Data Analysis Challenge 1: Astroinformatics

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Data Doubles Every Year

- Computing power doubles every 18 months (Moore’s Law) ...
  - 100x in 10 years

- I/O bandwidth increases ~10% / year
  - <3x in 10 years.

- Data doubles every year ...
  - 1000x in 10 years, and 1,000,000x in 20 yrs.

  - NCSA Example:
    - First 19 years: 1 PB
    - Year 20 (2007): 2 PB
    - Year 21 (2008): 4 PB
    - By 2020: ~20 Exabytes?

  - In the Year 2525: $10^{156}$ PB ?????

- As our data volumes grow, especially in the sciences (where scientific funding for research barely grows at all), we will fall farther and farther behind in our ability to analyze, assimilate, and extract knowledge from our data collections ... unless we develop and apply exponentially more powerful algorithms and methods.

(Illustration adapted from a slide by J. Heer, PARC User Interface Research Group)
Outline

• Astroinformatics
• Example Application: The LSST Project
• Informatics Use Cases in Astronomy
• Challenge Area: Distributed Data Mining
• Summary
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Astronomy: Data-Driven Science = Evidence-based Forensic Science
The Changing Landscape of Astronomical Research

• **Past:** 100’s to 1000’s of independent distributed heterogeneous data / metadata / information repositories.

• **Today:** Astronomical data are now accessible uniformly from federated distributed heterogeneous sources = the Virtual Observatory.

• **Future:** Astronomy is and will become even more data-intensive in the coming decade with the growth of massive data-producing sky surveys.

• **Challenge:** It will be prohibitively difficult to transport the data to the user application. Therefore … **SHIP THE CODE TO THE DATA!**
From Data-Driven to Data-Intensive

- Astronomy has always been a data-driven science.
- It is now a data-intensive science: welcome to Astroinformatics!

- Data-oriented Astronomical Research = "the 4th Paradigm"
- Scientific KDD (Knowledge Discovery in Databases):
  - Characterize the known (clustering, unsupervised learning)
  - Assign the new (classification, supervised learning)
  - Discover the unknown (outlier detection, semi-supervised learning)

- … Scientific Knowledge!

- Benefits of very large datasets:
  - best statistical analysis of "typical" events
  - automated search for "rare" events
Astronomy Data Environment: Sky Surveys

• To avoid biases caused by limited samples, astronomers now study the sky systematically = **Sky Surveys**

• Surveys are used to measure and collect data from all objects that are contained in large regions of the sky, in a systematic, controlled, repeatable fashion.

• These surveys include (... this is just a subset):
  – MACHO and related surveys for dark matter objects: ~ 1 Terabyte
  – Digitized Palomar Sky Survey: 3 Terabytes
  – 2MASS (2-Micron All-Sky Survey): 10 Terabytes
  – GALEX (ultraviolet all-sky survey): 30 Terabytes
  – Sloan Digital Sky Survey (1/4 of the sky): 40 Terabytes
  – and this one is just starting: Pan-STARRS: 40 Petabytes!

• **Leading up to the big survey next decade:**
  – LSST (Large Synoptic Survey Telescope): 100 Petabytes!
Sky Surveys: Partly the Solution and partly the Problem

As our chemistry friends say ....

If you're not part of the solution, you're part of the precipitate!
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LSST = Large Synoptic Survey Telescope
http://www.lsst.org/

(mirror funded by private donors)
8.4-meter diameter primary mirror = 10 square degrees!

Hello!

(designed, constructed, and operated by NSF; camera: DOE)
**LSST Key Science Drivers: Mapping the Universe**

- Solar System Map (moving objects, NEOs, asteroids: census & tracking)
- Nature of Dark Energy (distant supernovae, weak lensing, cosmology)
- Optical transients (of all kinds, with alert notifications within 60 seconds)
- Galactic Structure (proper motions, stellar populations, star streams, dark matter)

**LSST in time and space:**
- **When?** 2016-2026
- **Where?** Cerro Pachon, Chile
**Observing Strategy:** One pair of images every 40 seconds for each spot on the sky, then continue across the sky continuously every night for 10 years (2016-2026), with time domain sampling in log(time) intervals (to capture dynamic range of transients).

