are required in order to store a bucket, while d values are required to store each sampled point. In addition, a fixed amount of space C_T is required in order to store (the relevant segment of) the subspace tree. Thus, the total space requirement for this ensemble based procedure is given by $C_T + r_f \cdot (n_t \cdot 2 + n_s \cdot d)$. We note that C_T is likely to be (asymptotically) negligible for very large databases. The $r_f * n_t$ histogram buckets are divided among the different hyperplanes in the subspace tree. The number of buckets assigned to each hyperplane is proportional to the number of points assigned to it. Therefore, for a m-dimensional hyperplane with q assigned buckets, the number of intervals into which the data is discretized is given by $\lfloor q^{1/m} \rfloor$. This also results in adaptive bucket sizes and orientations depending upon the subspace specific data localities.

At query time, we determine all the buckets which intersect with user-specified query ranges. Let the total number of (extrapolated) points[4] in these buckets be denoted by s_1. Similarly, for the sampling component of the ensemble, we determine the total number of points s_2 from the random sample which lie in the user specified ranges. Then, the expected number of points from the second component of the ensemble was given by s_2/r_f. Therefore, the total selectivity estimated by the ensemble is given by $s_1 + s_2/r_f$. The histogram component can be significantly improved with the use of more sophisticated methods such as those in [10] though our aim in this section is to only show the effectiveness of the ensemble-based subspace decomposition principle. In the next section, we will show that this approach achieves much greater accuracy over random sampling for difficult high dimensional cases.

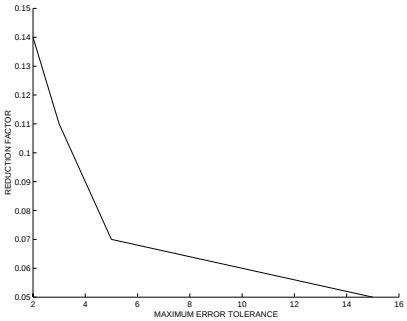
5. EMPIRICAL RESULTS

The system was implemented on an AIX 4.1.4 system with 233 MHz and 100 MB of main memory. The data was stored on a 2GB SCSI drive. We tested the subspace sampling method for the following measures: (1) Effectiveness of data reduction. (2) Efficiency of data reduction. (3) Effectiveness of the subspace tree for nearest neighbor indexing. (4) Effectiveness of the selectivity estimation procedure. Unless otherwise mentioned, the parametric values $k_{max} = minthresh = 2$, and $sampfactor = 10$ were used in the implementation.

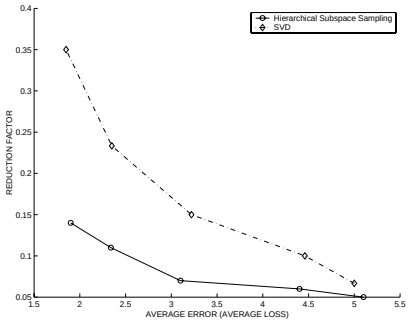
5.1 Performance of data reduction

For the purpose of testing, we used a combination of synthetic and real data sets. The synthetic data sets each contained $n_c = 20$ clusters which were gaussian in nature. The (relative) number of points in each cluster was determined by generating a uniform random number between 0 and 1. The centroids of the clusters were chosen randomly. The axis system of each gaussian cluster was arbitrarily oriented with respect to the original data set and the radius along each axis was chosen as an exponential distribution with 1% of the average distance between the clusters along the individual dimensions. We generated two data sets with dimensionalities 150 and 200 respectively. Each data set contained 100,000 records. We denote them as synthetic data sets 1 and 2 respectively. We also used a 64-dimensional color-histogram data set for testing purposes. In Figures 7(a), (c), and (e), we have illustrated the effect of the error tolerance threshold on the compression factor on each of the three data sets. The compression factor was defined as the fraction of the original data set size occupied by the reduced representation (including the subspace tree itself.) In each case, the compression was more effective at higher tolerance levels. This is because of the natural tradeoff between reduction quality and compactness. In order to get a better understanding of the effectiveness of the technique, we compared it to the Singular Value Decomposition method. Since the SVD technique does not provide worst-case bounds on the error tolerance, we compared the reduction factor of the two techniques using the average loss on the X-axis. The average loss was defined as the average distance between the original record and the projected record in the reduced representation. In each case of Figures 7(b), (d), and (f),

