Clustering with phylogenetic tools in astrophysics

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Abstract

Phylogenetic approaches are finding more and more applications outside the field of biology. Astrophysics is no exception since an overwhelming amount of multivariate data has appeared in the last twenty years or so. In particular, the diversification of galaxies throughout the evolution of the Universe quite naturally invokes phylogenetic approaches. We have demonstrated that Maximum Parsimony brings useful astrophysical results, and we now proceed toward the analyses of large datasets for galaxies. In this talk I present how we solve the major difficulties for this goal: the choice of the parameters, their discretization, and the analysis of a high number of objects with an unsupervised NP-hard classification technique like cladistics.

Keywords: multivariate classification; cladistics; Maximum Parsimony; galaxies.

1. Introduction

How do the galaxy form, and when? How did the galaxy evolve and transform themselves to create the diversity we observe? What are the progenitors to present-day galaxies? To answer these big questions, observations throughout the Universe and the physical modelisation are obvious tools. But between these, there is a key process, without which it would be impossible to extract some digestible information from the complexity of these systems. This is classification.

One century ago, galaxies were discovered by Hubble. From images obtained in the visible range of wavelengths, he synthetised his observations through the usual process: classification. With only one parameter (the shape) that is qualitative and determined with the eye, he found four categories: ellipticals, spirals, barred spirals and irregulars. This is the famous Hubble classification. He later hypothetized relationships between these classes, building the Hubble Tuning Fork.

The Hubble classification has been refined, notably by de Vaucouleurs, and is still used as the only global classification of galaxies. Even though the physical relationships proposed by Hubble are not retained any more, the Hubble Tuning Fork is nearly always used to represent the classification of the galaxy diversity under its new name the Hubble sequence (e.g. Delgado-Serrano, 2012). Its success is impressive and can be understood by its simplicity, even its beauty, and by the many correlations found between the morphology of galaxies and their other properties. And one must admit that there is no alternative up to now, even though both the Hubble classification and diagram have been recognised to be unsatisfactory. Among the most obvious flaws of this classification, one must mention its monovariate, qualitative, subjective and old-fashioned nature, as well as the difficulty to characterise the morphology of distant galaxies.

The first two most significant multivariate studies were by Watanabe et al. (1985) and Whitmore (1984). Since the year 2005, the number of studies attempting to go beyond the Hubble classification has increased largely. Why, despite of this, the Hubble classification and its sequence are still alive and no alternative have yet emerged (Sandage, 2005)?

My feeling is that the results of the multivariate analyses are not easily integrated into a one-century old practice of modeling the observations. In addition, extragalactic objects like galaxies, stellar clusters or stars do evolve. Astronomy now provides data on very distant objects, raising the question of the relationships between those and our present day nearby galaxies. Clearly, this is a phylogenetic problem.

Astrocladistics\(^1\) aims at exploring the use of phylogenetic tools in astrophysics (Fraix-Burnet et al., 2006a,b). We have proved that Maximum Parsimony (or cladistics) can be applied in astrophysics and provides a new exploration tool of the data (Fraix-Burnet et al., 2009, 2012; Cardone & Fraix-Burnet, 2013). As far as the classification of galaxies is concerned, a larger number of objects must now be analysed. In this paper, I

\(^1\)http://astrocladistics.org
2. Parameters as tracers of the evolutionary history: an illustration with stellar tracks

Let us consider the data shown on the left plot in Fig. 1. How many groups are there?

![Figure 1: Left: a sample data points. Right: the full stellar evolutionary tracks corresponding to the data points (51 points per track). Each track corresponds to the evolution of a star with an initial metallicity Z given in the inlet. All stars in this sample have an initial mass of 2.5 times the solar mass. The dotted line on the bottom left is the Main Sequence where the computations start.](image)

The answer is given on the right plot of Fig. 1: six. These plots give the luminosity log $L$ as a function of the surface temperature of the star log $T_{eff}$. They are known as the Hertzsprung-Russell (HR) diagram and are made using the Geneva stellar evolutionary models (Charbonnel et al., 1993; Mowlavi et al., 1998; Schaerer et al., 1993a,b; Schaller et al., 1992) that compute the stellar parameters for stars of masses from $M = 0.8$ to 120 Mo and metallicities $Z$ from $= 0.001$ to 0.1 at different ages (time steps or evolutionary stages). We have chosen six values of $Z$ and one mass (see Fig. 1). Each of our six tracks has 51 time steps which are our data points. The simulations provide 11 additional parameters which give the chemical composition of the stars. The analyses below are made with the 13 parameters.

![Figure 2: Left: the result of a k-medoids analysis assuming six clusters. The colors used to distinguish the groups are arbitrary. Right: the result of the cladistics analysis. The colors of the points corresponds to the true families of stars characterized by their initial metallicity (inlet). The black lines are the branches of the tree indicating the relationships between the data points. In other words, this plot is the projection of the tree on the bivariate diagram log $L$ vs log $T_{eff}$.](image)

A clustering approach like k-medoids would yield the result shown on the left of Fig. 2, while the cladistic analysis yields the result shown on the right plot. Obviously, cladistics does a pretty good job at recovering the
six evolutionary tracks. But there are some discrepancies which are due to the behaviour of the parameters with respect to the evolution. It can be seen below in Fig. 3 that a lot of parameters (shown here only for two tracks) are constant during the first half of the evolution, and at least one parameter shows a reversal (circle).

