A new approach to finding galaxy groups using Markov Clustering

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ABSTRACT

We present a proof of concept of a new galaxy group finder method, Markov graph CLustering (MCL; Van Dongen 2000) that naturally handles probabilistic linking criteria. We introduce a new figure of merit, the variation of information statistic (VI; Meila 2003), used to optimise the free parameter(s) of the MCL algorithm. We explain that the common Friends-of-Friends (FoF) method is a subset of MCL. We test MCL in real space on a realistic mock galaxy catalogue constructed from a N-body simulation using the GALFORM model. With a fixed linking length FoF produces the best group catalogues as quantified by the VI statistic. By making the linking length sensitive to the local galaxy density, the quality of the FoF and MCL group catalogues improve significantly, with MCL being preferred over FoF due to a smaller VI value. The MCL group catalogue recovers accurately the underlying halo multiplicity function at all multiplicities. MCL provides better and more consistent group purity and halo completeness values at all multiplicities than FoF. As MCL allows for probabilistic pairwise connections, it is a promising algorithm to find galaxy groups in photometric surveys.

Key words: galaxies: groups: general – galaxies : haloes – methods: statistical

1 INTRODUCTION

The fundamental assumption behind galaxy formation theory is that galaxies form inside dark matter haloes (White & Rees 1978). The hierarchical assembly of haloes and the timescale for galaxy mergers means that haloes often have a main or central galaxy, accompanied by distinct satellite galaxies. There are clear predictions for the properties of the galactic content of halos that can be tested if we can identify a high fidelity sample of galaxy groups from galaxy surveys that retains a connection to the underlying dark matter halos (Eke et al. 2004, 2005; van den Bosch et al. 2005; Yang et al. 2005a).

The identification of a galaxy group requires an algorithm to associate galaxies with a common, unique dark matter halo. Many ways have been explored to do this, with the most common being Friends-of-Friends (FoF; e.g. Huchra & Geller 1982; Zeldovich et al. 1982). For example, Eke et al. (2004) and Robotham et al. (2011) created FoF galaxy group catalogues from the 2dF Galaxy Redshift Survey (Colless et al. 2001) and the Galaxy And Mass Assembly survey (GAMA) (Driver et al. 2011). Liu et al. (2008) extended FoF for galaxies with photometric redshifts, which was then applied to the Pan-STARRS1 medium deep survey (Jian et al. 2014). Yang et al. (2005b) developed a halo based group finder that was used to construct a group catalogue using Sloan Digital Sky Survey (SDSS) galaxies (Yang et al. 2007).

However, despite the success of FoF-based methods they are far from perfect and struggle when applied to low density samples as is the case with galaxy catalogues. This should be contrasted with their application to numerical simulations where the particle distribution is thousands of times denser (if not more) than a typical galaxy distribution. When applied to galaxy catalogues, FoF tends to create either too many low multiplicity groups (by fragmentation of the larger ones) or groups that are too big (by spuriously joining smaller groups to bigger ones). Measures of purity and completeness are then used to rate the quality of the group catalogue and these statistics tend to be combined in some way, to create a statistic that should be minimized to ensure an ‘optimal’ set of groups (see, for example, Eke et al. 2004). It is worth noting that FoF does not use all of the available pairwise information, nor can it be extended naturally to handle probabilistic positional information, as is the case with e.g. photometric redshifts.

Here we show that the FoF approach to galaxy group finding is just one solution to the graph clustering problem
Graph clustering aims to find clusters of points given all pairwise connection amplitudes between them. It is a problem that occurs in many situations, such as detecting communities in social networks (e.g. Liu et al. 2014). We explain, in Section 2, how the FoF algorithm is a subset of the Markov graph CLustering algorithm MCL (Van Dongen 2000), which we apply to the problem of galaxy group detection. MCL has been widely used in the field of bioinformatics in detecting groups of proteins based on their pairwise interactions (e.g. Vlasblom & Wodak 2009).

Our overall aim is to construct a group catalogue using the narrow band PAU Survey (PAUS; e.g. Eriksen et al. 2019; Stothert et al. 2018). A PAUS group catalogue would probe significantly fainter galaxies than one built using SDSS or GAMA, and would cover a larger area with better completeness in both sampling and redshift than a group catalogue constructed using similar depth surveys such as zCOSMOS (Lilly et al. 2007) or VIPERS (Guzzo et al. 2014). Hence a PAUS group catalogue would provide a better probe of the redshift evolution of halos as traced by galaxy groups and better sampling of low mass halos. The challenge with finding galaxy groups in PAUS lies in the varying accuracy of the PAUS photometric redshifts. MCL is a promising approach as it allows probabilistic pairwise connections (see also Tempel et al. 2018, for another approach), something that could be useful for PAUS where it is more natural to frame pairwise connections as probabilities than as binary links.