- **LSST (Large Synoptic Survey Telescope):**
  - Ten-year time series imaging of the night sky – mapping the Universe!
  - **100,000 events each night** – anything that goes bump in the night!
  - *Cosmic Cinematography! The New Sky!* @ http://www.lsst.org/

**Education and Public Outreach** have been an integral and key feature of the project since the beginning – the EPO program includes formal Ed, informal Ed, Citizen Science projects, and Science Centers / Planetaria.
The LSST focal plane array

Camera Specs: (pending funding from the DOE)
201 CCDs @ 4096x4096 pixels each!
= 3 Gigapixels = 6 GB per image, covering 10 sq.degrees
= ~3000 times the area of one Hubble Telescope image

LSST Data Challenges

- Obtain one 6-GB sky image in 15 seconds
- Process that image in 5 seconds
- Obtain & process another co-located image for science validation within 20s (= 15-second exposure + 5-second processing & slew)
- Process the 100 million sources in each image pair, catalog all sources, and generate worldwide alerts within 60 seconds (e.g., incoming killer asteroid)
- Generate 100,000 alerts per night (VOEvent messages)
- Obtain 2000 images per night
- Produce ~30 Terabytes per night
- Move the data from South America to US daily
- Repeat this every day for 10 years (2016-2026)
- Provide rapid DB access to worldwide community:
  - 100-200 Petabyte image archive
  - 20-40 Petabyte database catalog
The LSST Data Challenges

- 100,000 events every night
- 100 PB image archive
- 50 billion object database
- 20 PB science catalog
The LSST Data Challenges

MANAGING AND MINING THE LSST DATA SETS

Astronomy is undergoing an exciting revolution -- a revolution in the way we probe the universe and the way we answer fundamental questions. New technology enables this: novel detectors are opening new windows on the universe, creating unprecedented volumes of high quality data, and computing technology is keeping up with this explosion. In turn, this is driving a shift in the way science is produced in astronomy and astrophysics: huge surveys of the sky over wide wavelengths can be analyzed statistically for low-level correlations and inverse problems may be solved by statistical inversion, producing new understanding of the underlying physics.

This parallels progress in high energy physics. Decades ago, a handful of photographs of events sufficed for ground-breaking discoveries. This gave way to experiments in which the systematic measuring (scanning) of many bubble chamber pictures allowed the measurement of statistical properties, such as lifetimes. Current experiments extend the technique by recording all events electronically and subjecting Petabyte data sets to rigorous statistical analysis.

A key ingredient in mining our astronomical science from such huge databases, efficient algorithms for statistical analysis, has been under-emphasized in the rush to utilize new technology and get the data products out to the science community. Past data sets in astronomy (and indeed in most areas of science) have been small enough that one individual could visualize the data and discover unanticipated correlations. This is often how major discoveries have been made. Data sets are now becoming sufficiently large that this is less possible -- even prescribed processing of the data to test a hypothesis is becoming challenging.

In the near future, analysis of Petabyte databases will require the solution of this problem.

New Horizons

It is worthwhile to briefly review this sea-change in the way astronomers produce science. A giant departure from the tradition of one astronomer and one modest data set per project has been the Sloan Digital Sky Survey: a 15TB imaging data set covering multiple wavelengths and up to 10,000 square degrees of the sky (http://www.sdss.org/). Nearly 100 Co-Is will mine these data in prescribed ways. Current plans do not include mining the 15TB. Rather, 1TB of catalogs of detected objects and another 2TB of their "cutout" pictures will be produced and mined. Nevertheless, this will surely result in new understanding of our universe. Imagine what might be discovered if the full 15TB could be explored efficiently! Another refreshing and very successful departure from tradition is the 2MASS infrared survey of the sky (http://irsa.ipac.caltech.edu). This group has poured major effort into usability of the data products and efficient remote searching.