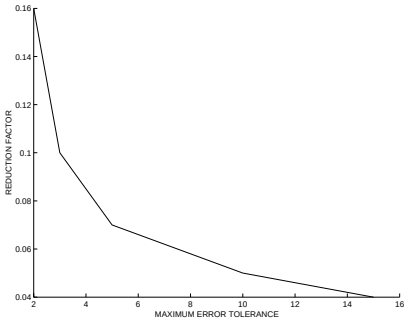
[4]For partially intersected buckets, we needed to find the fraction of the bucket inside user-specified ranges. In most cases, buckets were intersected by only one of the user specified constraints, in which case extrapolation was straightforward for 1- or 2-dimensional buckets. We included or omitted the entire count of buckets which were either greater than two dimensional or intersected with more than one constraint. This was determined by whether or not the bucket center lay inside the user specified range.



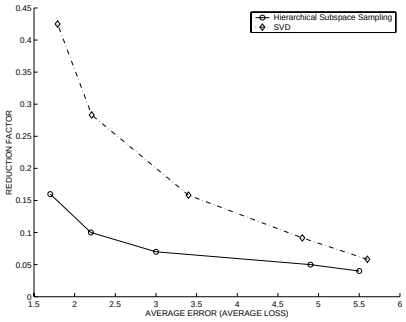
(a) Error Tolerance versus Reduction Factor (Synthetic Data Set 1)



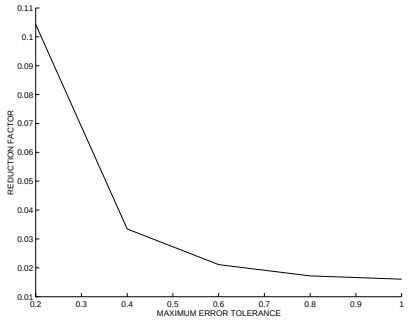
(b) Average Loss versus Reduction Factor (Comparison with SVD (Syn. 1))



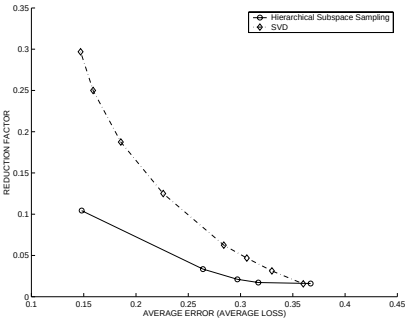
(c) Error Tolerance versus Reduction Factor (Synthetic Data Set 2)



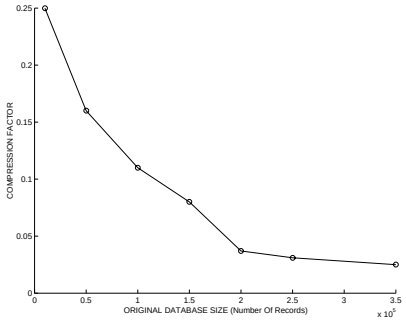
(d) Average Loss versus Reduction Factor (Comparison with SVD (Syn. 2))



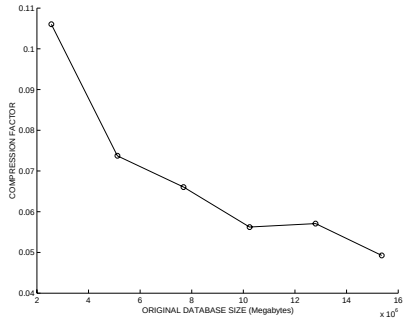
(e) Error Tolerance versus Reduction Factor (64-d histogram data sets)



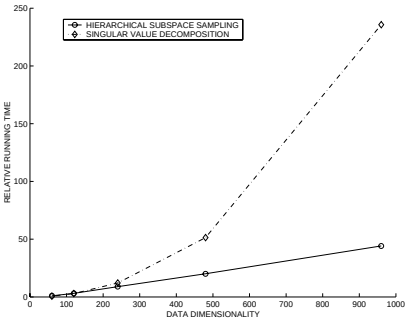
(f) Average Loss versus Reduction Factor (Comparison with SVD (64-d))



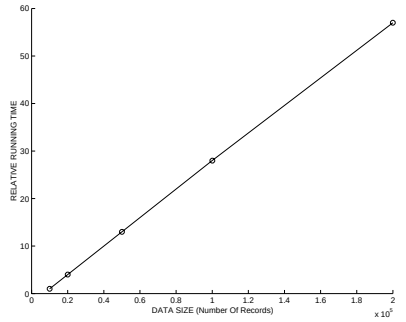
(g) Reduction Factor Improvement with data size (synthetic)