Section 2 presents the MCL algorithm and explains its relation to the standard FoF algorithm. Section 3 presents the mock catalogue which is used to test the algorithm. Section 4 summarises the metrics we use to assess the group finding performance. Section 5 presents the results in real space. We provide our conclusions and future prospects of finding performance. Section 6 summarises the metrics we use to assess the group finding performance. Section 5 presents the results in real space. We provide our conclusions and future prospects of finding performance. Section 6 summarises the metrics we use to assess the group finding performance. Section 5 presents the results in real space. We provide our conclusions and future prospects of finding performance. Section 6 summarises the metrics we use to assess the group finding performance. Section 5 presents the results in real space. We provide our conclusions and future prospects of finding performance. Section 6 summarises the metrics we use to assess the group finding performance. Section 5 presents the results in real space. We provide our conclusions and future prospects of finding performance. Section 6 summarises the metrics we use to assess the group finding performance. Section 5 presents the results in real space. We provide our conclusions and future prospects of finding performance. Section 6 summarises the metrics we use to assess the group finding performance. Section 5 presents the results in real space. We provide our conclusions and future prospects of finding performance. Section 6 summarises the metrics we use to assess the group finding performance. Section 5 presents the results in real space. We provide our conclusions and future prospects of finding performance. Section 6 summarises the metrics we use to assess the group finding performance.

We now explain each step in turn. The initial column-wise normalisation in step (i) above – and those that follow in step (iv) – are necessary to ensure that the pairwise connection elements relating to point i can be treated as probabilities. By squaring the pairwise connection matrix \( W_{k-1} \) to create a new pairwise connection matrix \( W_k \), the MCL algorithm approximately simulates a random walk on the graph by using the elements \( w_{ij}^k \) as transition probabilities to determine which pairs are more bound than others. Step (iii), raising the elements of \( w_{ij}^k \) to the power \( \Gamma \), is designed to boost the more travelled connections and reduce the less travelled inter-cluster ones. This process of matrix multiplication (here assumed to be squaring), element inflation (to the power of \( \Gamma \)) and column-wise normalisation is repeated until a predefined convergence criteria is met by the pairwise connection matrix \( W_k \). The convergence criterion is that the final matrix becomes idempotent, i.e. invariant under expansion and inflation. The exact criterion is expressed in terms of the maximum over all columns of the difference between the maximum value in a column and the sum of all elements squared of that column. Once converged, the matrix \( W_k \) is cleaned (by setting to zero all \( w_{ij}^k \) elements below a pruning value of \( 10^{-4} \)) and then rearranged with row replacement into a block diagonal matrix, with members of each group defined by the matrix blocks.

At face value MCL is an iterative \( N^2 \) process as all links between \( N \) points need to be defined at each iteration. The larger the value of the inflation parameter, \( \Gamma \), the more rapidly the pairwise connections tends towards zero during the iterations and the faster the MCL algorithm will split structures into smaller components. A structure that is split by inflation parameter \( \Gamma_1 \) will always be split by any structure that is split by inflation parameter \( \Gamma_2 \), where \( \Gamma_1 > \Gamma_2 \).

#### 2 Markov Clustering

The Markov Clustering algorithm (MCL) was developed as a fast, scalable approach to graph clustering\(^1\) (Van Dongen 2000). Graph clustering (e.g. Schaeffer 2007) is a solution to the problem of finding clusters of points given their pairwise connection amplitudes. One obvious and instructive example of a graph clustering problem is detecting communities within a social network (Liu et al. 2014). Here users are ‘friends’ with other users. The entire friendship network can be represented by a (symmetric) binary matrix, which we call the pairwise connection matrix \( W \), with elements \( w_{ij} \). If users \( i \) and \( j \) are friends, \( w_{ij} = 1 \) and is 0 otherwise. A graph clustering algorithm detects communities within this structure. MCL was chosen for two key reasons: (1) in one of its limits it tends to the standard FoF algorithm as explained later; (2) it supports probabilistic pairwise connections rather than just fixed binary links, which is essential for finding galaxy groups with photometric redshifts.

