



Master's thesis
Astronomy

Your Title Here

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1. Introduction

1.1 TL;DR version of prerequisite information

1. galaxies form
 - Why?
 - When?
 - How?
 - Where?
2. galaxies form in groups
3. our local group is one of these
4. something about large scale distribution of galaxies

1.2 History of Local Group Research

LG objects visible with naked eye -> realization they are something outside our galaxy -> realization they are something very much like our galaxy

First determining distance was difficult, now mass is more interesting question

1.3 Aim of This Thesis

Whatever the main results end up being, presented in somewhat coherent manner and hopefully sugar-coated enough to sound Important and Exciting.

2. Theoretical Background

Cosmology determines the properties of the Universe, including its origin, the rules by which it evolves and the structures that arise (Mo et al., 2010). Thus many fields of astronomy and astrophysics, including the study of galaxies and galaxy groups such as the Local Group and its members, is tightly connected to the study of cosmology. This section gives a brief explanation of the current cosmological understanding, its relevant implications and how the Local Group is currently viewed in the cosmological context.

2.1 Basics of Cosmology

Understanding processes that happen on large scales or take long times requires understanding some basic cosmology. The following sections will cover the most basic concepts of cosmology, the evolution of the Universe on both large and small scales, and the Λ CDM model which is currently the cosmological model that best matches the observations on multiple scales (Mo et al., 2010). Sections 2.1.1 and 2.1.2 cover large scales at which the cosmological principle applies and section 2.1.3 covers smaller scales of single dark matter halo.

2.1.1 Evolution of the Universe

Current cosmological understanding is based on a subset of the general theory of relativity together with simple hypotheses such as the cosmological principle, which

states that on large scales the Universe is spatially homogeneous and isotropic (Mo et al., 2010). At a given location, an observer might not see this, as is easy to understand when considering two observers located at the same point but moving relative to each other. In this situation, it is clear that at least one of the observers will see a dipole in the surrounding velocities and thus will not observe the universe to be isotropic. Nonetheless, in an isotropic universe, for every point in space we can define a so-called fundamental observer as the observer who sees the universe as isotropic (Mo et al., 2010). These fundamental observers correspond to a cosmological rest frame, which can be determined at a given location by e.g. observing the cosmic microwave background and subtracting the velocity corresponding to the observed dipole component (Mo et al., 2010).

The existence of such fundamental observer has interesting consequences. Existence of any large-scale flows are clearly prohibited, as these would violate the isotropy. In a three-dimensional universe any curl of the velocity field around the fundamental observer is also forbidden. This can be easily seen by considering the hairy ball theorem, which states that a sphere cannot have a nowhere-zero tangent vector field (Renteln, 2013). Thus if there was a curl in the surrounding velocity field, there would always be at least one direction in which the tangential velocity is zero and thus the field would not be isotropic. This means that there cannot be any tangential motion and thus the only allowed motion happens in the radial direction: the Universe can either expand or contract.

The expansion of the Universe can be parametrized by dimensionless scale factor a , whose time evolution is governed by the Friedmann equations

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3} \left(\rho + 3\frac{P}{c^2} \right) + \frac{\Lambda c^2}{3} \quad (2.1)$$

$$\left(\frac{\dot{a}}{a} \right)^2 = \frac{8\pi G}{3} \rho - \frac{Kc^2}{a^2} + \frac{\Lambda c^2}{3}, \quad (2.2)$$

where G is the gravitational constant, P is pressure, ρ is energy density and K and Λ are cosmology-related parameters (Mo et al., 2010). K specifies the curvature of

the universe, determined by the overall density of the universe (Mo et al., 2010). The allowed values for K are -1 corresponding to a hyperbolic universe, 0 to a flat one and 1 to a spherical universe (Mo et al., 2010). Modern measurements suggest that the Universe is flat within the measurement error, but small deviations from the $K = 0$ cannot be ruled out (Planck Collaboration, 2016). Λ is the cosmological constant driving the expansion of the universe, often described as dark energy or vacuum energy (Mo et al., 2010).

The scale factor a is important for this thesis as it both affects the distances and velocities measured and governs the structure formation. It increases or decreases as the universe expands or contracts, and thus it can be used to relate distances at different times (Mo et al., 2010). For a universe that is monotonically expanding the scale factor can also be used as an alternative time coordinate, as it has a one-to-one correspondence to time. It is often convenient to measure not the proper distance l between a pair of objects, but instead their so-called comoving distance r : (Mo et al., 2010)

$$r = \frac{l}{a} \quad (2.3)$$

For a pair of objects with no relative motion, the comoving distance will remain constant as the size of the universe changes. A comoving coordinate system is often used in cosmological simulations, as the expansion of the universe is included in the scale factor instead of all of the coordinates having to be recalculated as the size of the universe varies (Griebel et al., 2007).

