Visualization of Large Multi-Dimensional Datasets

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Abstract. Visualization techniques are well developed for many problem domains, but these systems break down for datasets which are very large or multidimensional. Techniques for data which is discrete rather than continuous are also less well studied. Astronomy datasets like the Sloan Digital Sky Survey are very much in this category. We propose the extension of information visualization techniques to these very large record-oriented datasets. Specifically, we describe the possible adaptation of the Visage information visualization tool to terabyte astronomy datasets.

1. Introduction

How can huge data sources (gigabytes up to terabytes) be quickly and easily analyzed? There is no off-the-shelf technology for this. There are devastating computational and statistical difficulties; manual analysis of such data sources is now passing from being simply tedious into a new, fundamentally impossible realm where the data sources are just too large to be assimilated by humans. The only alternative is to provide extensive computer support for the process of discovery.

The focus of this workshop is the challenge posed by the next generation of large astronomical sky surveys. Specifically, we concentrate on the Sloan Digital Sky Survey (SDSS), which will create over one terabyte of reduced data over the next 5 years: How does one navigate such a huge, multi-dimensional, dataset? The techniques of information visualization and visual discovery may be extended to such datasets, allowing the scientist to interactively explore and understand her results in real time.

This work is the product of a collaboration at Carnegie Mellon University and the University of Pittsburgh, involving astronomers, experts in traditional scientific visualization and interactive information visualization, and computer and computational scientists. Condensed data representations from the data mining and machine learning community (Nichol et al. in these proceedings) make it possible to explore these huge datasets interactively.
2. Visualization Challenges of the Virtual Observatory

Over the next ten years, we will witness a revolution in how astrophysical research is performed. This is primarily due to the large number of new sky surveys presently underway (or completed) that are designed to map the Universe to higher sensitivity and resolution than ever previously envisaged. We are quickly approaching the prospect of a Virtual Observatory, where one can digitally reconstruct the whole sky. These surveys, and the virtual observatory, present scientists with a “gold mine” that the next generation of astrophysicists will spend their whole careers exploring.

Two cornerstones of the Virtual Observatory are the 2 Micron All Sky Survey (2MASS) and the optical Sloan Digital Sky Survey (SDSS). The 2MASS survey (which is 91% released) is a near infrared imaging survey covering the full sky in three passbands (from 1-2.2 microns). The SDSS is an imaging and spectroscopic survey that will cover one quarter of the sky at five different wavelengths. Together these two surveys will detect over 200 million objects (galaxies and stars) and from these detections positions, fluxes, shapes, textures and bitmaps will be extracted. In addition to the scientific information will be book-keeping information that describes the observations themselves, e.g. whether the sky was cloudy or there were problems with the instrumentation. We must also understand these possible systematic uncertainties present within the data. The total 2MASS and SDSS surveys are expected to acquire 500 GB of cataloged attributes and 1 TB of postage stamp images (cutout images around each detected object) over the next 5 years of operation.

For each object detected hundreds of attributes will be recorded. The size and large dimensionality of these new data sets means that simple visualization and analysis techniques cannot be applied directly, because they do not scale effectively. The questions then become: How do we quickly determine the important dimensions within such a data set? Which dimensions tell us about how galaxies or stars form and how matter is distributed throughout the individual galaxies or, the Universe as a whole? New techniques developed for 2MASS and SDSS will be applicable to the analyses of all large observational data sets (such as the all-sky surveys of GALEX, ROSAT, MAP and PLANCK) and for the visualization of other large physical and biological experiments.

3. The Breakdown of Visual Discovery

Traditional astronomy has relied on the study of small numbers of rare objects. With hundreds of millions of objects in the Virtual Observatory, “rare” objects will themselves number in the millions. Statistical methods become necessary to group objects into classes for study.

This situation is opposite to that for which traditional visualization methods are best suited. Large dataset size alone kills interactivity. The record-oriented nature of the dataset makes it difficult to assimilate, because the brain is evolved to understand continuous systems that exist in three dimensions plus time. If too broad a view of the data is taken, important details can be literally too small to see. Too narrow a view is also disastrous. It becomes very easy to be distracted by structures that look important.
Supercomputer simulations routinely produce very large datasets. Standard methods of visualizing such data typically include the generation of one or more animations (assuming the system evolves in time), or interactive visualization of tiny subsets of the data. In most problem domains the researcher’s physical intuition applies, and can help her to assimilate the evolution of the system.

Large computing facilities are developing interactive visualization tools for these terabyte-sized datasets. Direct application of traditional visualization typically requires a supercomputer, and even with one available interactivity is very difficult to attain. Current rendering hardware can draw at most about 10 million polygons per second (though this number is rising), so interactive drawing of hundreds of millions of objects is simply impossible.

4. Desirable Capabilities

Here are illustrative questions that astrophysicists will want to ask of the data:

- A range of counting queries such as:
  - How many elliptical galaxies, with a redshift above 0.3, are there?
  - What is the mean and variance of ellipticity among radio galaxies within clusters of galaxies compared to outside clusters of galaxies?
  - How does the distribution of galaxy colors observed on 1 May 2001 compare to those seen on 1 June 2002?

- Sophisticated statistical queries that require the clustering, classification, regression, filtering and newer probabilistic inference techniques.

