SCIENTIFIC DATA MINING IN ASTRONOMY

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Abstract

We describe the application of data mining algorithms to research problems in astronomy. We posit that data mining has always been fundamental to astronomical research, since data mining is the basis of evidencebased discovery, including classification, clustering, and novelty discovery. These algorithms represent a major set of computational tools for discovery in large databases, which will be increasingly essential in the era of data-intensive astronomy. Historical examples of data mining in astronomy are reviewed, followed by a discussion of one of the largest data-producing projects anticipated for the coming decade: the Large Synoptic Survey Telescope (LSST). To facilitate data-driven discoveries in astronomy, we envision a new data-oriented research paradigm for astronomy and astrophysics - astroinformatics. Astroinformatics is described as both a research approach and an educational imperative for modern data-intensive astronomy. An important application area for large timedomain sky surveys (such as LSST) is the rapid identification, characterization, and classification of real-time sky events (including moving objects, photometrically variable objects, and the appearance of transients). We describe one possible implementation of a classification broker for such events, which incorporates several astroinformatics techniques: user annotation, semantic tagging, metadata markup, heterogeneous data integration, and distributed data mining. Examples of these types of collaborative classification and discovery approaches within other science disciplines are presented.

1 Introduction

It has been said that astronomers have been doing data mining for centuries: "the data are mine, and you cannot have them!". Seriously, astronomers are trained as data miners, because we are trained to: (a) characterize the known (i.e., unsupervised learning, clustering); (b) assign the new (i.e., supervised learning, classification); and (c) discover the unknown (i.e., semi-supervised learning, outlier detection) [12, 13]. These skills are more critical than ever

since astronomy is now a data-intensive science, and it will become even more data-intensive in the coming decade [25, 72, 9].

We describe the new data-intensive research paradigm that astronomy and astrophysics are now entering [33, 19, 20]. This is described within the context of the largest data-producing astronomy project in the coming decade - the LSST (Large Synoptic Survey Telescope). The enormous data output, database contents, knowledge discovery, and community science expected from this project will impose massive data challenges on the astronomical research community. One of these challenge areas is the rapid machine learning (ML), data mining, and classification of all novel astronomical events from each 3-gigapixel (6-GB) image obtained every 20 seconds throughout every night for the project duration of 10 years. We describe these challenges and a particular implementation of a classification broker for this data fire hose. But, first, we review some of the prior results of applying data mining techniques in astronomical research. A similar, more thorough survey of data mining and ML in astronomy was published [7] after this paper was published¹.

2 Data Mining Applications in Astronomy

Astronomers classically have focused on clustering and classification problems as standard practice in our research discipline. This is especially true of observational (experimental) astronomers who collect data on objects in the sky, and then try to understand the objects' physical properties and hence understand the underlying physics that leads to those properties. This invariably leads to a partitioning of the objects into classes and subclasses, which reflect the manifestation of different physical processes that appear dominant in different classes of objects. Even theoretical astrophysicists, who apply pure physics and applied mathematics to astronomy problems, are usually (though not always) governed by the results of the experimentalists – to identify classes of behavior within their models, and to make predictions about further properties of those classes that will enhance our understanding of the underlying physics.

2.1 Clustering

Clustering usually has a very specific meaning to an astronomer – that is "spatial clustering" (more specifically, angular clustering on the sky). In other words, we see groupings of stars close together in the sky, which we call star clusters. We also see groupings of galaxies in the sky, which we call galaxy clusters (or clusters of galaxies). On even larger spatial scales, we see clusters of clusters of galaxies (superclusters) – e.g., our Milky Way galaxy belongs to the Local Group of Galaxies, which belongs to the Local Supercluster. Most of these cluster classes can be further subdivided and specialized: e.g., globular star clusters versus open star clusters; or loose groups of galaxies versus compact groups of

 $^{^1}$ Borne, K., "Scientific Data Mining in Astronomy," in Next Generation of Data Mining (Taylor & Francis: CRC Press), pp. 91-114 (2009)

galaxies; or rich clusters of galaxies versus poor clusters of galaxies. Two of the research problems that are addressed by astronomers who study these objects are discovery and membership – i.e., discovering new clusters, and assigning objects as members of one or another cluster. These astronomical applications of clustering are similar to corresponding ML applications. Because clustering is standard research practice in astronomy, it is not possible to summarize the published work in this area, since it would comprise a significant fraction of all research papers published in all astronomy journals and conference proceedings over the last century. Specific data mining applications of clustering in astronomy include the search for rare and new types of objects [31, 32, 35].

More generally, particularly for the ML community, clustering refers to class discovery and segregation within any parameter space (not just spatial clustering). Astronomers perform this general type of clustering also [30, 33]. For example, there are many objects in the Universe for which at least two classes have been discovered. Astronomers have not been too creative in labeling these classes, which include: Types I and II supernovae, Types I and II Cepheid variable stars, Populations I and II (and maybe III) stars, Types I and II active galaxies, and so on, including further refinement into subclasses for some of these. These observationally different types of objects (segregated classes) were discovered when astronomers noticed clustering in various parameter spaces (i.e., in scatter plots of measured scientific parameters).