The MCL algorithm has one free parameter, the inflation parameter \( \Gamma \), which has to be greater than or equal to unity. The algorithm takes the initial pairwise connection matrix, \( W_0 \) (specified by its elements \( w_{ij}^0 \)), as an input and assigns points to clusters following an iterative process, where \( W_k \) is the pairwise connection matrix after \( k \) steps:

1. **Normalise** \( w_{ij}^0 \) column-wise such that \( \sum_j w_{ij}^0 = 1 \).
2. **At step** \( k \), create \( W_k \) by squaring the pairwise connection matrix \( W_{k-1} \), i.e. \( W_k = W_{k-1}^2 \).
3. **Raise every element of** \( w_{ij}^k \) **to the power of** \( \Gamma \), i.e. \( (w_{ij}^k)^\Gamma \).
4. **Renormalise** \( w_{ij}^k \) column-wise such that \( \sum_j w_{ij}^k = 1 \).
5. **Repeat from** (ii) **until all elements of** \( W_k \) **have converged individually to within a specified tolerance.**
6. **Rearrange the converged cleaned** \( W_k \) **matrix into a block diagonal matrix and read off the groups.**

\(^1\) The MCL code is publicly available at http://micans.org/mcl/.

\(^2\) See e.g. Van Dongen (2000) for a discussion of why this approach produces a similar result to a standard random walk, while strictly speaking it is not a random walk.
3 MOCK CATALOGUE

To test the MCL approach to galaxy group finding we apply it to a realistic real space galaxy mock catalogue. We use real space rather than redshift space to better understand the impact of changing the clustering algorithm. We use a $z = 0$ snapshot of the Galform model presented in Gonzalez-Perez et al. (2018), implemented in the 125 $h^{-1}$Mpc per side MilliGas simulation cube. Note that this simulation has the same cosmology and number of snapshots as the 500$h^{-1}$Mpc MR7 simulation (Guo et al. 2013). We use a smaller simulation to speed up the calculations, as deciding between methods of linking galaxies and optimisation of free parameters requires running the algorithm many times. The catalogue is limited in the rest frame r-band to $M_r - 5 \log h \sim -20.0$ and contains $\sim 20,000$ galaxies, corresponding to a galaxy density of $\sim 10^{-2} (h^{-1} \text{Mpc})^{-3}$, comparable to the GAMA survey at $z \sim 0.15$ (Driver et al. 2011; Liske et al. 2015; Baldry et al. 2018). By construction each galaxy belongs to a unique dark matter halo and each halo contains one or more galaxies. See Stothert (2018) for further details of how the mock catalogue was constructed.

4 GOODNESS OF FIT METRICS

We assess the quality of group finding using the measures of purity and completeness. Group purity, $P$, quantifies the extent to which galaxies in the same group are actually in the same halo (e.g. Manning et al. 2008; Wu et al. 2009):

$$P = \frac{1}{N_G} \sum_{i=1}^{N_G} \max_{j}(n_{ij})$$

where $n_{ij}$ is the number of galaxies in group $i$ and halo $j$, $N_G$ is the total number of groups and $N_H$ is the total number of halos. Similarly, we define the halo completeness, $C$, which quantifies the extent to which galaxies in the same halo are placed in the same galaxy group:

$$C = \frac{1}{N_H} \sum_{j=1}^{N_H} \max_{i}(n_{ij}).$$

We also use the associated cumulative measures $C(\geq M)$ and $P(\geq M)$ defined, respectively, as the completeness of halos and the purity of groups with multiplicity (i.e. number of members) greater than or equal to $M$. For the cumulative measures, the multiplicity cut is only applied to the halos for $C(\geq M)$ and groups for $P(\geq M)$.

To optimise the parameters of the MCL algorithm a single statistic is desirable. Here we would like a problem agnostic measure to build an ‘optimal’ group catalogue. Most astrophysical applications invoke combinations of bijective measures of completeness and purity (Gerke et al. 2005; Robotham et al. 2011; Knobel et al. 2012; Jian et al. 2014). Instead we follow Wu et al. (2009) who tested multiple goodness of fit metrics in a statistical context and choose to use the variation of information (VI) (Meil˘ a 2003). VI, also called the shared information distance, quantifies the extent to which the catalogue stops splitting, as all clusters become fully connected sub-graphs with equal pairwise connections, i.e. all points in every cluster are connected only to all other points within the same cluster with the same $w_{ij}$ value (and such clusters are not split by MCL). We note that a $\Gamma$ value of unity will connect any structure that has any path connecting it. In that case MCL tends to converge extremely slowly as no links are ever trimmed from the matrix (see Section 4 for a practical application).

In the astrophysical case we first have a connection criterion that sets the values of $w_{ij}$ between galaxies $i$ and $j$. This is normally based on a distance criterion between two galaxies, setting $w_{ij}$ to 1 if the galaxies are closer to each other than some specified linking length and 0 otherwise. The standard FoF algorithm connects all points that could be reached via a succession of links between points. This outcome is exactly the same as that for MCL with the inflation parameter $\Gamma$ set to unity. Therefore the FoF algorithm should be considered as the limit towards which MCL converges when $\Gamma$ tends to unity, i.e. formally FoF is a subset of MCL. An advantage of MCL over FoF is that, even though MCL like FoF uses all pairwise links, MCL gives higher priority to points that are more connected than those with fewer connections, unlike FoF. By carefully using the inflation parameter, the less well connected points (or less important pairwise links) can be broken up. Only through detailed tests on mocks (see Section 5) can the accuracy of the MCL algorithm be assessed against e.g. FoF.