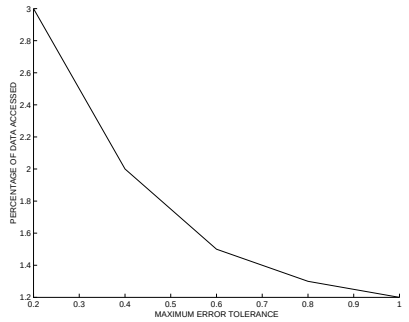
(h) Reduction Factor Improvement with data size (64-d histograms)



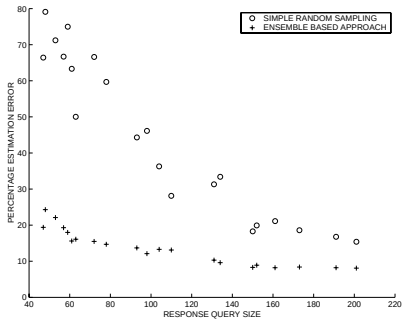
(i) Reduction Efficiency (Increasing Dimensionality)



(j) Reduction Efficiency (Increasing Database Size)



(k) Nearest Neighbor Pruning Performance (64-d color histograms)



(l) Selectivity Estimate Accuracy (64-d color histograms)

Figure 7: Effectiveness of Hierarchical Subspace Sampling and its Applications

we have plotted the average compression factor versus the average loss of each record for both methods. It is clear that the subspace sampling technique is significantly more effective than the standard dimensionality reduction technique. Another interesting observation from the charts is that the relative compression performance of the subspace sampling technique improves with reduced error tolerances. This is because for very relaxed (high) loss rates, it suffices to represent the data in 1- or 2-dimensional format for either of the two methods. As the error tolerances are tightened, the advantages of localized subspace sampling begin to show up, and the method is able to represent the data in a much smaller number of dimensions. As a result, the overall space required by the subspace tree representation is significantly lower than the standard dimensionality reduction method. Furthermore, we note that these improved results are in spite of the fact that the subspace sampling method provides hard guarantees on the error tolerances, whereas this is not achieved by the standard dimensionality reduction method. It is evident by comparing[5] the different charts in Figure 7 that in each case the average loss was about 50% of the error tolerance for the subspace sampling method.

We also tested the performance of the hierarchical subspace sampling technique with increasing database size. In Figure 7(g), we have illustrated the behavior of the reduction factor with database generations of different sizes for the parameters of the first synthetic data set (Syn. 1). On the X-axis, we have illustrated the database size in records whereas the reduction factor is illustrated on the Y-axis. The maximum error tolerance was kept constant at 2% of the standard deviation of the data. It is clear that the reduction factor improves with increasing database size. In Figure 7(h), we have illustrated the same results by sampling an increasing number of records from the 64-dimensional color histogram data set. In this case, the error tolerance was set at $\epsilon = 0.3$. The results show a similar trend as the synthetic data set. It was our experience over a number of data sets that the *reduction factor always improved with increasing database size.* This is a very useful property of the subspace sampling technique, since the data reduction problem is motivated by the large size of data sets. There are two reasons for this behavior:

(1) The size of the subspace tree itself scales sublinearly with database size. In fact, for most data sets that we tested, the subspace tree size increased only marginally for database sizes above 100,000 points. At this point, all the major subspace patterns are already significantly represented in the tree structure as well as the database. In all cases, the total number of nodes in the subspace tree was only about 0.5-10% of the maximum limit $L = 10,000$ nodes.
(2) For larger data sets, the local subspaces determined by the sampling technique are more refined. These refined nodes are reflected in the lower levels of the subspace tree. As a result, a large number of points which would otherwise get classified as outliers are reflected in some lower dimensional projection in the subspace tree. The basic intuition is that in larger data sets, all the natural local data patterns can be reflected in a refined way, which leads to a more optimized representation.

[5]For example, by matching the common axis value (reduction factor) of Figure 7(a) and (b), one can obtain the relationship between the error tolerance and average loss. Explicit charts were omitted for lack of space.