2.2 Classification

The other major dimension of astronomical research is the assignment of objects to classes. This was historically carried out one-at-a-time, as the data were collected one object at a time. ML and data mining classification algorithms were not explicitly necessary. However, in fact, the process is the same in astronomy as in data mining: (1) class discovery (clustering); (2) discover rules for the different classes (e.g., regions of parameter space); (3) build training samples to refine the rules; (4) assign new objects to known classes using new measured science data for those objects. Hence, it is accurate to say that astronomers have been data mining for centuries. Classification is a primary feature of astronomical research. We are essentially zoologists – we classify objects in the astronomical zoo.

As the data sets have grown in size, it has become increasingly appropriate and even imperative to apply ML algorithms to the data in order to learn the rules and to apply the rules of classification. Algorithms that have been used include Bayesian analysis, decision trees, neural networks, and (more recently) support vector machines. The ClassX project has used a network of classifiers in order to estimate classes of X-ray sources using distributed astronomical data collections [70, 71].

We will now briefly summarize some specific examples of these. But first we present a more general survey of data mining research in astronomy.

2.3 General Survey of Astronomical Data Mining

A search of the online astronomical literature database ADS (NASA's Astrophysics Data System) lists only 63 refereed astronomy research papers (765 abstracts of all types – refereed and unrefereed) that have the words "data mining" or "machine learning" in their abstracts. (Note that ADS searches a much broader set of disciplines than just astronomy when non-refereed papers are included – most of these search results are harvested from the ArXiv.org manuscript repository.) Of course, there are many fine papers related to astronomical data mining in the SIAM, ACM, IEEE, and other journals and proceedings that are not harvested by ADS.

Within the ADS list of refereed papers, the earliest examples that explicitly refer to "data mining" in their abstract are two papers that appeared in 1997 – these were general perspective papers. (Note that there are many papers, including [12] and [13] that were not in the refereed literature but that pre-date the 1997 papers.) The first of the refereed data mining application papers that explicitly mentions "data mining" in the abstract and that focused on a specific astronomy research problem appeared in 2000 [58]. This paper described all-sky monitoring and techniques to detect millions of variable (transient) astronomical phenomena of all types. This was an excellent precursor study to the LSST (see §4.1).

Among the most recent examples of referred papers in ADS that explicitly refer to data mining (not including this author's work [17]) is the paper [47] that addresses the same research problem as [58]: the automated classification of large numbers of transient and variable objects. Again, this research is a major contributor and precursor to the LSST research agenda (§4.3).

A very recent "data mining" paper focuses on automatic prediction of Solar CMEs (Coronal Mass Ejections), which lead to energetic particle events around the Earth-Moon-Mars environment, which are hazardous to astronauts outside the protective shield of the Earth's magnetosphere [61]. This is similar to the data mining research project just beginning at George Mason University with this author [56].

Additional recent work includes investigations into robust ML for terascale astronomical datasets [5],

In addition to these papers, several astronomy-specific data mining projects are underway. These include AstroWeka (http://astroweka.sourceforge.net/), Grist (Grid Data Mining for Astronomy; http://grist.caltech.edu), the Laboratory for Cosmological Data Mining (http://lcdm.astro.uiuc.edu/), the LSST Data Mining Research study group ([18]), the Transient Classification Project at Berkeley [11], and the soon-to-be commissioned Palomar Transient Factory.

We will now look at more specific astronomical applications that employed ML and data mining techniques. We have not covered everything (e.g., other methods that have been applied to astronomical data mining include principal component analysis, kernel regression, random forests, and various nearest-neighbor methods, such as [80, 30, 36, 21, 27, 6]).

2.3.1 Bayesian Analysis

A search of ADS lists 575 refereed papers in which the words Bayes or Bayesian appear in the paper's abstract. For comparison, the same search criteria returned 2313 abstracts of all papers (referred and non-referred). Seven of the refereed papers were published before 1980 (none published before 1970). One of these was by Sebok [67]. He applied Bayesian probability analysis to the most basic astronomical classification problem – distinguishing galaxies from stars among the many thousands of objects detected in large images. This is a critical problem in astronomy, since the study of stars is a vastly different astrophysics regime than the study of galaxies. To know which objects in the image are stars, and hence which objects are galaxies, is critical to the science. It may seem that this is an obvious distinction, but that is only true for nearby galaxies, which appear large on the sky (with large angular extent). This is not true at all for very distant galaxies, who provide the most critical information about the origin and history of our Universe. These distant galaxies appear as small blobs on images, almost indistinguishable from stars – nearly 100% of the stars are in our Milky Way Galaxy, hence very very nearby (by astronomical standards), and consequently stars therefore carry much less cosmological significance.

A more recent example is the application of Bayesian analysis to the problem of star formation in young galaxies [45]: the authors applied a Bayesian Markov Chain Monte Carlo method to determine whether the stars in the galaxies form in one monolithic collapse of a giant gas cloud, or if they form in a hierarchical fashion (with stars forming in smaller galaxies forming first, then those galaxies merge to become larger galaxies, and so on). The latter seems to be the best model to fit the observational data.

The above examples illustrate a very important point. The large number of papers that refer to Bayes analysis does not indicate the number that are doing data mining. This is because Bayesian analysis is used primarily as a statistical analysis technique or as a probability density estimation technique. The latter is certainly applicable to classification problems, but not on a grand scale as we expect for data mining (i.e., discovering hidden knowledge contained in large databases).

