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► To cite this version:

Didier Fraix-Burnet. Grand Challenges in Astrostatistics. Frontiers in Astronomy and Space Sciences, 2020, 10.3389/fspas.2020.00011 . hal-02524124

HAL Id: hal-02524124

<https://hal.science/hal-02524124>

Submitted on 30 Mar 2020

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Grand Challenges in Astrostatistics

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Astrostatistics is not really a new discipline since it has been long recognised as a fundamental requirement for astrophysics (Feigelson and Babu, 1992a). However, it has been only quite recently accepted as a part of the astronomical activity with the official creation of a commission of the International Astronomical Union. But more importantly, sophisticated statistical tools have pervaded the literature.

We can regret the lengthy time it took before astrostatistics became openly spread, but the success is here. I see cosmology as the more spectacular demonstration of the usefulness, and even the absolute necessity, of sophisticated statistical analyses: it first started with the determination of the structure of the cosmic web (Barrow et al., 1985), but the more popular outcome emerged in the derivation of the properties of our Universe through Bayesian analyses.

As was already obvious long time ago (Feigelson and Babu, 1992a), astronomers are not experts in statistics and interdisciplinary collaborations are necessary. This is routine practice in cosmology, but still much less elsewhere even though things are changing quickly.

The advent of Big Data in astrophysics is a more recent argument in favour of astrostatistics. New telescopes such as the LSST and SKA, among many others, have given birth to astroinformatics to manage the foreseen avalanche of data. As a consequence, statistical tools appear in the landscape of astrophysics and naturally foster interest for their use in data analysis.

It is striking to see that many techniques explored in the case of a particular astrophysical problem are never used again in other papers. I think one of the challenges of astrostatistics is to understand why. Is this because it is so technical that only a very few people can use them? Is this because the interdisciplinary collaboration collapsed due to career pressures or lack of funds? Is this because the results did not convince the other astronomers since they might not trust a method that they do not understand? Is this because the results are not easily connectible with the current physical knowledge and understanding of the subject? Or is this simply because statistical methods introduce a different avenue from the traditional way of doing astrophysics?

Doing physics with Machine Learning outcomes is not a specific difficulty of astrophysics, and it appears as a cultural revolution, sometimes referred to as the transition from object-driven to data-driven science. Physics is deterministic, but cosmology has largely proven that we can use likelihoods to predict and assess the most probable parameter values from observations. Indeed, the relative popularity of the Bayesian approach in astrophysics is certainly related to the uncertainties that are unavoidably attached to astronomical data and can seemingly be incorporated easily in such methods. Uncertainties and noise are a specificity of astronomical data that may deter some statisticians or motivate others.

A counter example to the success of Bayesian statistics in astrophysics is that, despite a very pedagogical paper by Feigelson and Babu (1992b), astronomers use nearly exclusively the χ -square minimization

regression-type problems generally without checking its validity for the case under study. The other methods are not part of the basic toolbox of most astronomers, in particular for the so common truncated and censored data. In the same manner, it is not because the Bayesian approach is popular that it is always fully understood: in particular, it is sometimes forgotten that the choice of the prior is arbitrary and can have a significant influence on the result.

It is true that statistics is a huge domain, and every single astrophysical analysis could benefit from more or less sophisticated methods and algorithms. It is thus very difficult for an astronomer to be aware of the state of the art of another discipline. But there are plethora of robust available techniques which are mathematically not too difficult to understand. Thanks to many training sessions, workshops, books and of course papers, it is now getting easier and easier to fill the gap between the two disciplines.

I strongly believe that the main difficulty is somehow cultural. Astronomers were used to work with small data sets, describing the diversity by eye, and concentrating on the detailed physics of so-called typical objects. The big challenge of the XXIth century is certainly that eye examination is not possible any more, and consequently the scientists have to rely on automatic machines to do the job. This causes serious issues, and I present only a few of them here.

Grouping objects obtained from the astronomical observations into distinct categories has always been a necessity imposed by their vast diversity. This is the case for stars, galaxies, asteroids, supernova, active galactic nuclei, gamma-ray bursts and many others. This clustering (unsupervised classification) is a prerequisite to any physical modelling. For this purpose, astronomers have always used heuristic, simple and subjective techniques, based on only one or two physical parameters, most often with the help of a visual examination. But the classification algorithms do not always respect the physical properties, they merely distinguish classes on purely mathematical grounds. It often means that the classification is justified only in a multivariate space, that cannot be summarized by a very few physical characteristics. Then, what can the astronomer make of such a classification (e.g. Fraix-Burnet et al., 2015)?

