

A Technology for Retrieval of Volume Images from Biomedical Databases*

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Abstract—To facilitate the retrieval of volume images from a biomedical database (e.g., images of proteins from a macromolecular database), it is necessary to obtain concise descriptors of the images. Relatively recently developed successful algorithms for high-resolution three-dimensional reconstruction of biomedical structures from projections produce volume images represented as linear combinations of spherically symmetric basis functions (called blobs). In this paper, we discuss our work toward obtaining topological and geometric descriptors in the form of Betti triple sequences from such a linear combination of blobs, and give some preliminary experimental results.

I. INTRODUCTION

The goal of this work is to ease the retrieval, from a database, of information relevant to a given biomedical structure.

We assume that we have access to a large database containing volume images. Suppose now that—for example, as a result of reconstruction from projections—we have a new volume image and we wish to see if anything similar is in the database. This is difficult to achieve if the structures in the database are described either as a collection of atoms at specific locations or as gray-level volumes, not only because of the enormous size of such descriptions but also because, due to the variety of ways an object can be prepared and imaged, there may be differences (both in shape and in the values) between gray-level volumes associated with the same type of biomedical object imaged at different times. We need structural descriptors (both of the things in the database and the new thing that we have) that are easier to match than the atom collection or volume information.

In addition to being “signatures” of volume images for searches in databases, accurate topological and geometrical descriptors are likely to lead to better understanding of the structural properties of the biomedical specimens under investigation. We report on our preliminary work toward obtaining topological and geometrical structural descriptors.

II. ART WITH BLOBS

Algebraic Reconstruction Techniques (ART) assume that a specimen can be approximated by a linear combination of a finite set of known basis functions, and their task is to estimate

the weights of these basis functions based on projection data. The conventional choice is to use basis functions that have value 1 inside a voxel and 0 outside it; typical voxels are cube-shaped volume elements arranged on a simple cubic grid (so that the union of all voxels covers the volume of interest). Some very successful algorithms that have been developed for the three-dimensional reconstruction of biomedical structures from projections produce descriptions of volumes as linear combinations of spherically symmetric basis functions; they use a certain family of Kaiser-Bessel window functions (“blobs”) that can be arranged on various grids [1]. Blobs have bell-shaped radial profiles, and they go to zero at their boundaries. Each blob overlaps with its neighbors on the grid. The blobs we use are twice differentiable—an important property that also holds for their finite linear combinations. Their invariance under rotation and their smoothness make them well suited for representing natural structures of all physical sizes. It has been found that ART with blobs produces high-quality reconstructions and is superior (for many tasks) to other well-established algorithms [2].

In view of this, we have aimed our initial investigation at obtaining topological and geometrical descriptors of volumes from their blob representations (which are provided by our reconstruction algorithms).

III. METHODS

The three Betti numbers of spatial objects are the number b_0 of components, the number b_1 of “holes or tunnels,” and the number b_2 of cavities. Edelsbrunner et al. [3] advocate the use of sequences related to Betti numbers to represent a volume that is originally described as a collection of atoms. Inspired by this work, we aim to produce something similar to represent a real-valued function given by a linear combination of blobs. A topological descriptor of such a function is the sequence of Betti number triples of the spatial objects obtained by thresholding it, as we lower the threshold from the maximum value of the function to the minimum value. Combined with the threshold values at which the triples of Betti numbers change, the sequence also contains non-topological geometric information.

To compute these sequences, we first convert the linear combination of blobs into a voxel-based gray-valued image

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(of suitably high resolution) on a Cartesian grid, by sampling. We then consider the sequence of binary images that would be obtained if we thresholded the gray-valued image repeatedly, as we lowered the threshold from the highest gray value in the image to the lowest. We compute the Betti number triples of these binary images and the thresholds at which the triple changes. Usually, there are very many such binary images—just as many as there are distinct gray-values in the gray-valued image—and so it would be very expensive to calculate the Betti triple of each binary image independently. Instead, we use the method described in the following paragraphs to more efficiently compute the Betti triples of all the binary images. (We actually compute the Betti numbers b_0 and b_2 , and the so-called *Euler number* E ; the Betti number b_1 is calculated from the relationship $E = b_0 - b_1 + b_2$. We define Euler and Betti numbers of binary images using 6-connectivity for foreground voxels and 26-connectivity for background voxels [4].)

To compute E and the number b_0 of connected components of foreground voxels at each threshold, we grow a set of voxels: we start with the empty set and add all voxels (one at a time) in non-increasing order of their gray values.

The Euler number E is initialized to 0, and is recalculated each time we add a new voxel to the set. In computing the change in E when we add a voxel, we need only consider the eight $2 \times 2 \times 2$ -voxel subunits that contain the new voxel. The contribution of each $2 \times 2 \times 2$ -voxel subunit to the Euler number of a voxel set is given by a 256-element lookup array [5].

To track the number b_0 of connected components as we grow the set of voxels, we give each new voxel a label when we add it to our set, and we maintain equivalence classes of labels, where each class represents a component. If the new voxel has no 6-neighbor in our voxel set, we give it a new label and create a singleton equivalence class consisting of just that label. Otherwise, we merge the equivalence classes of the labels of the new voxel's 6-neighbors, and give the voxel a label that is representative of the resulting class. Each class is implemented as a tree in a disjoint set forest (DSF) of labels, and when merging classes we use union-by-rank with path compression [6]. The number b_0 is just the number of classes.

For the sequence of cavity counts b_2 we grow the set of background voxels, adding voxels in non-decreasing order of their gray values. We use a new DSF and proceed as in the case of b_0 , but consider the 26-neighbors of each new voxel rather than its 6-neighbors. Components that extend into the image's bounding box are not cavities and so are not counted.

Our program calculates Betti triple sequences very efficiently. For example, the production (including disk writes) of the Betti triple sequence from a $128 \times 128 \times 128$ voxel-based gray-valued image took 28 seconds (on a 1.7GHz Intel® Xeon™ with ≈ 1 GB RAM running Linux).

IV. PRELIMINARY RESULTS

The approach of the previous section produces from linear combinations of voxels or blobs a finite sequence of triples of

Betti numbers. It produces the mathematically correct sequences for sufficiently fine voxel images derived from mathematical descriptions of phantom images that consist of the superimposition of homogenous (single intensity contribution) simple regions (ellipsoids); see Fig. 1, left (the correct Betti sequence for this three dimensional phantom has 6 triples). However, for images converted from blob-images (obtained from reconstruction procedures based on projections of the phantom; see Fig. 1, right), we get sequences that are very long (e.g., more than 100,000 triples) and reflect more the inaccuracies of reconstruction than the inherent topology of the underlying phantom.



Fig. 1. A slice from a voxelization of the phantom (left) and the corresponding slice obtained from a reconstruction (right). A very narrow display window was chosen to emphasize their difference.

V. FUTURE CHALLENGES

We hope to reduce the currently obtained long sequences into shorter, more useful sequences. Preliminary attempts at achieving this indicate that we need to consider geometrical (as well as topological) information; for example, by introducing notions corresponding to that of persistent Betti numbers in [3].

Our approach so far has involved conversion of blob representations into voxel representations before further processing. Some information is lost, and some errors are introduced if the output resolution is not high enough. A mathematically challenging task is to develop a method for recovering useful sequences of Betti number triples directly from blob descriptions of volumes.

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