One significant recent paper that applies Bayesian analysis in a data mining sense focuses on a very important problem in large-database astronomy: cross-identification of astronomical sources in multiple large data collections [26]. In order to match the same object across multiple catalogs, the authors have proposed the use of more than just spatial coincidence, but also include numerous physical properties, including colors, redshift (distance), and luminosity. The result is an efficient algorithm that is ready for petascale astronomical data mining.

2.3.2 Decision Trees

A search of ADS lists 21 refereed papers (166 abstracts of all types) in which "Decision Tree" appears in the abstract. One of the earliest (non-refereed) conference papers was the 1994 paper by Djorgovski, Wier, and Fayyad [34], when Fayyad was working at NASA's Jet Propulsion Lab. This paper described the SKICAT classification system, which was the standard example of astronomical data mining quoted in many data mining conference talks subsequently. The earliest paper we could find in astronomy was in 1975 [43], 16 years before the next paper appeared. The 1975 paper addressed a "new methodology to integrate planetary quarantine requirements into mission planning, with application to a Jupiter orbiter".

Decision trees have been applied to another critical research problem in astronomy by [66] – the identification of cosmic ray (particle radiation) contamination in astronomical images. Charge-coupled device (CCD) cameras not only make excellent light detectors, they also detect high-energy particles that permeate space. Cosmic-ray particles deposit their energy and create spikes in CCD images (in the same way that a light photon does). The cosmic-ray hits are random (as the particles enter the detector randomly from ambient space) – they have nothing to do with the image. Understanding the characteristics of these bogus "events" (background noise) in astronomical images and being able to remove them are very important steps in astronomical image processing. The decision tree classifiers employed by [66] produced 95% accuracy. Recently, researchers have started to investigate the application of neural networks to the same problem [78] (and others).

2.3.3 Neural Networks

A search of ADS lists 418 refereed papers in which the phrases "Neural Net" or "Neural Network" appear in the paper's abstract. For comparison, the same search criteria returned over 10,000 abstracts of all papers (refereed and non-refereed, most of which are not in astronomy; see §2.3). The earliest of these refereed papers that appeared in an astronomical journal [44] (published in 1986) addressed neural networks and simulated annealing algorithms in general. One of the first real astronomical examples that was presented in a refereed paper [2] applied a neural network to the problem of rapid adaptive mirror adjustments in telescopes in order to dramatically improve image quality.

As mentioned above, artificial neural networks (ANN) have been applied to the problem of cosmic-ray detection CCD images. ANN have also been applied to another important problem mentioned earlier: star-galaxy discrimination (classification) in large images. Many authors have applied ANN to this problem, including [54, 55, 8, 48, 1, 29, 59, 62]. Of course, this astronomy research problem has been tackled by many algorithms, including decision trees [4].

Two other problems that have received a lot of astronomical research attention using neural networks are: (a) the classification of different galaxy types within large databases of galaxy data (e.g., [68, 53, 40, 3]); and (b) the determinant

nation of the photometric redshift estimate, which is used as an approximator of distance for huge numbers of galaxies, for which accurate distances are not known (e.g., [37, 28, 74, 57]). The latter problem has also been investigated recently using random forests [27] and support vector machines.

2.3.4 Support Vector Machines (SVM)

ADS lists 154 abstracts (refereed and non-refereed) that include the phrase "Support Vector Machine", of which 21 of these are refereed astronomy journal papers. Three of the latter focus on the problem mentioned earlier: determination of the photometric redshift estimate for distant galaxies [76, 79, 77]. Note that [77] also applies a kernel regression method to the problem – the authors find that kernel regression is slightly more accurate than SVM, but they discuss the positives and negatives of the two methods. SVM was used in conjunction with a variety of other methods to address the problem of cross-identification of astronomical sources in multiple data collections that was described earlier [64, 65]. SVM has also been used by several authors for forecasting solar flares and solar wind-induced geostorms, including [38, 63, 61].

3 Data-Intensive Science

The development of models to describe and understand scientific phenomena has historically proceeded at a pace driven by new data. The more we know, the more we are driven to tweak or to revolutionize our models, thereby advancing our scientific understanding. This data-driven modeling and discovery linkage has entered a new paradigm [49]. The acquisition of scientific data in all disciplines is now accelerating and causing a nearly insurmountable data avalanche [10]. In astronomy in particular, rapid advances in three technology areas (telescopes, detectors, and computation) have continued unabated - all of these advances lead to more and more data [9]. With this accelerated advance in data generation capabilities, humans will require novel, increasingly automated, and increasingly more effective scientific knowledge discovery systems [16].

To meet the data-intensive research challenge, the astronomical research community has embarked on a grand information technology program, to describe and unify all astronomical data resources worldwide. This global interoperable virtual data system is referred to as the National Virtual Observatory (NVO, at www.us-vo.org) in the U.S., or more simply the "Virtual Observatory" (VO). Within the international research community, the VO effort is steered by the International Virtual Observatory Alliance (IVOA at www.ivoa.net). This grand vision encompasses more than a collection of data sets. The result is a significant evolution in the way that astrophysical research, both observational and theoretical, is conducted in the new millennium [51]. This revolution is leading to an entirely new branch of astrophysics research - Astroinformatics - still in its infancy, consequently requiring further research and development as a discipline in order to aid in the data-intensive astronomical science that is

emerging [22].