In addition, with more and more data, the diversity increases, populating the parameter space which, in astrophysics, is essentially a continuum of object properties without clear boundaries. As a consequence, any reasonable classification is fuzzy, which is not simple to summarise with simple schemes.

One illustrative instance of this issue is the classification of galaxies. A quantitative and objective classification of the morphologies of galaxies is still an unsolved problem. From dimensionality reduction with Principal Component Analysis first attempted nearly forty years ago (Whitmore, 1984; Watanabe et al., 1985) to computationally heavy Deep Learning techniques, no satisfactory solution has been yet found. It is clear that the visual Hubble morphological classification is too much appealing emotionally (simple and beautiful) to be easily replaced by something more thorough but more complex. Nevertheless, "Nature dictates the classification to the scientists", not the reverse (Adanson, 1763).

The classification of galaxy spectra suffers from the same fate (e.g. Connolly et al., 1995) and this again is due to our inability to see in a high-dimensional space. One can argue that the stellar classification seems to be robust and multivariate, but stars are obviously less complex objects than galaxies.

A big issue of science is robustness and reproducibility. Astronomers are used to check the validity of a result by examining visually any image or summarizing plot. This is unfortunately not objective, quantitative, nor reproducible. Supervised machine learning triggered a lot of promises since the philosophy is to teach the algorithm what we would like it to yield, including the human subjectivity. The control is straightforward. But is this really feasible? On the contrary, the exploration of the data

requires unsupervised learning, but how can we trust the findings of the algorithms? How can we describe them in a multivariate configuration? How can we summarize the results in simple terms?

Most importantly, even if there are statistical tools to assess the robustness and reproducibility of the outcomes of algorithms, only the physics can validate a result in the sense that it can be useful to our understanding of the Universe. But how can we reconcile these new kinds of data analysis with the physical models? Most theoretical calculations are devised to mimic a single object, and they can be repeated by varying the input parameters. However, the more sophisticated the models are, the heavier is the computational cost, so it is probably illusory in many cases to produce a statistical analysis of the outcomes of models. Different approaches are used to fit different kinds of objects, such as interpolation, but this might not fully answer our concern.

Numerical simulations are a recent tool in astrophysics, in particular the cosmological ones which create a very large diversity of galaxies. It seems to be possible to compare these data with real observations using the same statistical tools. But would it be enough to constrain the very complicated physics that are introduced in the simulations and test various hypotheses or some ad hoc recipes that are often necessary to lighten somewhat the computation?

In a multivariate world, the selection of the attributes is useful, if not crucial. This is often necessary to perform the analysis, and very useful for the interpretation. This is called dimensionality reduction, and among them the Principal Component Analysis is well known in astrophysics. But there are others, such as Discriminant Analysis or Independent Component Analysis. They all have their interest and limitation, but they all share the common drawback of providing unphysical components in the form of combinations of the real observables or physical parameters. Probably astronomers have to learn to do physics in these artificial spaces as they already do for instance to separate stars from galaxies in Principal Component bivariate plots. They may even create many artificial features to improve their regression analyses (e.g. D'Isanto et al., 2018), and envisage clustering of variables.

Time series are ubiquitous in astrophysics, from celestial mechanics to gravitational waves, from exoplanets to quasars, with phenomena that are periodic (orbits, cycles, pulses, rotations...), transient (explosions, bursts, stellar activity...), random (accretion, ejection...) or regular (apparent motions...). In astrophysics, the detection can be immediate to alert other telescopes, or very detailed to identify some exoplanets or probe the interior of stars. The characterization of the light curves is required for the physical modelling and understanding. Classification is of course necessary to organize the observations. Time series analysis is widespread in many other disciplines (meteorology, finance, economy, medical sciences...) and is an important branch of research in statistics with huge developments that astronomers often ignore. There is here an important potential of new studies and discoveries.

Graphical methods are relatively under-explored in astrophysics. Yet, the Hubble tuning fork diagram may be seen as a rather old and still extremely popular graphics depicting the evolution of galaxies. Also, the Minimum Spanning Tree method was used early on to map the cosmic web using two spatial coordinates and the redshift (Barrow et al., 1985). These tools are particularly suited to represent evolutionary paths and are heavily used in bioinformatics. Their use in astrophysics is recent (Fraix-Burnet et al., 2006) with already many applications to small solar system bodies, stars, stellar clusters, Gamma Ray Bursts, galaxies and quasars.

Astrostatistics is thus full of challenges and opportunities. We hope that this section of *Frontiers in Astronomy and Space Sciences* will become the home of experiments, discussions, propositions, solutions, a place where astronomers and statisticians can come together, where anyone can find research articles,

reviews, opinions, codes, tutorials, that could accompany the data science revolution astrophysics is beginning to experience.

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