Observations have confirmed that the universe is indeed expanding, first observed by Hubble (1929). The rate of the expansion is denoted with the Hubble parameter $H(t)$, which is defined using the proper distance and the rate of change of the proper distance between a pair of fundamental observers:

$$H(t) \, l = \frac{dl}{dt} \quad (2.4)$$

The Hubble parameter is also closely related to the scale factor, as (Mo et al., 2010)

$$H(t) = \frac{\dot{a}(t)}{a(t)} \quad (2.5)$$

The first measurements trying to determine the current value of the Hubble parameter, often called the Hubble constant, were prone to error as the distance estimates to extragalactic objects were inaccurate, but later estimates offer reasonably accurate results such as Planck Collaboration (2014) value of 67.77 ± 0.77 km/s/Mpc for the current expansion speed.

Another factor affecting measurements based on extragalactic objects is that the observed proper velocities contain not only the expansion of the universe but also peculiar motions of the objects, which is why measurements based on other probes such as the cosmic microwave background in case of Planck Collaboration (2016) are valuable. Information contained in the peculiar motions can still be interesting. In this thesis, the mass of the Local Group is estimated using radial velocity measurements within a few megaparsecs of a number of simulated Local Universe analogues. At scales this small, the expansion of the universe is greatly affected by local gravity fields, and thus expansion measurements can be used to infer the mass enclosed within the Local Group.

While the scale factor is one possible way of expressing time, it is not the only one. As the universe expands and we observe objects receding, the emitted light from them is shifted to longer wavelengths. The further away the emitter is, the more the space between the observer and emitter will expand making the effect stronger. The relative change in the wavelength is called redshift z , defined as

$$z \equiv \frac{\lambda_o - \lambda_e}{\lambda_e} \quad (2.6)$$

where λ_o is the observed and λ_e the emitted wavelength (Mo et al., 2010). If the effect of peculiar motions is ignored, redshift is directly related not only to the distance to the emitter but also to the scale factor at the time of the emission. For arbitrary scale factors at the time of the emission and observation, the relation

between z and a is (Mo et al., 2010)

$$1 + z = \frac{a(t_o)}{a(t_e)} \quad (2.7)$$

2.1.2 Composition of the Universe

Using the Friedmann equations 2.1 and 2.2 to model the evolution of the Universe requires not only the equations and cosmological parameters introduced in section 2.1.1, but also the composition of the Universe has to be known in order to determine the density, pressure, cosmological constant and ultimately even the curvature of the Universe. According to the current understanding, the Universe is made of three components: non-relativistic matter, relativistic matter and vacuum energy (Mo et al., 2010). At present time, about 69 % of the energy density ρ in the Universe is vacuum energy and 31 % is non-relativistic matter, including both baryonic and dark components (Planck Collaboration, 2016). Most of the non-relativistic matter, around 84 %, is dark matter, with baryonic matter only contributing around 16 % of total matter energy density (Planck Collaboration, 2016). The energy density of relativistic matter i.e. photons and standard-model neutrinos in the present-day universe is negligible (Mo et al., 2010).

This has not always been true, as these ratios change over time as the Universe evolves. It is easy to see that, as the Universe expands, the energy density of matter behaves as a^{-3} , as the volume of the Universe increases as a^3 and in an adiabatic system no new matter is created or disappears. Radiation is diluted similarly to matter, but in addition to the effect of increasing volume, the growing universe also causes the wavelength of the radiation to increase, resulting in the energy density decreasing as a^{-4} . The vacuum energy, as the name suggests, can be thought as arising from the space itself, and thus a change in a does not affect the energy density of the component (Mo et al., 2010). The change of energy density of a component may also correspond to a change in the pressure or temperature of the component

Component	ρ	P	T
Matter	a^{-3}	a^{-5}	a^{-2}
Radiation	a^{-4}	a^{-4}	a^{-1}
Dark energy	a^0	a^0	

Table 2.1: Evolution of energy density, pressure and temperature of the Universe as the scale factor varies. Adapted from Mo et al. (2010).

changing (Mo et al., 2010). These effects are shown in table 2.1.

The different time evolutions of the components also mean that the dominant component of the Universe changes as the scale factor grows. At very early times the Universe was radiation dominated, but as the radiation energy density decreases faster than the energy densities of the two other components, a matter dominated era followed. As the dark energy is the only component with constant energy density, it will be the final dominant energy component. This transition from matter to dark energy dominated era has happened in the recent past (Mo et al., 2010).