The VO effort enables discovery, access, and integration of data, tools, and information resources across all observatories, archives, data centers, and individual projects worldwide [60]. However, it remains outside the scope of the VO projects to generate new knowledge, new models, and new scientific understanding from the huge data volumes flowing from the largest sky survey projects [8, 9]. Even further beyond the scope of the VO is the ensuing feedback and impact of the potentially exponential growth in new scientific knowledge discoveries back onto those telescope instrument operations. In addition, while the VO projects are productive science-enabling I.T. research and development projects, they are not specifically *scientific* (astronomical) research projects. There is still enormous room for scientific data portals and data-intensive science research tools that integrate, mine, and discover new knowledge from the vast distributed data repositories that are now VO-accessible [16, 19].

The problem therefore is this: astronomy researchers will soon (if not already) lose the ability to keep up with any of these things: the data flood, the scientific discoveries buried within, the development of new models of those phenomena, and the resulting new data-driven follow-up observing strategies that are imposed on telescope facilities to collect new data needed to validate and augment new discoveries.

4 Astronomy Sky Surveys as Data Producers

A common feature of modern astronomical sky surveys is that they are producing massive (terabyte) databases. New surveys may produce hundreds of terabytes (TB) up to 100 (or more) petabytes (PB) both in the image data archive and in the object catalogs (databases). Interpreting these petabyte catalogs (*i.e.*, mining the databases for new scientific knowledge) will require more sophisticated algorithms and networks that discover, integrate, and learn from distributed petascale databases more effectively [42], [46].

4.1 The LSST Sky Survey Database

One of the most impressive astronomical sky surveys being planned for the next decade is the Large Synoptic Survey Telescope project (LSST at www.lsst.org) [73]. The three fundamental distinguishing astronomical attributes of the LSST project are:

1. Repeated temporal measurements of all observable objects in the sky, corresponding to thousands of observations per each object over a 10-year period, expected to generate 10,000-100,000 alerts each night - an alert is a signal (e.g., XML-formatted news feed) to the astronomical research community that something has changed at that location on the sky: either the brightness or position of an object, or the serendipitous appearance of some totally new object;

- 2. Wide-angle imaging that will repeatedly cover most of the night sky within 3 to 4 nights (= tens of billions of objects); and
- 3. Deep co-added images of each observable patch of sky (summed over 10 years: 2016-2026), reaching far fainter objects and to greater distance over more area of sky than other sky surveys [69].

Compared to other astronomical sky surveys, the LSST survey will deliver time domain coverage for orders of magnitude more objects. It is envisioned that this project will produce ~ 30 TB of data per each night of observation for 10 years. The final image archive will be ~ 70 PB (and possibly much more), and the final LSST astronomical object catalog (object-attribute database) is expected to be ~ 10 -20 PB.

LSST's most remarkable data product will be a 10-year "movie" of the entire sky = "Cosmic Cinematography". This time-lapse coverage of the night sky will open up time-domain astronomy like no other project has been able to do previously. In general, astronomers have a good idea of what things in the sky are varying and what things are not varying, as a result of many centuries of humans staring at the sky, with and without the aid of telescopes. But, there is so much more possibly happening that we are not aware of at the very faintest limits simply because we have not explored the sky systematically night after night on a large scale. When an unusual time-dependent event occurs in the sky (e.g., a gamma-ray burst, supernova, or in-coming asteroid), astronomers (and others) will not only want to examine spatial coincidences of this object within the various surveys, but they will also want to search for other data covering that same region of the sky that were obtained at the same time as this new temporal event. These contextual data will enable more robust classification and characterization of the temporal event. Because of the time-criticality and potential for huge scientific payoff of such follow-up observations of transient phenomena, the classification system must also be able to perform time-based searches very efficiently and very effectively (i.e., to search all of the distributed VO databases as quickly as possible). One does not necessarily know in advance if such a new discovery will appear in any particular waveband, and so one will want to examine all possible astronomical sky surveys for coincidence events. Most of these "targets of opportunity" will consequently be added immediately to the observing programs of many ground-based and space-based astronomical telescopes, observatories, and on-going research experiments worldwide.

4.2 The LSST Data-Intensive Science Challenge

LSST is not alone. It is one (likely the biggest one) of several large astronomical sky survey projects beginning operations now or within the coming decade. LSST is by far the largest undertaking, in terms of duration, camera size, depth of sky coverage, volume of data to be produced, and real-time requirements on operations, data processing, event-modeling, and follow-up research response. One of the key features of these surveys is that the main telescope facility will be

dedicated to the primary survey program, with no specific plans for follow-up observations. This is emphatically true for the LSST project [52]. Paradoxically, the follow-up observations are scientifically essential - they contribute significantly to new scientific discovery, to the classification and characterization of new astronomical objects and sky events, and to rapid response to short-lived transient sky phenomena.

Since it is anticipated that LSST will generate many thousands (probably tens of thousands) of new astronomical event alerts per night of observation, there is a critical need for innovative follow-up procedures. These procedures necessarily must include modeling of the events - to determine their classification, time-criticality, astronomical relevance, rarity, and the scientifically most productive set of follow-up measurements. Rapid time-critical follow-up observations, with a wide range of time scales from seconds to days, are essential for proper identification, classification, characterization, analysis, interpretation, and understanding of nearly every astrophysical phenomenon (e.g., supernovae, novae, accreting black holes, microquasars, gamma-ray bursts, gravitational microlensing events, extrasolar planetary transits across distant stars, new comets, incoming asteroids, trans-Neptunian objects, dwarf planets, optical transients, variable stars of all classes, and anything that goes "bump in the night").