![Figure 3](image)

**Figure 3:** Evolution of the 13 parameters for two tracks (i.e. two metallicities) as a function of the time steps. The circle indicates a reversal in the evolution of the parameter \( \log T_{\text{eff}} \).

Reversals, convergences or parallel evolutions are called homoplasies and tend to destroy the phylogenetic signal. The Maximum Parsimony technique minimizes these homoplasies and maximizes the synapomorphies. So the crucial point in phylogenetic methods is the selection of the parameters that are synapomorphies, which keep the traces of the ancestorships. There is no method to detect them except trial-and-error approaches, and some a priori knowledge help to eliminate obvious homoplasies.

3. **Discretizing the Parameters**
Cladistics has initially been devised for qualitative and discrete parameters (called characters), each bin representing an evolutionary state for that parameter. The use of continuous data has long been debated but seems now to be accepted (Goloboff et al., 2006) and even justified (Thuillard & Fraix-Burnet, 2009). Since there is yet no phylogenetic algorithm using continuous parameters and adapted to the kind of evolution processes for galaxies, we have to bin our data. Of course, there is no unique choice:

1. taking a small number of bins could reduce the number of distinct objects, but we have noted that the result depends significantly on the precise number of bins below, say, fifteen bins. In any case, should the bin be equal? And if not, where should we place the limits?

2. taking more bins more or less respects the continuous nature of the parameters, but this may question the meaning of the bins as evolutionary states.

We have always adopted the second choice, and used most often 32 bins, noting that in any case this is the physical interpretation that ensures the relevance of the binning.

4. **Unknown Species and the High Number of Individuals: the Example of Galaxies**
Maximum Parsimony is a NP-hard problem: it looks for all the possible arrangements of objects on a tree and then selects the most parsimonious one. Above a thousand individuals, this takes too much CPU time, especially if we have to repeat the analysis a large number of times, either to select the most satisfactory subsets of parameters, or to assess the robustness of the result via a bootstrap method.

The problem here is that there is no multivariate classification of galaxies so that the species are not known at all. We thus have to make the hypothesis that each individual is an exemplar of a class to be identified. Up to now, we have analysed only a few hundreds galaxies at a time, as shown on the tree below (Fig. 4 left; Fraix-Burnet et al., 2012). The groups or classes are defined from the tree, and the average properties for each class are computed. This constitutes a first and partial phylogeny of galaxies that must be extended.

One important consequence of our analysis is that the correlations (scaling relations) must be revisited since they often vary depending on the class or even disappear within the classes. A spectacular example is the well-known scaling relation between the velocity dispersion $\sigma$ and the metallicity (here the Mg$_2$ index). The Maximum Parsimony result (top right in Fig. 4) shows that the correlation is absent in most if not all of the groups. Indeed, the global correlation appears to be caused by the diversification of galaxies: the relative position of the groups in the plot follows exactly the relative position on the tree. This is a clear evidence that a confounding factor explains this correlation.

On the contrary, the three morphological classes present in the sample show the same correlation (bottom right diagram in Fig. 4). This would indicate that all galaxies have the same history, which is not plausible.

4. Selecting Smaller Representative Subsets

Our current goal is to extend the application of Maximum Parsimony to much larger samples of galaxies. To keep the problem computationally tractable, there are two pathways:

Figure 4: Left: tree of galaxies, from Fraix-Burnet et al. (2012). Top right: metallicity indicator Mg$_2$ vs the velocity dispersion log $\sigma$ with the colors corresponding to the groups of the tree to the left. Bottom right: same diagram with the color-coded morphological classes.
1. keep the already established phylogeny, define an exemplar for each class, and add new objects progressively;

2. define small sub-samples, determine the phylogenies and combine them with supertree techniques.

The first approach is easier with discrete data since a species can be characterized precisely. For continuous data, the class limits are necessarily overlapping, and a parameter specific to a class is defined by its quantiles. This requires a sufficient number of individuals for these quantiles to be representative enough of a given class. Hence this approach is quite interesting when a significant fraction of the whole sample has been analysed, the already established phylogeny serving as a backbone tree to constrain the Maximum Parsimony search.

The second approach randomly selects a tractable subset of the data. For this, it appears necessary that the subset is representative of the whole sample, ideally with the same distribution for each parameter. Subsequently, a supertree can be built using all the sub-trees if the latter are sufficiently robust.

The two approaches are indeed complementary and can be run in parallel.

5. Conclusion
To be able to replace the one-century old Hubble Tuning Fork with a multivariate phylogenetic classification, the phylogenetic approach has now proven to be a viable pathway. To tackle larger samples of galaxies, astrocladistics faces several challenges which seem to be surmountable. The Maximum Parsimony is not the only phylogenetic tool. More generally, distance-based techniques – phylogenetic, partitioning or hierarchical – are much more computationally efficient. However, I think that the cladistics method allows for a clearer conceptual clarification of the diversification processes. This was obviously a necessary step before performing large scale multivariate clustering analyses of complex objects in evolution.

References


Schaller, G., Schaerer, D., Meynet, G., & Maeder, A. (1992). New grids of stellar models from 0.8 to 120 solar masses at z = 0.020 and z = 0.001. *Astronomy and Astrophysics Supplement Series, 96*, 269–331.