A New Collaboration

We see this research program attracting a broad range of mathematical, computer and physical scientists. In addition to the obvious connections to astronomy, statistics and large-scale computation, this program would also include probability, data visualization and data management. We would also seek to include representatives from the high-energy physics community, who have faced somewhat different problems involving massive data sets and immense data streams for many years now. Some representation from theoretical cosmologists who simulate universes would add to the mix and allow the question of comparing simulated universes to the actual universe to be more profitably addressed.

It will be particularly useful to study the characteristics of spatial processes, since it nicely combines the central computational and statistical challenges. Very little work has been done to date in this area, although a recent paper by Moore et al. (2001) recognizes the importance of this problem and describes an algorithm for computing estimates of higher order correlation functions that, for sufficiently large data sets, is much more efficient than the obvious approach.

We need not simply a theoretical study of how massive astronomical data sets should be analyzed, but major efforts to analyze the most recently available data sets. Data from the Sloan Digital Sky Survey should be publicly available by 2003. It will be useful to work with this database in new ways, searching for low-level correlations. Deeper imaging surveys, such as the Deep Lens Survey, are producing imaging data and catalogs nearly to the depth that LSST will reach, but over a very small area of sky by comparison to a decade of LSST operations. Such surveys are precursors to LSST and their data products will prove to valuable sand boxes for development of new algorithms.

A common technique in modern high-energy physics experiments is the "mock data challenge." The data stream, from detector, through data acquisition and processing, to final science analysis, is simulated at the appropriate level of detail. This allows a final acceptance testing of all data systems to be completed along with the hardware, so that full-up science operations can begin on a much better schedule, with good diagnostics in place. For the science, these studies are just as important. Analysis teams combing for subtle effects can, in then end, compare their result (and error estimate) with the "true" values of parameters that were in the simulation. Often, a sample of "real" data is used to get the background distribution of events correct. Using catalogs from the SDSS and the Deep Lens Survey as a basis for the mock data challenge for the LSST will make it more effective.
Bytes/flop? ... Flops/byte?
XLDB: an approach to petascale databases

• XLDB = eXtremely Large Databases
• Since 2007: 3 XLDB Workshops and 1 working meeting
• XLDB4 conference:
  – October 5-7, 2010 at Stanford/SLAC
  – Expect ~200 attendees
• The result is a new design for petabyte-scale scientific databases = SciDB
  – SciDB is based on the new array-based data model
  – Relational data model (RDBMS) is so “last century”
• References:
  – XLDB: http://xldb.org
  – SciDB: http://scidb.org
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The clustering problem:
- Finding clusters of objects within a data set
- What is the significance of the clusters (statistically and scientifically)?
- What is the optimal algorithm for finding friends-of-friends or nearest neighbors?
  - N is $>10^{10}$, so what is the most efficient way to sort?
  - Number of dimensions $\sim 1000$ – therefore, we have an enormous subspace search problem
- Are there pair-wise (2-point) or higher-order (N-way) correlations?
  - N is $>10^{10}$, so what is the most efficient way to do an N-point correlation?
    - algorithms that scale as $N^2\log N$ won’t get us there
Outlier detection: (unknown unknowns)

- Finding the objects and events that are outside the bounds of our expectations (outside known clusters)
- These may be real scientific discoveries or garbage
- Outlier detection is therefore useful for:
  - Novelty Discovery – *is my Nobel prize waiting?*
  - Anomaly Detection – *is the detector system working?*
  - Data Quality Assurance – *is the data pipeline working?*
- How does one optimally find outliers in $10^3$-D parameter space? or in interesting subspaces (in lower dimensions)?
- How do we measure their “interestingness”? 
The dimension reduction problem:

- Finding correlations and “fundamental planes” of parameters
- Number of attributes can be hundreds or thousands
  - The Curse of High Dimensionality!
- Are there combinations (linear or non-linear functions) of observational parameters that correlate strongly with one another?
- Are there eigenvectors or condensed representations (e.g., basis sets) that represent the full set of properties?
The superposition / decomposition problem:

- Finding distinct clusters (Classes of Object) among objects that overlap in parameter space.