4.3 Petascale Data Mining with the LSST

LSST and similar large sky surveys have enormous potential to enable countless astronomical discoveries. Such discoveries will span the full spectrum of statistics: from rare one-in-a-billion (or one-in-a-trillion) type objects, to a complete statistical and astrophysical specification of a class of objects (based upon millions of instances of the class). One of the key scientific requirements of these projects therefore is to learn rapidly from what they see. This means: (a) to identify the serendipitous as well as the known; (b) to identify outliers (e.g., "front-page news" discoveries) that fall outside the bounds of model expectations; (c) to identify rare events that our models say should be there; (d) to find new attributes of known classes; (e) to provide statistically robust tests of existing models; and (f) to generate the vital inputs for new models. All of this requires integrating and mining of all known data: to train classification models and to apply classification models.

LSST alone is likely to throw such data mining and knowledge discovery efforts into the petascale realm. For example: astronomers currently discover ~ 100 new supernovae (exploding stars) per year. Since the beginning of human history, perhaps $\sim 10,000$ supernovae have been recorded. The identification, classification, and analysis of supernovae are among the key science requirements for the LSST Project to explore Dark Energy - *i.e.*, supernovae contribute to the analysis and characterization of the ubiquitous cosmic Dark Energy. Since supernovae are the result of a rapid catastrophic explosion of a massive star, it is imperative for astronomers to respond quickly to each new event with rapid follow-up observations in many measurement modes (light curves; spectroscopy; images of the host galaxy's environment). Historically, with <10 new supernovae

being discovered each week, such follow-up has been feasible. But now, LSST promises to produce a list of 1000 new supernovae each night for 10 years [69], which represent a small fraction of the total (10-100 thousand) alerts expected each night! Astronomers are faced with the enormous challenge of efficiently mining, correctly classifying, and intelligently prioritizing a staggering number of new events for follow-up observation each night for a decade.

The major features and contents of the LSST scientific database include:

- -->100 database tables
- Image metadata = 675M rows
- Source catalog = 260B rows
- Object catalog = 22B rows, with 200+ attributes
- Moving Object catalog
- Variable Object catalog
- Alerts catalog
- Calibration metadata
- Configuration metadata
- Processing metadata
- Provenance metadata

Many possible scientific data mining use cases are anticipated with the LSST database, including:

- Provide rapid probabilistic classifications for all 10,000 LSST events each night;
- Find new "fundamental planes" of parameters (e.g., the fundamental plane of Elliptical galaxies);
- Find new correlations, associations, relationships of all kinds from 100+ attributes in the science database;
- Compute N-point correlation functions over a variety of spatial and astrophysical parameters;
- Discover voids or zones of avoidance in multi-dimensional parameter spaces (e.g., period gaps);
- Discover new and exotic classes of astronomical objects, while discovering new properties of known classes;
- Discover new and improved rules for classifying known classes of objects (e.g., photometric redshifts);
- Identify novel, unexpected behavior in the time domain from time series data of all known variable objects;
- Hypothesis testing verify existing (or generate new) astronomical hypotheses with strong statistical confidence, using millions of training samples;

- Serendipity discover the rare one-in-a-billion type of objects through outlier detection; and
- Quality assurance identify glitches, anomalies, image processing errors through deviation detection.

Some of the data mining research challenge areas posed by the petascale LSST scientific database include:

- scalability (at petabytes scales) of existing ML and data mining algorithms;
- development of grid-enabled parallel data mining algorithms;
- designing a robust system for brokering classifications from the LSST event pipeline;
- multi-resolution methods for exploration of petascale databases;
- visual data mining algorithms for visual exploration of the massive databases;
- indexing of multi-attribute multi-dimensional astronomical databases (beyond sky-coordinate spatial indexing); and
- rapid querying of petabyte databases.

5 A Classification Broker for Astronomy

We are beginning to assemble user requirements and design specifications for a ML engine (data integration network plus data mining algorithms) to address the petascale data mining needs of the LSST and other large data-intensive astronomy sky survey projects. The data requirements surpass those of the current Sloan Digital Sky Survey (SDSS, at www.sdss.org) by 1000-10,000 times, while the time-criticality requirement (for event/object classification and characterization) drastically drops from months (or weeks) down to minutes (or tens of seconds). In addition to the follow-up classification problem (described above), astronomers also want to find every possible new scientific discovery (pattern, correlation, relationship, outlier, new class, etc.) buried within these new enormous databases. This might lead to a petascale data mining compute engine that runs in parallel alongside the data archive, testing every possible model, association, and rule. We will focus here on the time-critical data mining engine (i.e., classification broker) that enables rapid follow-up science for the most important and exciting astronomical discoveries of the coming decade, on a wide range of time scales from seconds to days, corresponding to a plethora of exotic astrophysical phenomena.