5.2 Efficiency of Data Reduction

We tested the efficiency of the scheme for dimensionality reduction. In order to test the efficiency, we need a data set in which the dimensionality can be varied effectively, while retaining the basic structure of the data. To this effect, we found the market basket data generator of [3] useful. This data set was derived[6] from the set T20.I20.D100K by using random projections of varying dimensionality. The error tolerance was fixed at 5% of the standard deviation. In Figure 7(i), we have illustrated the scalability of the approach with increasing data dimensionality. It is clear that for lower dimensionalities, the standard SVD approach performs more effectively, but for dimensionalities 80 and higher, the hierarchical subspace sampling technique performed more effectively. This is because of the (almost) linear scalability of the subspace sampling technique with respect to data dimensionality, whereas the SVD method had worse than quadratic scalability with increasing dimensionality. We have also illustrated the scalability of the subspace sampling technique with increasing data set size in Figure 7(j). In this case, we used a 100-dimensional projection of the data set T20.I20.D"x". Here the value of x was varied in order to control the database size. It is clear that the subspace sampling technique scales almost linearly with database size. The straightforward sampling approach is the key to the tremendous efficiency of subspace sampling.

5.3 Application Performance

We applied the subspace sampling method for approximate nearest neighbor search on the 64-dimensional color histogram data set. A direct application of the branch and bound method [16] on the R^*-Tree structure leads to 100% of the data being accessed. When we modified the branch and bound method to allow pruning even within predefined error bounds, the R^*-Tree structure continued to access the entire data set for error bounds ranging between 0.2 and 1.0. Then, we tried to use the R^*-Tree structure to index a data set which was reduced using SVD, but with similar *average* error as the reduced data created by the subspace sampling technique with error guarantees between 0.2 and 1.0. This results in loss of error guarantees. In this case, the performance improved only because of the reduced data set size, whereas 100% of the index continued to be accessed. Since the results of Figure 7(f) indicate that the SVD method does not reduce the data as efficiently as the subspace sampling technique anyway, it is clear that the dimensionality reduction method cannot hope to qualitatively compete with the subspace sampling method even with the loss in error guarantees. In Figure 7(k), we have illustrated the performance of the hierarchical subspace sampling index for the same error ranges. It is clear that for all ranges tested, the hierarchical subspace index tree accessed between 1% to 3% of the original data set size. This improvement was *both* because of more effective pruning and the advantages of a reduced representation. Typically, between $60 - 90\%$ of the (reduced) data was pruned during the branch and bound

[6]We are using notations from [3].

search. Unlike the R^*-Tree which used axis-parallel rectangles in characterizing the nodes of the partitions, the arbitrary hyperplanes of the subspace sampling technique provided tight bounds which helped in effective pruning during the nearest neighbor search procedure.

We also tested the ensemble-based approach for selectivity estimation on the 64-d color histogram data set. The queries were all range queries in which we intersected 10% on the ranges on two randomly picked dimensions. For the 64-dimensional case, simple random sampling is the most realistic alternative [10] for effective selectivity estimation. In Figure 7(l), we have illustrated the performance of the ensemble-based approach on the color histogram data set. We used a representation factor of 3% and a maximum dimensionality of $q_{max} = 2$ for the ensemble-based estimator. Both approaches were implemented so that they required the same amount of storage space. In Figure 7(l), we have illustrated the estimation accuracy on the same queries for both methods. It is clear that the ensemble-based approach performs significantly more effectively than the simple random sampling procedure, especially for queries with small responses. Since the estimation of queries with small responses is the most inaccurate for most selectivity estimators, the overall robustness of the ensemble system was significantly better. The reason for this improvement was twofold: (1) Since the histogram component of the ensemble was built in a lower dimensional space, it was more compact. Therefore, a greater amount of selectivity information could be stored in the same amount of space. (2) The primary reason for the effectiveness of the ensemble approach was its ability to decompose the data depending upon its natural degree of difficulty and use suitably optimized approaches for each of the portions. This generic approach can be leveraged to good use in a number of other high dimensional problems. We are currently exploring the use of this technique for high dimensional classification.

6. CONCLUSIONS AND SUMMARY

In this paper, we discussed the novel technique of hierarchical subspace sampling, a method for effective high dimensional data reduction. As indicated by the empirical results, the hierarchical subspace sampling technique is both effective and efficient and can achieve a clear advantage over widely used dimensionality reduction techniques such as SVD, while providing worst-case bounds on the error of each record. The technique shows the interesting behavior of improved reduction ratios with increasing database size. In addition, the technique shows almost linear scalability of running time with increasing database size and dimensionality. This results in an approach which is significantly more efficient than SVD for data sets of higher dimensionality. The reason for the efficiency is rooted in its straightforward sampling approach, while retaining the power of finding local subspaces of appropriate dimensionality. Since the hierarchical subspace sampling method reveals important local subspace properties of the data, these can also be utilized for decomposable solutions to problems such as nearest neighbor search and selectivity estimation.

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