- What if there are $10^{10}$ objects that overlap in a $10^3$-D parameter space?

- What is the optimal way to separate and extract the different unique classes of objects?

- How are constraints applied (as in operations research or linear programming)?
The optimization problem:
- Finding the optimal (best-fit, global maximum likelihood) solution to complex multivariate functions over very high-dimensional spaces.
Example: Beyond Exascale Computational & Data Science Challenge problem for LSST

• Find the optimal simultaneous solution for 20,000,000,000 objects’ shapes across 2000 image planes, each of which has 201x4096x4096 pixels ... $10^{23}$ floating-point operations!
  – This illustrates an example for just one such object:

References:
http://universe.ucdavis.edu/docs/MultiFit-ADASS.pdf
http://code.google.com/p/multifit/
The LSST Petascale Challenges


LSST Petascale Data R&D Challenges

Achieving scalability and reliability in LSST computing, storage, and network resources

The design of the DM system architecture is influenced by the technology. We expect to be available to implement it, starting with construction in 2011 – 2014 and continuing through the five-year period until 2024. This technology includes not only more powerful components, but completely new system architectures and potentially disruptive technologies. Most computing throughout improvements will come not from increased CPU clock speeds as in the past, but from larger concentrations of CPUs/cores and advanced computing architectures. Solid state technology may change storage and the way we physically organize data. Hardware failures will be routine for the LSST data system due to the large number of CPU's and disk drives, and reliance on high-speed network connectivity. It is a challenge to create a system sufficiently robust to these failures. We need to predict the characteristics of CPU, network, storage hardware, and system software sufficiently well that our design is appropriate. Further, we must insulate the design as much as possible from underlying platform dependencies.

Reliability and performance issues for very large databases

LSST’s main data products from the 20,000 square degree survey with 2000 images over ten years per patch of sky are in the form of relational database tables. These tables are very large (30 billion rows in the Object table, 600 billion rows in the Source table). They must be extensible, and partitioned and indexed to facilitate high query performance, and replicated across multiple centers. Queries in the time domain (Source table) are likely to be of equal importance to those in the spatial domain. Since these are traditionally optimized by different database organizations, it is unclear what choices will perform best for LSST. Some intensive applications will involve n-point correlations of object attributes over all objects. All these factors suggest that database performance and reliability are risk areas.

Efficient automated data quality assessment

LSST will produce large volumes of science data. The Data Management System (DMS) produces derived products for scientific use both during observing (e.g., alerts and supporting image and source data) and in daily and periodic reprocessing. The periodic reprocessing also results in released science products. Analysis of the nightly data will also provide insights into the health of the telescope/camera system. An automated data quality assessment system must be developed, which efficiently searches for outliers in raw image data and unusual correlations. This will involve aspects of machine learning.

Operational control and monitoring of the DMS

The DMS will be a complex distributed system with enormous data flows that operates 24/7. The DMS must be continuously monitored and controlled to ensure the proper functioning of all computing hardware, software, network connections, and software, including the data quality of the science pipelines. Most of the monitoring tasks, and some of the control tasks, must be highly automated, since the data volumes preclude human examination of all but a tiny fraction of the data.

Achieving acceptably low False Transient Alert Rate

The science mission places high demand on the LSST’s ability to rapidly and accurately detect and classify varying and transient objects and to achieve a low false alarm rate. Given the very high data volume produced by the LSST, the corresponding large number of detections in each image (up to one million objects detected per image), as well as the likelihood that the entire new class of transients will not be able to rely on traditional labor-intensive validation of detections, classifications, and alerts. To achieve the levels of accuracy required, new algorithms for detection and classification must be created, as well as innovative automated techniques for alert filtering and validation.