5.1 Broker Specifications: AstroDAS

The classification broker's primary specification is to produce and distribute scientifically robust near-real-time classification of astronomical sources, events, objects, or event host objects (i.e., the astronomical object that hosts the event; e.g., the host galaxy for some distant supernova explosion – it is important to measure the redshift distance of the host galaxy in order to interpret and to classify properly the supernova). These classifications are derived from integrating and mining data, information, and knowledge from multiple distributed data repositories. The broker feeds off existing robotic telescope and astronomical alert networks world-wide, and then integrates existing astronomical knowledge (catalog data) from the VO. The broker may eventually provide the knowledge discovery and classification service for LSST, a torrential fire hose of data and astronomical events.

Incoming event alert data will be subjected to a suite of ML algorithms for event classification, outlier detection, object characterization, and novelty discovery. Probabilistic ML models will produce rank-ordered lists of the most significant and/or most unusual events. These ML models (e.g., Bayesian networks, decision trees, multiple weak classifiers, Markov models, or perhaps scientifically derived similarity metrics) will be integrated with astronomical taxonomies and ontologies that will enable rapid information extraction, knowledge discovery, and scientific decision support for real-time astronomical research facility operations - to follow up on the 10-100K alertable astronomical events that will be identified each night for 10 years by the LSST sky survey.

The classification broker will include a knowledgebase to capture the new labels (tags) that are generated for the new astronomical events. These tags are annotations to the events. "Annotation" refers to tagging the data and metadata content with descriptive terms. For this knowledgebase, we envision a collaborative tagging system, called AstroDAS (Astronomy Distributed Annotation System) [24]. AstroDAS is similar to existing science knowledgebases, such as BioDAS (biodas.org), WikiProteins (www.wikiprofessional.info), the Heliophysics Knowledgebase (HPKB; www.lmsal.com/helio-informatics/hpkb/), and The Entity Describer [41]. AstroDAS is "distributed" in the sense that the source data and metadata are distributed, and the users are distributed. "Annotation" refers to tagging the data and metadata content with descriptive terms, which apply to individual data granules or to subsets of the data. It is a "system" with a unified schema for the annotation database, where distributed data are perceived as a unified data system to the user. One possible implementation of AstroDAS could be as a Web 2.0 scientific data and information mashup (=Science2.0). AstroDAS users will include providers (authors) and annotation users (consumers). Consumers (humans or machines) will eventually interact with AstroDAS in four ways:

- 1. Integrate the annotation database content within their own data portals, providing scientific content to their own communities of users.
- 2. Subscribe to receive notifications when new sources are annotated or clas-

sified.

- 3. Use the classification broker as a data integration tool to broker classes and annotations between sky surveys, robotic telescopes, and data repositories.
- 4. Query the annotation database (either manually or through web services).

In the last case, the users include the astronomical event message producers, who will want to issue their alerts with their best-estimate for the astronomical classification of their event. The classification will be generated through the application of ML algorithms to the networked data accessible via the VO, in order to arrive at a prioritized list of classes, ordered by probability of certainty. In order to facilitate these science use cases (and others not listed here), AstroDAS must have the following features: (a) it must enable collaborative, dynamic, distributed sharing of annotations; (b) it must access databases, data repositories, grids, and web services; (c) it must apply ontologies, semantics, dictionaries, annotations, and tags; and (d) it must employ data/text mining, ML, and information extraction algorithms.

5.2 Collaborative Annotation of Classes

Machine learning and data mining algorithms, when applied to very large data streams, could possibly generate the classification labels (tags) autonomously. Generally, scientists do not want to leave this decision-making to machine intelligence alone - they prefer to have human intelligence in the loop also. When humans and machines work together to produce the best possible classification label(s), this is collaborative annotation. Collaborative annotation is a form of Human Computation [75]. Human Computation refers to the application of human intelligence to solve complex difficult problems that cannot be solved by computers alone. Humans can see patterns and semantics (context, content, and relationships) more quickly, accurately, and meaningfully than machines. Human Computation therefore applies to the problem of annotating, labeling, and classifying voluminous data streams. Of course, the application of autonomous machine intelligence (data mining and ML) to the annotation, labeling, and classification of data granules is also valid and efficacious. The combination of both human and machine intelligence is critical to the success of AstroDAS as a classification broker for enormous data-intensive astronomy sky survey projects, such as LSST.

5.3 A Research Agenda

We identify some of the key research activities that must be addressed, in order to promote the development of a ML-based classification broker for petascale mining of large-scale astronomy sky survey databases. Many of these research activities are already being pursued by other data mining and computational science researchers - we hope to take advantage of all such developments, many

of which are enabled through advanced next-generation data mining and cyber-infrastructure research:

- 1. Before the classification labels can be useful, we must reach community consensus on the correct set of semantic ontological, taxonomical, and classification terms. There are ontologies under development in astronomy already their completeness, utility, and usability need to be researched.
- Research into user requirements and scientific use cases will be required in order that we design, develop, and deploy the correct user-oriented petascale data mining system.
- 3. A complete set of classification rules must be researched and derived for all possible astronomical events and objects. For objects and events that are currently unknown, we need to identify robust outlier and novelty detection rules and classifiers. These need to be researched and tested.
- 4. We need to research and collect comprehensive sets of training examples for the numerous classes that we hope to classify. With these samples, the classification broker will be trained and validated.
- 5. Algorithms for web services-based (perhaps grid-based or peer-to-peer) classification and mining of distributed data must be researched, developed, and validated. These mining algorithms should include text mining as well as numeric data mining, perhaps an integrated text-numeric data mining approach will be most effective and thus needs to be researched.
- 6. User interface and interaction models will need to be researched through prototypes and demonstrations of the classification broker.
- Research into the robust integration of the many AstroDAS system components will be needed. This will require investigation of different modes of interaction and integration, such as grids, web services, RSS feeds, ontologies (expressed in RDF or OWL), linked databases, etc.
- 8. Deploy a working classification broker on a live astronomical event message stream, to research its functionality, usefulness, bottlenecks, failure modes, security, robustness, and (most importantly) scalability (from the current few events per night, up to many tens of thousands of events per night in the coming decade). Fortunately, there are such event message feeds available today, though on a much smaller scale than that anticipated from LSST.

Clearly, this is an ambitious research agenda. It will not be fully accomplished in just a year or two. It will require several years of research and development. This is fortunate, since the most dramatic need for the classification broker system for astronomy will come with the start-up of LSST sky survey operations in 2016, lasting ten years (until 2026). So, we have a few years to get it right, and we will need all of those years to complete the challenging research program described above.

6 Introducing the New Science of Astroinformatics

As described above, today's astronomical research environment is highly focused on the design, implementation, and archiving of very large sky surveys. Many projects today (e.g., Palomar-Quest Synoptic Sky Survey [PQ], Sloan Digital Sky Survey [SDSS], and 2-Micron All Sky Survey [2MASS]) plus many more projects in the near future (e.g., LSST, Palomar Transient Factory [PTF], Supernova Acceleration Probe [SNAP], Panoramic Survey Telescope And Rapid Response System [Pan-STARRS], and Dark Energy Survey [DES]) are destined to produce enormous catalogs of astronomical sources. The virtual collection of these gigabyte, terabyte, and (eventually) petabyte catalogs will significantly increase science return and enable remarkable new scientific discoveries through the integration and cross-correlation of data across these multiple survey dimensions. Astronomers will be unable to tap the riches of this data lode without a new paradigm for astroinformatics that involves distributed database queries and data mining across distributed virtual tables of de-centralized, joined, and integrated sky survey catalogs. The challenges posed by this problem are daunting, as in most disciplines today that are producing data floods at prodigious rates.

The development and deployment of the astronomy Virtual Observatory (VO) is perceived by some as the solution to this problem. The VO provides one-stop shopping for all end-user data needs, including access to distributed heterogeneous data, services, and other resources (e.g., the GRID). Some grid-based data mining services are already envisioned or in development (e.g., GRIST at http://grist.caltech.edu/, the Datamining Grid, and F-MASS at http://www.itsc.uah.edu/f-mass/). However, processing and mining the associated distributed and vast data collections are fundamentally challenging since most off-the-shelf data mining systems require the data to be downloaded to a single location before further analysis. This imposes serious scalability constraints on the data mining system and fundamentally hinders the scientific discovery process. If distributed data repositories are to be really accessible to a larger community, then technology ought to be developed for supporting distributed data analysis that can reduce, as much as possible, communication requirements.

The new science of astroinformatics will emerge from this large and expanding distributed heterogeneous data environment. We define astroinformatics as the formalization of data-intensive astronomy for research and education [19, 20]. Astroinformatics will borrow heavily from concepts in the fields of bioinformatics and geoinformatics (i.e., GIS = Geographic Information Systems). The main features of this new science are: it is data-driven, data-centric, and data-inspired. As bioinformatics represents an entirely new paradigm for research in the biological sciences, beyond computational biology, so also does astroinformatics represent a new mode of data-intensive scientific research in astronomy that is cognizant of and dependent on the astronomical flood of astronomical

data that is now upon us. Data mining and knowledge discovery will become the killer apps for this mode of scientific research and discovery. Scientific databases will be the "virtual sky" that astronomers will study and mine. New scientific understanding will flow from the discovered knowledge, which is derived from the avalanche of information content, which is extracted from the massive data collections.

6.1 Distributed Scientific Data Mining

Distributed data mining (DDM) of large scientific data collections will become the norm in astronomy, as the data collections (from the numerous large sky surveys) become so large that they cannot all be downloaded to a central site for mining and analysis. DDM algorithms will be an essential tool to enable discovery of the hidden knowledge buried among geographically dispersed heterogeneous databases [14, 15, 50, 39, 35].

As an example of the potential astronomical research that DDM will enable, we consider the large survey databases being produced (now and in the near future) by various NASA missions. GALEX is producing all-sky surveys at a variety of depths in the near-UV and far-UV. The Spitzer Space Telescope is conducting numerous large-area surveys in the infrared, including regions of sky (e.g., the Hubble Deep Fields) that are well studied by the Hubble Space Telescope (optical), Chandra X-ray Observatory, and numerous other observatories. The WISE mission (to be launched circa 2009) will produce an all-sky infrared survey. The 2-Micron All-Sky Survey (2MASS) has catalogued millions of stars and galaxies in the near-infrared. Each of these wavebands contributes valuable astrophysical knowledge to the study of countless classes of objects in the astrophysical zoo. In many cases, such as the young star-forming regions within starbursting galaxies, the relevant astrophysical objects and phenomena have unique characteristics within each wavelength domain. For example, starbursting galaxies are often dust-enshrouded, yielding enormous infrared fluxes. Such galaxies reveal peculiar optical morphologies, occasional X-ray sources (such as intermediate black holes), and possibly even some UV bright spots as the shortwavelength radiation leaks through holes in the obscuring clouds. All of these data, from multiple missions in multiple wavebands, are essential for a full characterization, classification, analysis, and interpretation of these cosmologically significant populations.

