Statistical Challenges in Modern Astronomy

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Despite centuries of close association, statistics and astronomy are surprisingly distant today. Most observational astronomical research relies on an inadequate toolbox of methodological tools. Yet the needs are substantial: astronomy encounters sophisticated problems involving sampling theory, survival analysis, multivariate classification and analysis, time series analysis, wavelet analysis, spatial point processes, nonlinear regression, bootstrap resampling and model selection. We review the recent resurgence of astrostatistical research, and outline new challenges raised by the emerging Virtual Observatory. Our essay ends with a list of research challenges and infrastructure for astrostatistics in the coming decade.

1. THE GLORIOUS HISTORY OF ASTRONOMY AND STATISTICS

Astronomy is perhaps the oldest observational science[1]. The effort to understand the mysterious luminous objects in the sky has been an important element of human culture for at least 10^4 years. Quantitative measurements of celestial phenomena were carried out by many ancient civilizations. The classical Greeks were not active observers but were unusually creative in the applications of mathematical principles to astronomy. The geometric models of the Platonists with crystalline spheres spinning around the static Earth were elaborated in detail, and this model endured in Europe for 15 centuries. But it was another Greek natural philosopher, Hipparchus, who made one of the first applications of mathematical principles that we now consider to be in the realm of statistics. Finding scatter in Bablylonian measurements of the length of a year, defined as the time between solstices, he took the middle of the range – rather than the mean or median – for the best value.

This is but one of many discussions of statistical issues in the history of astronomy. Ptolemy estimated parameters of a non-linear cosmological model using a minimax goodness-of-fit method. Al-Biruni discussed the dangers of propagating errors from inaccurate instruments and inattentive observers. While some Medieval scholars advised against the acquisition of repeated measurements, fearing that errors would compound rather than compensate for each other, the usefulnes of the mean to increase precision was demonstrated with great success by Tycho Brahe.

During the 19th century, several elements of modern mathematical statistics were developed in the context of celestial mechanics, where the application of Newtonian theory to solar system phenomena gave astonishingly precise and self-consistent quantitative inferences. Legendre developed L_2 least squares parameter estimation to model cometary orbits. The least-squares method became an instant success in European astronomy and geodesy. Other astronomers and physicists contributed to statistics: Huygens wrote a book on probability in games of chance; Newton developed an interpolation procedure; Halley laid foundations of actuarial science; Quetelet worked on statistical approaches to social sciences; Bessel first used the concept of "probable error"; and Airy wrote a volume on the theory of errors.

But the two fields diverged in the late-19th and 20th centuries. Astronomy leaped onto the advances of physics – electromagnetism, thermodynamics, quantum mechanics and general relativity – to understand the physical nature of stars, galaxies and the Universe as a whole. A subfield called "statistical astronomy" was still present but concentrated on rather narrow issues involving star counts and Galactic structure [30]. Statistics concentrated on analytical approaches. It found its principle applications in social sciences, biometrical sciences and in practical industries (*e.g.*, Sir R. A. Fisher's employment by the British agricultural service).

2. STATISTICAL NEEDS OF ASTRONOMY TODAY

Contemporary astronomy abounds in questions of a statistical nature. In addition to exploratory data analysis and simple heuristic (usually linear) modeling common in other fields, astronomers also often interpret data in terms of complicated non-linear models based on deterministic astrophysical processes. The phenomena studied must obey known behaviors of atomic and nuclear physics, gravitation and mechanics, thermodynamics and radiative processes, and so forth. 'Modeling' data may thus involve both the se-

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[1] The historical relationship between astronomy and statistics is described in references [15], [38] and elsewhere. Our *Astrostatistics* monograph gives more detail and contemporary examples of astrostatistical problems [3].

lection of a model family based on an astrophysical understanding of the conditions under study, and a statistical effort to find parameters for the specified model. A wide variety of issues thus arise:

- Does an observed group of stars (or galaxies or molecular clouds or γ-ray sources) constitute a typical and unbiased sample of the vast underlying population of similar objects?

- When and how should we divide/classify these objects into 2, 3 or more subclasses?

- What is the intrinsic physical relationship between two or more properties of a class of objects, especially when confounding variables or observational selection effects are present?