The geometry of the Universe is also determined by the contents of it. A density threshold known as critical density and defined as

$$\rho_{crit,0} \equiv \frac{3H_0^2}{8\pi G} \quad (2.8)$$

acts as a threshold value that separates the different geometries (Mo et al., 2010). Subscript zero comes from $z = 0$ and denotes present-day values, but all introduced quantities can also be determined at any other time. The overall density of the universe can be parametrized using this critical density:

$$\Omega_0 \equiv \frac{\bar{\rho}_0}{\rho_{crit,0}} \quad (2.9)$$

where $\bar{\rho}_0$ is the mean density of the universe and Ω_0 is known as the density parameter (Mo et al., 2010). Different values of Ω_0 correspond to different geometries: for

values of $\Omega_0 < 1$ the Universe is hyperbolic, for $\Omega_0 = 1$ flat and for $\Omega_0 > 1$ spherical (Mo et al., 2010).

As the contents of the Universe can be divided into the three categories of vacuum energy and relativistic and non-relativistic matter, the total density parameter is also a sum of three density parameters:

$$\Omega_0 = \Omega_{m,0} + \Omega_{r,0} + \Omega_{\Lambda,0} \quad (2.10)$$

where m , r and Λ stand for non-relativistic matter ("matter"), relativistic matter ("radiation") and vacuum energy (Mo et al., 2010). Each of these can be calculated similarly to the equation 2.9 but replacing the overall density with density of the corresponding component (Mo et al., 2010). As in the Universe the value of Ω_0 is very close to unity, the different density parameters conveniently correspond the relative densities of the components.

2.1.3 Structure Formation

All structures in the Universe arise from the small perturbations in the matter density in the early universe and the physics that govern their evolution. Starting at the end of inflation, small density contrasts in the dark matter start to grow. These primordial density fluctuations that later develop into the structures such as galaxy clusters and voids separating them can still be seen in the cosmic microwave background (CMB) (Planck Collaboration, 2016). Starting from the end of inflation, the density contrast of such perturbations in the dark matter begin to grow. While the DM is collisionless, the pressure experienced by baryons slows their structural evolution down. Consequently, their evolution is delayed relative to the dark matter, and baryons sink into potential wells already formed from the dark matter.

At $z \approx 1100$, the time of recombination and origin of the CMB photons, these fluctuations are still very small, having $\Delta\rho/\rho \approx 10^{-4}$, but sufficiently overdense regions have already collapsed (Mo et al., 2010). The gas inside these structures

seen as hot spots in the CMB has just reached a density maximum and is shock-heated, while gas inside smaller fluctuations has already begun expanding again, and larger scales have not yet reached their maximum density at the time of the CMB.

At first, the evolution of overdense regions that will later collapse differ from the evolution of the surroundings only by the speed of the expansion of the Universe in that region: denser regions expand slower. Later some of these volumes will start to collapse. This requires the volume to be sufficiently dense to allow gravity to overcome the expansion of the universe as described by the Friedmann equations.

To understand the evolution of density perturbations at early times when the perturbations are still small and evolve linearly, let us consider an ideal fluid of density ρ , moving at proper velocity \mathbf{v} and experiencing the gravitational field with potential ϕ . Growth of a perturbation in this medium is governed by three equations: the equation of continuity describing the conservation of mass, Euler equation governing the motions in the fluid and the Poisson equation describing the gravitational field, or

$$\frac{D\rho}{Dt} + \rho \nabla_{\mathbf{x}} \cdot \mathbf{v} = 0, \quad (2.11)$$

$$\frac{D\mathbf{v}}{Dt} = -\frac{\nabla_{\mathbf{x}} P}{\rho} - \nabla_{\mathbf{x}} \phi \quad (2.12)$$

and

$$\nabla_{\mathbf{x}}^2 \phi = 4\pi G \rho \quad (2.13)$$

respectively (Mo et al., 2010). Here \mathbf{x} denotes proper coordinates and $\frac{D}{Dt}$ is the convective time derivative, defined as

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} \quad (2.14)$$

and describing the time derivative when moving with the fluid (Mo et al., 2010).

Next let us introduce a small perturbation by replacing \mathbf{v} , ρ , P and ϕ with $\mathbf{v}_0 + \delta\mathbf{v}$, $\rho_0 + \delta\rho$, $P_0 + \delta P$ and $\phi_0 + \delta\phi$ respectively, having subscript zero represent the properties of the unperturbed medium. Now equations 2.11–2.13 are

$$\frac{D\rho_0}{Dt} + \frac{D\delta\rho}{Dt} + \rho_0 \nabla_{\mathbf{x}} \cdot \mathbf{v}_0 + \rho_0 \nabla_{\mathbf{x}} \cdot \delta\mathbf{v} + \delta\rho \nabla_{\mathbf{x}} \cdot \mathbf{v}_0 + \delta\rho \nabla_{\mathbf{x}} \cdot \delta\mathbf{v} = 0, \quad (2.15)$$