In order to reap the full potential of scientific data mining, analysis, and discovery that this distributed data environment enables, it is essential to bring together data from multiple heterogeneously distributed data sites. For the all-sky surveys in particular (such as 2MASS, WISE, GALEX, SDSS, LSST), it is impossible to access, mine, navigate, browse, and analyze these data in their current distributed state. To illustrate this point, suppose that an all-sky catalog contains descriptive data for one billion objects; and suppose that these descriptive data consist of a few hundred parameters (which is typical for the 2MASS and Sloan Digital Sky Surveys). Then, assuming simply that each parameter requires just 2-byte representation, then each survey database will

consume one terabyte of space. If the survey also has a temporal dimension (such as the LSST, which will re-image each object 1000-2000 times), then massively more data handling is required in order to mine the enormous potential of the database contents. If each of these catalog entries and attributes requires only one CPU cycle to process it (e.g., in a data mining operation), then many teraflops (up to petaflops) of computation will be required even for the simplest data mining application on the full contents of the databases.

It is clearly infeasible, impractical, and impossible to drag these terabyte (and soon, petabyte) catalogs back and forth from user to user, from data center to data center, from analysis package to package, each time someone has a new query to pose against these various data collections. Therefore, there is an urgent need for novel DDM algorithms that are inherently designed to work on distributed data collections. We are consequently focusing our research efforts on these problems [39, 35].

6.2 Beyond the Science

Before we conclude, it is important to mention how these scientific data mining concepts are also relevant to science, mathematics, and technical education in our society today [20]. The concept of "Using Data in the Classroom" is developing quite an appeal among inquiry-based learning proponents². Astronomy data and images in particular have a special universal appeal to students, general public, and all technical experts. Student-led data mining projects that access large astronomical databases may lead to discoveries of new comets, asteroids, exploding stars, and more. Members of both the LSST and the NVO project scientific teams are especially interested in this type of collaboration among scientists, data mining experts, educators, and students. The classroom activities (involving "cool astronomy data") are engaging and exciting to students and thus contribute to the overall scientific, technical, and mathematical literacy of the nation. Astroinformatics enables transparent data sharing, reuse, and analysis in inquiry-based science classrooms. This allows not only scientists, but also students, educators, and citizen scientists to tackle knowledge discovery problems in large astronomy databases for fun and for real. This integrated research and education activity matches well to the objectives of the new CODATA ADMIRE (Advanced Data Methods and Information technologies for Research and Education) initiative (www.iucr.org/iucr-top/data/docs/codataga2006_beijing.html). Students are trained: (a) to access large distributed data repositories; (b) to conduct meaningful scientific inquiries into the data; (c) to mine and analyze the data; and (d) to make data-driven scientific discoveries [23].

6.3 Informatics for Scientific Knowledge Discovery

Finally, we close with discussions of BioDAS (the inspiration behind AstroDAS) and of the relevance of informatics (e.g., Bioinformatics and Astroinformatics) to the classification broker described earlier. Informatics is the discipline

 $^{^2}$ http://serc.carleton.edu/usingdata/

of organizing, accessing, mining, analyzing, and visualizing data for scientific discovery. Another definition says informatics is the set of methods and applications for integration of large datasets across spatial and temporal scales to support decision-making, involving computer modeling of natural systems, heterogeneous data structures, and data-model integration as a framework for decision-making³.

Massive scientific data collections impose enormous challenges to scientists: how to find the most relevant data, how to reuse those data, how to mine data and discover new knowledge in large databases, and how to represent the newly discovered knowledge. The bioinformatics research community is already solving these problems with BioDAS (Biology Distributed Annotation System). The DAS provides a distributed system for researchers anywhere to annotate (markup) their own knowledge (tagged information) about specific gene sequences. Any other researcher anywhere can find this annotation information quickly for any gene sequence. Similarly, astronomers can annotate individual astronomical objects with their own discoveries. These annotations can be applied to observational data/metadata within distributed digital data collections. The annotations provide mined knowledge, class labels, provenance, and semantic (scientifically meaningful) information about the experiment, the experimenter, the object being studied (astronomical object in our case, or gene sequence in the case of the bioinformatics research community), the properties of that object, new features or functions discovered about that object, its classification, its connectiveness to other objects, and so on.

Bioinformatics (for biologists) and Astroinformatics (for astronomers) provide frameworks for the curation, discovery, access, interoperability, integration, mining, classification, and understanding of digital repositories through (human plus machine) semantic annotation of data, information, and knowledge. We are focusing new research efforts on further development of Astroinformatics as: (1) a new subdiscipline of astronomical research (similar to the role of bioinformatics and geoinformatics as stand-alone subdisciplines in biological and geoscience research and education, respectively); and (2) the new paradigm for data-intensive astronomy research and education [19, 20], which focuses on existing cyberinfrastructure such as the astronomical Virtual Observatory.

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