- How do we answer such questions in the presence of observations with measurement errors and flux limits?

- When is a blip in a spectrum (or image or time series) a real signal rather than a random event from Gaussian (or often Poissonian) noise or confounding variables?

- How do we interpret the vast range of temporally variable objects: periodic signals from rotating stars or orbiting extrasolar planets, stochastic signals from accreting neutron stars or black holes, explosive signals from magnetic reconnection flares or γ-ray bursts?

- How do we model the points in 2, 3, ..., 6-dimensional points representing photons in an image, galaxies in the Universe, Galactic stars in phase space?

- How do we quantify continuous structures seen in the sky such as the cosmic microwave background, the interstellar and intergalactic gaseous media?

- How do we fit astronomical spectra to highly non-linear astrophysical models based on atomic physics and radiative processes, including confidence limits on the best-fit parameters?

From a superficial examination of the astronomical literature[2], we can show that such questions are very common today. Of $\simeq 15,000$ refereed papers published annually, 1% have "statistics" or "statistical" in their title, 5% have "statistics' in their abstract,

10% treat time-variable objects, $5-10\%$ (est.) present or analyze multivariate datasets, and $5-10\%$ (est.) fit parametric models. Accounting for overlaps, we roughly estimate that around $\simeq 3,000$ distinct studies each year require non-trivial statistical methodologies. Roughly 10% of these are principally involved with statistical methods; indeed, some of these purport to develop new methods or improve on established ones.

3. ASTROSTATISTICS TODAY

We thus find that astronomy and astrophysics today require a vast range of statistical capabilities. In statistical jargon, it helps for astronomers to know something about: sampling theory, survival analysis with censoring and truncation, measurement error models, multivariate classification and analysis, harmonic and autoregressive time series analysis, wavelet analysis, spatial point processes and continuous surfaces, density estimation, linear and non-linear regression, model selection, and bootstrap resampling. In some cases, astronomers need combinations of methodologies that have not yet been fully developed (§7 below).

Faced with such a complex of challenges, mechanical exposure to a wider variety of techniques is a necessary but not sufficient prerequisite for high-quality statistical analyses. Astronomers also need to be imbued with established principles of statistical inference; *e.g.*, hypothesis testing and parameter estimation, nonparametric and parametric inference, Bayesian and frequentist approaches, and the assumptions underlying and applicability conditions for any given statistical method.

Unfortunately, we find that the majority of the thousands of astronomical studies requiring statistical analyses use a very limited set of classical methods. The most common tools used by astronomers are: Fourier transforms for temporal analysis (developed by Fourier in 1807), least squares regression and χ^2 goodness-of-fit (Legendre in 1805, Pearson in 1900, Fisher in 1924), the nonparametric Kolmogorov-Smirnov 1- and 2-sample nonparametric tests (Kolmogorov in 1933), and principal components analysis for multivariate tables (Hotelling in 1936).

Even traditional methods are often misused. Feigelson & Babu [9] found that astronomers use interchangeably up to 6 different fits for bivariate linear least squares regression: ordinary least squares (OLS), inverse regression, orthogonal regression, major axis regression, the OLS mean, and the OLS bisector. Not only did this lead to confusion in comparing studies (*e.g.*, in measuring the expansion of the Universe via Hubble's constant, H_o), but astronomers did not realize that the confidence intervals on the fitted parameters can not be correctly estimated with standard analytical formulae. Similarly, Protassov et al. [24] found that the majority of astronomical applications of the

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[2]Such bibliometric measures are easily accomplished as the entire astronomical research literature is on-line (in full text at subscribing institutions) through the NASA-supported *Astrophysics Data System*, http://adsabs.harvard.edu/abstract_service.html.

F test, or more generally the likelihood ratio test, are inconsistent with asymptotic statistical theory.

But, while the *average* astronomical study is limited to often-improper usage of a limited repertoire of statistical methods, a significant *tail of outliers* are much more sophisticated. The maximization of likelihoods, often developed specially for the problem at hand, is perhaps the most common of these improvements. Bayesian approaches are also becoming increasingly in vogue.