3 MOCK CATALOGUE

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Figure 1. Variation of information (VI; top), group purity and halo completeness ($P(\geq M)$ and $C(\geq M)$; main panel) as a function of linking length in a standard FoF approach to galaxy group finding for three values of minimum group/halo multiplicity $M$. The minimum of VI provides a good compromise between group purity and halo completeness at all multiplicities.
Figure 2. Group purity, $P(\geq M)$ (left panel), and halo completeness, $C(\geq M)$ (right panel), as a function of minimum multiplicity, $M$, for different VI minimised galaxy group catalogues: simple FoF (dotted), FoF with density enhancement (dashed) and MCL with density enhancement group catalogues (solid). The purity and completeness of the MCL group catalogue is the most consistent as a function of multiplicity, and has undoubtedly the best halo completeness.

Figure 3. The cumulative multiplicity function, $N(\geq M)$, for halos (truth, thick black line) and three groups catalogues (green lines), which are the simple FoF (dotted), FoF with density enhancement (dashed) and MCL with density enhancement (solid). The bottom panel shows the ratio of the multiplicity functions to the truth, $N(\geq M)/N_H$. MCL with density enhancement recovers the true halo multiplicity function extremely well (to better than 7% at all multiplicities).

5 RESULTS

We compare the results of applying two different clustering methods (MCL and FoF) to the mock galaxy catalogue. In each case the free parameters are found by minimizing VI (Eq. 3). All models set the binary connection between galaxies $i$ and $j$, $w_{ij}$, to unity if the pairwise separation $r_{ij}$ is smaller than the linking length $L_{ij}$, and 0 otherwise.

In our first groupings we adopt a constant linking length, i.e. $L_{ij}$ is fixed. For FoF this is the only free parameter. Fig. 1 indicates that the optimal value is $L_{ij} = 0.55h^{-1}$Mpc. The optimal solution with MCL using a fixed linking length is achieved, according to VI, when the inflation, $\Gamma$, tends to unity, indicating that the FoF algorithm is preferred over MCL in this fixed linking length scenario. This is because with a fixed linking length small structures have poor purity and large structures have poor completeness, and increasing $\Gamma$ only splits the larger structures further.
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6 CONCLUSIONS

For the first time in an astronomical context we apply the Markov Clustering algorithm (MCL; Van Dongen 2000), which is part of the more general graph clustering algorithms, to identify galaxy groups. MCL has one free parameter, inflation, $\Gamma$. We show that the widely used FoF algorithm is a subset of MCL; with $\Gamma = 1$, MCL produces the same result as the deterministic FoF algorithm. We apply MCL to detect galaxy groups in a real space galaxy mock catalogue. We minimize the variation of information (VI; Meilă 2003) to compare group catalogues to real halos. We validate this choice by showing that the minimum value of VI for a simple FoF approach is found at linking lengths that are in good agreement with previous values (e.g. Eke et al. 2004).

For a constant linking length FoF produces the best group catalogue. Nevertheless, FoF returns too many spurious small groups and too few large groups: increasing inflation away from unity only makes this discrepancy worse. Using a linking length sensitive to the local density to account for the scale dependence of the grouping, MCL is superior to FoF (i.e. VI is minimised with $\Gamma > 1$). In both cases the group purity and halo completeness are improved over a fixed linking length FoF for all multiplicities. The MCL group catalogue has better halo completeness and group purity than the comparable FoF catalogues, with a completeness and purity that is approximately independent of multiplicity. As a result, MCL provides a better estimate of the number of groups at all multiplicities tested here to better than 7%, and often to better than 3%. This is to be compared to the best FoF performance which underestimates the number of halos by as much as 25% from the truth at $N \geq 5$ and ~15% for most multiplicities. Note these results were not used to identify the optimal group finder, which is determined by minimizing the variation of information (VI) for each clustering model.

Our results show that MCL can better address the stochastic nature of ‘bridges’ connecting structure that appear with FoF. FoF needs to be more cautious about the connection criterion as there is a large penalty if even a single link is found between two large structures, whereas MCL reduces this penalty by using inflation to break loosely connected structures. These ‘bridges’ cause the number of high multiplicity FoF groups to be underestimated (see Fig. 3), and their group purity to be low (see Fig. 2). Both aspects are improved significantly upon using MCL.
real space, where pairwise connections are not probabilistic, MCL produces better group catalogues than FoF. Future work will test MCL on more detailed mock galaxy catalogues in redshift space with photometric errors.

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