Efficient detection and orbit determination for solar system objects

One of the LSST’s science missions is to catalog the population of solar system objects, with a particular focus on potentially hazardous objects. Due to the depth of LSST’s images, about 300 solar system objects per square degree will be detected near the ecliptic. The LSST cadence on the sky is not optimized solely for tracking solar system objects, so this dense swarm of objects must be reliably tracked through considerable gaps in time. Algorithms must be developed that are robust to possible mis-associations of detections at different epochs, and have acceptable computational scalability.

Achieving required photometric accuracy and precision

The LSST Science Requirements Document (SRD) requires a level of photometric (intensity data) accuracy and precision that may be difficult to achieve over the entire sky, particularly since the LSST will be operating in a wide variety of seeing, sky brightness, and atmospheric extinction. To achieve this requires a thoroughly tested calibration procedure and associated image processing pipeline. In addition to the point-source requirements in the SRD, accurate photometric redshifts require precision photometry for spatially extended objects.

Achieving required astrometric accuracy and precision

The LSST SRD requires a level of astrometric (position on the sky) accuracy and precision that is difficult to achieve over the entire sky. Achieving this astrometric performance requires a global, whole-sky, numerical solution for all per-frame astrometric quantities that minimizes a cost function. Considerable work will be required to develop an effective cost function.

Achieving optimal object detection and shape measurement from stacks of images

Most objects that will be used for dark matter and energy science are too faint to be usefully measured in a single LSST exposure. Instead, the LSST must detect and measure the properties of objects combining information from multiple exposures of the same region of sky (image stacks). Weak lensing galaxy shape measurements are particularly vulnerable to systematic effects introduced by errors in the local point-spread function (PSF) determination, and these systematic effects must be minimized. Exposures may vary significantly in their signal-to-noise and PSF quality, and defining how to optimally combine information from all of them is a research problem.

Need to develop a flexible approach that enables highly reliable classification of objects

Classification of astronomical objects is important and difficult. A wide variety of information must be assessed to reliably classify an object. This includes spatial morphology in multiple colors, photometry in multiple colors, time dependent behavior, and astrometric motion. Further, the best classifications will make use of surveys in other wavelength regimes and spectral information where available, not solely information from the LSST. Experience from many surveys has shown that no single algorithm can do a good job on all objects. Rather, good algorithms tend to be specialists, limited to particular objects classes, e.g., eclipsing binaries or supernovae. A successful system must allow the development and incorporation of a wide variety of algorithms in a flexible manner.

Adaptive retuning of algorithm behavior

Several key algorithms employed in the LSST application pipelines are complex, containing many data-dependent decisions and a large number of tuning parameters that affect their behavior. As observing conditions change, an algorithm may begin to perform for a particular choice of tuning parameters. LSST’s extremely large data volume makes human intervention in such cases impractical, but it is essential that the pipelines continue to function successfully.

Need to verify scientific usefulness of the LSST database schema and its implementation against realistic queries

The LSST database schema must efficiently support queries of data that have many relationships between multiple locations on the sky, epochs of observation, and filters employed. A high performance has motivated this schema has many features of the current large scale database architecture and analysis task. The ultimate test of how well these tasks have been carried out is to perform science with the database. To do this usefully, we are simulating LSST data, using data from current surveys, and engaging the LSST Science Collaborations and scientific community.
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Distributed Data

- Distributed data are the norm (across people, institutions, projects, agencies, nations, ...)
- Data are usually heterogeneous (e.g., databases, images, catalogs, file systems, web interfaces, document libraries, binary, text, structured, unstructured, ...)
- Scientists want to query and to mine these data (= 2 different user scenarios)
- Virtual Observatory implementations enable data discovery and integration, but do not yet facilitate large-scale data mining
Data Bottleneck