In a number of cases, sometimes buried in technical appendices of observational papers, astronomers independently develop statistical methods. Some of these are rediscoveries of known procedures; for example, Avni et al. [2] and others recovered elements of survival analysis for treatments of left-censored data arising from nondetections of known objects. Some are quite possibly mathematically incorrect; such as various revisions to χ^2 for Poissonian data that assume the resulting statistic still follows the χ^2 distribution. On rare occasions, truly new and correct methods have emerged; for example, astrophysicist Lynden-Bell [19] discovered the maximum-likelihood estimator for a randomly truncated dataset, for which the theoretical validity was later established by statistician Woodroofe [31].

A growing group of astronomers, recognizing the potential for new liaisons with the accomplishments of modern statistics, have promoted astrostatistical innovation through cross-disciplinary meetings and collaborations. Fionn Murtagh, an applied mathematician at Queen's University (Belfast) with long experience in astronomy, and his colleagues have run conferences and authored many useful monographs (*e.g.*, [16], [17], [22] and [27]). We at Penn State have run a series of *Statistical Challenges in Modern Astronomy* meetings with both communities in attendance (*e.g.*, [3] and [10]). Alanna Connors has organized brief statistics sessions at large astronomy meetings, and we have organized brief astronomy sessions at large *Joint Statistical meetings*. We wrote a short volume called *Astrostatistics* [3] intended to familiarize scholars in one discipline with relevant issues in the other discipline. Other series conferences are devoted to technical issues in astronomical data analysis but typically have limited participation by statisticians. These include the dozen *Astronomical Data Analysis Software and Systems* (*e.g.*, [23]), several Erice workshops on *Data Analysis in Astronomy* (*e.g.*, [8]), and the new SPIE *Astronomical Data Analysis* conferences (*e.g.*, [26]).

Most importantly, several powerful astrostatistical research collaborations have emerged. At Harvard University and the Smithsonian Astrophysical Observatory, David van Dyk worked with scientists at the *Chandra*[3] X-ray Center on several issues, particularly Bayesian approaches to parametric modeling of spectra in light of complicated instrumental effects. At Carnegie Mellon University and the University of Pittsburgh, the Pittsburgh Computational Astrophysics group addressed several issues, such as developing powerful techniques for multivariate classification of extremely large datasets and applying nonparametric regression methods to cosmology. Both of these groups involved academics, researchers and graduate students from both fields working closely for several years to achieve a critical mass of cross-disciplinary capabilities.

Other astrostatistical collaborations must be mentioned. David Donoho (Statistics at Stanford University) works with Jeffrey Scargle (NASA Ames Research Center) and others on applying advanced wavelet methods to astronomical problems. James Berger (Statistics at Duke University) has worked with astronomers William Jefferys (University of Texas), Thomas Loredo (Cornell University), and Alanna Connors (Eureka Inc.) on Bayesian methodologies for astronomy. Bradley Efron (Statistics at Stanford University) has worked with astrophysicist Vehé Petrosian (also at Stanford) on survival methods for interpreting γ-ray bursts. Philip Stark (Statistics at University of California, Berkeley) has collaborated with solar physicists in the *GONG* program to improve analysis of oscillations of the Sun (helioseismology). More such collaborations exist in the U.S., Europe and elsewhere.

4. THE VIRTUAL OBSERVATORY: A NEW IMPERATIVE FOR ASTROSTATISTICS

A major new trend is emerging in observational astronomy with the production of huge, uniform, multivariate databases from specialized survey projects and telescopes[4]. But they are heterogeneous in character, reside at widely dispersed locations, and ac-

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[3]The *Chandra* X-ray Observatory is one of NASA's Great Observatories. It was launched in 1999 with a total budget around $2 billion.