- Visualization requests to answer questions such as:
  - Give me a smoothed map of all X-ray detected galaxies.
  - Display all emission-line galaxies in detected clusters of galaxies; are they in the center or on the outskirts?

5. XGobi, a Simple Tool for Visualizing Multidimensional Data

XGobi, one of the most widely used information visualization tools, was written at Lucent Technologies (Swayne, Cook, & Buja 1998). This tool interactively produces arbitrary 3D projections of n-dimensional data. For example, figure shows the correspondence between data groups which differ in one projection but are cluster together in another. XGobi deals only with scalar data, and is designed for relatively small datasets.

XGobi supports a method called brushing, whereby the user selects data items in one window and the selection is propagated to the corresponding items in all other windows. This has proven to be a useful technique for mentally integrating multiple views.

1XGobi is freely available from http://www.research.att.com/areas/stat/xgobi
At Carnegie Mellon University, in collaboration with Maya Design Group, we have already developed an interactive data exploration system called Visage (Kolojejchick, Roth, & Lucas 1997). It is effective for analyzing high dimensional data, but it uses only 2D visualizations and is limited to small discrete datasets. Below, we describe Visage’s features, while in the next subsection, we discuss our plans to generalize these features and expand the capacity of Visage to handle massive datasets. We call this new system TeraVisage.

Visage presents data as graphemes (visual elements) organized by frames (lightweight nestable windows that impose some visualization discipline on the graphemes presented within them). Within a frame, the data are presented by graphemes such as bars, text labels, marks and gauges. The visual properties of the graphemes (e.g., the color or size of a plot point) encode attributes of the objects they represent (e.g., a galaxy). While each grapheme stands for one object, an object may be represented by many graphemes of varying appearance in different frames.

Some of the basic operations provided by Visage are:

- Drag-and-drop objects from one frame to another,
- Navigate (drill-down) from an object along a relation creates graphemes for the related objects,
- Aggregate (roll-up) a set of selected objects to create a new object with properties computed from its members,
- Brush an object or a set of objects in a choice of colors, as described in Section 5,
- Dynamically query by an attribute to render invisible all objects within a frame whose values for that attribute fall outside a range selected by a slider widget.

The results of these operations depend only on the underlying data object, and are uniformly applicable in any type of Visage frame.
6.1. Going to Large Datasets

In this subsection, we discuss the methods by which we propose to adapt Visage to very large datasets. Interactive visualization requires interactive speeds; the challenge is to maintain these speeds during interrogation of a large (500GB) database. Our plan is to maintain a hierarchy of representations and subsets, with a hierarchy of access speeds.

Figure 2 presents our vision of how this would play out for exploring an astronomical dataset. The data comes from a simulation of the coming merger of our Milky Way galaxy with the Andromeda galaxy\(^2\).

The dataset we examine here corresponds to the last frame of the simulation. In the course of the collision large "tidal tails" of stars, dust, and gas have been drawn from both galaxies. At the moment in question the bulk of the galactic matter has formed a roughly elliptical collision remnant, but two tidal tails remain. The matter in one tail is to be selected and examined.

In the left frame labeled "All Star Groups", the astronomer has displayed 7 attributes of all the star groups in the two galaxies. The 3D visualization shows spatial position (x, y, and z). The histograms additionally show the distribution of distance from the center of the galaxy, magnitude of velocity, x component of velocity, and original galaxy each star group belonged to. On the galaxy histogram the astronomer has brushed the Milky Way star groups purple and the Andromeda ones yellow. The relative distributions can be seen in the other histograms and the density plot. It is apparent that star groups that originated in the Milky Way dominate the streamers. The astronomer selects a group of stars from one of the streamers using a bounding box. These stars are brightened in the 3D density plot. The brushing and selection operations should take about one second.

The astronomer then creates a new frame with a density plot showing the x, y, and z components of the velocities and drags (copies) the selected star groups there. She labels the new frame "+Z Tail" (right), and copies the histograms as well. Appropriate condensed representations should allow this operation to be carried out in about 10 seconds. Being interested in the relationship between the distance from the center and the magnitude of the velocity, she creates a 2D scatter plot of those variables. By moving the distance slider, she controls which stars remain fully visible and which are grayed out. Feedback from slider changes should occur in roughly 100ms.

It is easy to see how to extend most of the graphemes of Visage to large datasets. Sets of individual marks become density distributions in some space, and are selected by selecting regions in the space and/or using DQ filters. Gauges remain gauges, but now represent statistical summaries of subsets of the data. Text labels remain, but become labels for sub-aggregates found in traversing kd-trees or in more sophisticated models. Many confusing issues remain, however.

\(^2\)Welling carried out the simulation using conditions specified by John Dubinski and code by Lars Hernquist and others [Mihos, 1998 #176]; further information is available from http://www.cita.utoronto.ca/~dubinski/index.html. An animation of the merger can be found at http://www.psc.edu/~welling/big-merger.mpg.
7. Interactive Visualization Through Condensed Representations

In addition to facilitating machine learning and database operations, appropriate condensed representations can accelerate such tasks as volume rendering by allowing data items to be grouped and drawn together if they are similar to within specified error bounds. A large dataset can easily have more data elements than there are pixels on the display, and there is no sense rendering at a level of detail which will be invisible to the user. These hierarchical rendering methods are well studied in computer graphics and map well to condensed representations for knowledge discovery. For example, see Laur & Hanrahan (1991).

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