• **Mismatch:**
  • Data volumes increase 1000x in 10 yrs
  • I/O bandwidth improves ~3x in 10 years

• DOE-identified problem areas: “(1) data movement, rather than computational operations, will be the limiting factor for exascale systems; (2) memory per core is expected to decline sharply; (3) the performance of storage systems will continue to lag far behind.”  (Ref: Exascale Co-Design Centers)

• Therefore . . . **Distributed Data Mining**
Distributed Data Mining (DDM)

- DDM comes in 2 types:
  1. **Distributed Mining** of Data
  2. Mining of **Distributed Data**

- Type 1 requires sophisticated algorithms that operate with data *in situ* ...
  - *Ship the Code to the Data*

- Type 2 takes many forms, with data being centralized (in whole or in partitions) or data remaining in place at distributed sites

Why Distributed Data Mining (DDM)?

Because ...

... many great scientific discoveries have come from inter-comparisons of diverse data sources:
- Quasars
- Gamma-ray bursts
- Ultraluminous IR galaxies
- X-ray black-hole binaries
- Radio galaxies
- ...

"Just checking."
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  1. Data Science Research Challenges
  2. Data Science in Education
Data Science Challenge Areas in Astronomy over the next 10 years – addressable by Astroinformatics

- Scalability of statistical, computational, & data mining algorithms to peta- and exa- scales
- Algorithms for optimization of simultaneous multi-point fitting across massive multi-dimensional data cubes
- Multi-resolution, multi-pole, fractal, hierarchical methods and structures for exploration of condensed representations of petascale databases
- Petascale analytics for visual exploratory data analysis of massive databases (including feature detection, pattern & interestingness discovery, correlation mining, clustering, class discovery, eigen-monitoring, dimension reduction)
- Indexing and associative memory techniques (trees, graphs, networks) for highly-dimensional petabyte databases
- Rapid query and search algorithms for petabyte databases
Astroinformatics Research paper available!

Addresses the data science challenges, research agenda, application areas, use cases, and recommendations for the new science of Astroinformatics.


See also http://arxiv.org/abs/0909.3892

State of the Profession position paper, submitted to the Astro2010 Decadal Survey
3/15/2009

Astroinformatics: A 21\textsuperscript{st} Century Approach to Astronomy

Authorship: This Position Paper was prepared and endorsed by the following team of 91 astronomers and information scientists (listed separately). The lead author is Kirk D. Borne (Dept. of Computational and Data Sciences, George Mason University, kborne@gmu.edu). The team maintains a web site that hosts information about the authors (including email addresses and links to web sites) and supporting information for this document: http://inference.astro.cornell.edu/Astro2010/.
Education in Data-Intensive Computational Science

Computational and Data Sciences

Combining science and computing to meet human needs ...

http://cds.gmu.edu/
Dept of Computational & Data Sciences
@ GMU (George Mason University)
Fairfax, VA
Informatics-based Science Education

- Informatics enables transparent reuse and analysis of scientific data in inquiry-based classroom learning (http://serc.carleton.edu/usingdata/).
- **Students are trained:**
  - to access large distributed data repositories
  - to conduct meaningful scientific inquiries into the data
  - to mine and analyze the data
  - to make data-driven scientific discoveries
- The 21st century workforce demands training and skills in these areas, as all agencies, businesses, and disciplines are becoming flooded with data.
- Numerous Data Sciences programs now starting at several universities (GMU, Caltech, RPI, Michigan, Cornell, ...).
- **CODATA ADMIRE** initiative: Advanced Data Methods and Information technologies for Research and Education
Computational & Data Sciences @ GMU  http://cds.gmu.edu/

• Primary Goal:
  – to increase student’s understanding of the role that data plays across the sciences as well as to increase the student’s ability to use the technologies associated with data acquisition, mining, analysis, and visualization.