[4]An enormous collection of catalogs, and some of the underlying imaging and spectral databases, are already available on-line. Access to many catalogs is provided by Vizier (http://vizier.u-strasbg.fr). The NASA Extragalactic Database (NED, http://ned.ipac.caltech.edu), SIMBAD stellar database (http://simbad.u-strasbg.fr), and ADS (footnote 2) give integrated access to many catalogs and bibliographic information. Raw data are available from all U.S. space-based observatories; see, for example, the Multi-mission Archive at Space Telescope (MAST, http://archive.stsci.edu) and High Energy Astrophysics Science Archive Research Center (HEASARC, http://heasarc.gsfc.nasa.gov).

cessed through different database systems. Examples include:

1. $10^8 - 10^9$-object catalogs of stars and stellar extragalactic objects (*i.e.*, quasars). These include the all-sky photographic optical USNO-B1 catalog, the all-sky near-infrared 2MASS catalog, and the wide-field Sloan Digital Sky Survey (SDSS). Five to ten photometric values, each with measured heteroscedastic measurement errors (*i.e.*, different for each data point), are available for each object.

2. $10^5 - 10^6$-galaxy redshift catalogs from the 2-degree Field (2dF) and SDSS spectroscopic surveys. The main goal is characterization of the hierarchical, nonlinear and anisotropic clustering of galaxies in a 3-dimensional space. But the datasets also include spectra for each galaxy each with 10^3 independent measurements.

3. $10^5 - 10^6$-source catalogs from various multi-wavelength wide-field surveys such as the NRAO Very Large Array Sky Survey in one radio band, the InfraRed Astronomical Satellite Faint Source catalog in four infrared bands, the Hipparcos and Tycho catalogs of star distances and motions, and the X-ray Multimirror Mission Serendipitous Source Catalogue in several X-ray bands now in progress. These catalogs are typically accompanied by large image libraries.

4. $10^2 - 10^4$-object samples of well-characterized pre-main sequence stars, binary stars, variable stars, pulsars, interstellar clouds and nebulae, nearby galaxies, active galactic nuclei, gamma-ray bursts and so forth. There are dozens of such samples with typically $10 - 20$ catalogued properties and often with accompanying 1-, 2-, or 3-dimensional images or spectra.

5. Perhaps the most ambitious of such surveys is the planned Large-aperture Synoptic Survey Telescope (LSST) which will survey much of the entire optical sky every few nights. It is expected to generate raw databases in excess of 10 PBy (petabyte) and catalogs with 10^{10} entries.

An international effort known as the Virtual Observatory (VO) is now underway to coordinate and federate these diverse databases, making them readily accessible to the scientific user [6, 29]. Considerable progress is being made in the establishment of the necessary data and metadata infrastructure and standards, interoperability issues, data mining, and technology demonstration prototype services[5]. But

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[5]See http://www.ivoa.net and /http://us-vo.org for entry into Virtual Observatory projects.

scientific discovery requires more than effective recovery and distribution of information. After the astronomer obtains the data of interest, tools are needed to explore the datasets. How do we identify correlations and anomalies within the datasets? How do we classify the sources to isolate subpopulations of astrophysical interest? How do we use the data to constrain astrophysical interpretation, which often involve highly non-linear parametric functions derived from fields such as physical cosmology, stellar structure or atomic physics? These questions lie under the aegis of statistics.

A particular problem relevant to statistical computing is that, while the speed of CPUs and the capacity of inexpensive hard disks rise rapidly, computer memory capacities grow at a slower pace. Combining the largest optical/near-infrared object catalogs today produces a table with > 1 billion objects and up to a dozen columns of photometric data. Such large datasets effectively preclude use of all standard multivariate statistical packages and visualization tools (*e.g.*, R and GGobi) which are generally designed to place the entire database into computer memory. Even sorting the data to produce quantiles may not be computationally feasible.

The Virtual Observatory of the 21st century thus presents new challenges to statistical capability in two ways. First, some new methodological developments are needed (§5). Second, efficient access to both new and well-established statistical methods are needed. No single existing software package can provide the vast range of needed methods. We are now involved in developing a prototype system called *VOStat* to provide statistical capabilities to the VO astronomer. It is based on concepts of Web services and distributed Grid computing. Here, the statistical software and computational resources, as well as the underlying empirical databases, may have heterogeneous structures and can reside at distant locations.

5. SOME GRAND METHODOLOGICAL CHALLENGES FOR THE COMING DECADE

While it is risky to prognosticate the directions of future research, and judgments will always differ regarding the relative importance of research goals, we can outline a few "grand challenges" for astrostatistical research for the next decade or two.

5.1. Multivariate analysis with measurement errors and censoring

Traditional multivariate analysis is designed mainly for applications in the social and human sciences where the sources of variance are largely unknowable.

Measurement errors are usually ignored, or are considered to be exogenous variables in the parametric models [12]. But astrophysicists often devote as much effort to precise determination of their errors as they devote to the measurements of the quantities of interest. The instruments are carefully calibrated to reduce systematic uncertainties, and background levels and random fluctuations are carefully evaluated to determine random errors. Except in the simple case of bivariate regression [1, 5, 9], this information on measurement errors is usually squandered.

While heteroscedastic measurement errors with known variances is common in all physical sciences, only astronomy frequently has nondetections when observations are made at new wavelengths of known objects. These are datapoints where the signal lies below (say) 3 times the noise level. Here again, modern statistics has insufficient tools. Survival analysis for censored data assumes that the value below which the data point must lie is known with infinite precision, rather than being generated from a distribution of noise. Astronomer Herman Marshall [20] makes an interesting attempt to synthesize measurement errors and nondetections, but statistician Leon Gleser [14] argues that he has only recovered Fisher's failed theory of fiducial distributions. Addressing this issue in a self-consistent statistical theory is a profound challenge that lies at the heart of interpreting the data astronomers obtain at the telescope.

5.2. Statistical inference and visualization with very-large-N datasets

The need for computational software for extremely large databases – multi-terabyte image and spectrum libraries and multi-billion object catalogs – is discussed in section 4. A suite of approximate methods based on flowing data streams or adaptive sampling of large datasets resident on hard disks should be sought. Visualization methods involving smoothing, multidimensional shading and variable transparency, should be brought into the astronomer's toolbox. Here, considerable work is being conducted by computer scientists and applied mathematicians in other applied fields so that independent development by astrostatisticians might not be necessary to achieve certain goals.

5.3. A cookbook for construction of likelihoods and Bayesian computation

While the concepts of likelihoods and their applications in maximum likelihood estimation, Bayes Theorem and Bayes factors are becoming increasingly well-known in astronomical research, the applications to real-life problems is still an art for the expert rather than a tool for the masses. Part of the problem is conceptual; astronomers need training in how to construct likelihoods for familiar parametric situations (*e.g.*, power law distributions or a Poisson process). Part of the problem is computational; astronomers need methods and software for the oft-complex computations. Many such methods, such as Markov chain Monte Carlo, are already well-established and can be directly adopted for astronomy [13]. For example, astronomers are often not fully aware of the broad applicability of the EM Algorithm for maximizing likelihoods [21][6].

5.4. Links between astrophysical theory and wavelets

Wavelet analysis has become a powerful and sophisticated tool for the study of features in data. Originally intended mainly for modelling time series, astronomers also use it increasingly for spatial analysis of images [11, 25]. In some ways it can be viewed as a generalization of Fourier analysis in which the basis function need not be sinusoidal in shape and, most importantly, the pattern need not extend over the entire dataset. Wavelets are thus effective in quantitatively describing complicated overlapping structures on many scales, and can also be used for signal denoising and compression. In addition, wavelets have a strong mathematical foundation.

Despite its increasing popularity in astronomical applications, wavelet analysis suffers a profound limitation in comparison with Fourier analysis. A peak in a Fourier spectrum is immediately interpretable as a vibrational, rotational or orbital rotation of solid bodies. A bump or a continuum slope in a wavelet decomposition often has no analogous physically intuitive interpretation. We therefore recommend that astrophysicists seek links between physical theory – often involving continuous media such as turbulent plasmas in the interstellar medium and hierarchical structure formation in the early Universe – and wavelets. One fascinating example is the demonstration that the wavelet spectrum and Lyapunov exponent of the quasi-periodic X-ray emission from Sco X-1, which reflects the processes in an accretion disk around a neutron star, exhibit a transient chaotic behavior similar to that of water condensing and dripping onto an automobile windshield or a dripping handrail [32].

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[6]The seminal study of the EM Algorithm is Dempster, Laird & Rubin in 1977 [7], which is one of the most frequently cited papers in statistics. However, the method was independently derived three years earlier by astronomer Leon Lucy [18] as an "iterative technique for the rectification of observed distributions" based on Bayes' Theorem. This study is widely cited in the astronomical literature; its most frequent application is in image deconvolution where it is known as the Lucy-Richardson algorithm.

5.5. Time series models for astrophysical phenomena

The quasi-periodic oscillation of Sco X-1 is only one of many examples of complex accretional behavior onto neutron stars and black holes seen in X-ray and γ-ray astronomy. The accreting Galactic black hole GRS 1915+105 exhibits a bewildering variety of distinct states of stochastic, quasi-periodic and explosive behaviors. The prompt emission from gamma-ray bursts shows a fantastic diversity of temporal behaviors from simple smooth fast-rise-exponential-decays to stochastic spiky profiles. Violent magnetic reconnection flares on the surfaces of the Sun and other magnetically active stars also show complex behaviors. Many of these datasets are multivariate with time series available in several spectral bands often showing lags or hardness ratio variations of astrophysical interest.

There are also important astronomical endeavors which seek astrophysically interesting signals amidst the oft-complex noise characteristics of the detectors. The Arecibo, Parkes and VLA radio telescopes, for example, conduct searches for new radio pulsars or for extraterrestrial intelligences in nearby planetary systems. The Laser Interferometer Gravitational-Wave Observatory (LIGO) and related detectors search for both continuing periodic signals and brief bursts from perturbations in space-time predicted by Einstein's General Relativity. Here the signals sought are orders of magnitude fainter than instrumental variations.

6. INFRASTRUCTURE NEEDED TO ADVANCE ASTROSTATISTICS

The current quality of statistical analyses in astronomical research often begs for improvment. There is both inadequate research on important new challenges (§5) and inadequate application of known advanced methods to astronomical problems (§3). Astronomy clearly needs needs a strong and rapid surge of energy in statistical expertise. Three types of activities should be promoted:

Cross-training In the U.S., the typical curriculum leading to a career in astronomical research requires zero or one course in statistics at the undergraduate level, and zero at the graduate level. Analogously, the curriculum of statisticians includes virtually no coursework in astronomy or other physical science. While statisticians can learn basics from "Astronomy 101" courses given at all universities, the statistical training of astronomers is not as easily accomplished. New curricular products summarizing the applicable statistical subfields, short training workshops for graduate students and young

scientists, and effective statistical consulting are all needed.

Increased collaborative research While several astrostatistical research groups are making exciting progress (§3), the total effort is too small to impact the bulk of astronomical research. Very roughly, astrostatistical funding is currently \$1M of the \$1B spent annually on astronomical research. This fraction is far below that spent in biomedical or other non-physical-science fields. Though top academic leaders of statistics have expressed great enthusiasm for astronomy and astrostatistics, we can not pull them away from biostatistics and business applications without a major increase in funding. We might seek, for example, $10-20$ cross-disciplinary research groups active at any one time at the end of a decade's growth.

Statistical software For various policy and cultural reasons, astronomers rarely purchase the large commercial statistical software packages, preferring to write their own software as needs arise. This approach has contributed to the narrow methodological scope of astronomical research. Avenues for improving this situation are emerging. R is a large statistical software package with the flexible command-line interface preferred by astronomers that has recently emerged (http://www.r-project.org). A wide variety of specialized packages and codes are also available on-line (http://www.astro.psu.edu/statcodes). The new Web services concept being developed within the context of a Virtual Observatory permits coordinated access to heterogeneous software developed specifically for astronomical applications.

At Penn State, we are in the early stages of developing a Center for Astrostatistics to help attain these goals (http://www.astrostatistics.psu.edu). This is an inter-disciplinary Center to serve the astronomy and statistics communities around the nation and worldwide, seeking to bring advances in statistics into the toolbox of astronomy and astrophysics. The Center's Web site will maintain the popular *StatCodes*, build an instructional library of R programs, coordinate with the nascent *VOStat* Web service, and develop an archive of annotated links to selected statistical literature applicable to astronomy (and vice versa). The site is also planned to include tutorial handbooks and curricular products developed specifically for astrostatistical needs.

Acknowledgments

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