$$\frac{D\mathbf{v}_0}{Dt} + \frac{D\delta\mathbf{v}}{Dt} = -\frac{\nabla_{\mathbf{x}}(P_0 + \delta P)}{\rho_0 + \delta\rho} - \nabla_{\mathbf{x}}\phi_0 - \nabla_{\mathbf{x}}\delta\phi \quad (2.16)$$

and

$$\nabla_{\mathbf{x}}^2 \phi_0 + \nabla_{\mathbf{x}}^2 \delta\phi = 4\pi G \rho_0 + 4\pi G \delta\rho. \quad (2.17)$$

These equations can be greatly simplified by subtracting the unperturbed versions from each and assuming that the initial state is homogeneous and isotropic i.e. $\nabla P_0 = 0$ and $\nabla \rho_0 = 0$. Using the knowledge that in the linear regime the perturbations are small and thus discarding second order terms, the equations take the following forms:

$$\frac{D}{Dt} \frac{\delta\rho}{\rho_0} = -\nabla_{\mathbf{x}} \cdot \delta\mathbf{v} \quad (2.18)$$

$$\frac{\partial \delta\mathbf{v}}{\partial t} + (\delta\mathbf{v} \cdot \nabla_{\mathbf{x}}) \mathbf{v}_0 = -\frac{\nabla_{\mathbf{x}} \delta P}{\rho_0} - \nabla_{\mathbf{x}} \delta\phi \quad (2.19)$$

$$\nabla_{\mathbf{x}}^2 \delta\phi = 4\pi G \delta\rho \quad (2.20)$$

As the Universe is expanding, it is natural to transit to comoving coordinates, defined in equation 2.3 and denoted by \mathbf{r} . This also affects the velocities, and using the dot to denote time derivative we can write

$$\mathbf{v} = \dot{\mathbf{x}} = \dot{a}(t) \mathbf{r} + a(t) \dot{\mathbf{r}} = \dot{a}(t) \mathbf{r} + \mathbf{u}, \quad (2.21)$$

where \mathbf{u} denotes the perturbed comoving velocity. From this it follows that $\delta\mathbf{v} = a\mathbf{u}$. In comoving coordinates the operator $\nabla_{\mathbf{x}}$ is also replaced with $\frac{1}{a}\nabla_{\mathbf{r}}$. Using these

and $(a\mathbf{u} \cdot \nabla_{\mathbf{x}})\dot{a}\mathbf{r} = \mathbf{u}\dot{a}$, the equations can be written as

$$\frac{D}{Dt} \frac{\delta\rho}{\rho_0} = -\nabla_{\mathbf{r}} \cdot \mathbf{u} \quad (2.22)$$

$$\frac{\partial \mathbf{u}}{\partial t} + 2\frac{\dot{a}}{a}\mathbf{u} = -\frac{\nabla_{\mathbf{r}}\delta P}{\rho_0 a^2} - \frac{1}{a^2}\nabla_{\mathbf{r}}\delta\phi. \quad (2.23)$$

$$\nabla_{\mathbf{r}}^2\delta\phi = 4\pi G\delta a^2\rho \quad (2.24)$$

Taking the comoving divergence, equation 2.23 gives

$$\nabla_{\mathbf{r}} \cdot \dot{\mathbf{u}} + 2\frac{\dot{a}}{a}\nabla_{\mathbf{r}} \cdot \mathbf{u} = -\frac{\nabla_{\mathbf{r}}^2\delta P}{\rho_0 a^2} - \frac{1}{a^2}\nabla_{\mathbf{r}}^2\delta\phi. \quad (2.25)$$

There the last term on the right side contains the left side of equation 2.24, the first term on the left can be found in equation 2.22 after taking the convective time derivative and the second term on the left already contains the right side of 2.22.

Inserting these yields

$$\frac{D^2}{D^2t} \frac{\delta\rho}{\rho_0} + 2\frac{\dot{a}}{a} \frac{D}{Dt} \frac{\delta\rho}{\rho_0} = \frac{\nabla_{\mathbf{r}}^2\delta P}{\rho_0 a^2} + 4\pi G\delta\rho. \quad (2.26)$$

The overdensities in the Universe are often denoted using a density contrast $\Delta = \delta\rho/\bar{\rho}$, where the bar denotes the universal mean (Mo et al., 2010). In this case the unperturbed density ρ is the mean density, so the left side of equation 2.27 can be expressed using Δ . If the density perturbations are assumed to be adiabatic, the adiabatic sound speed c_s relates perturbations in density and pressure as $\delta P/\delta\rho = c_s^2$.

Inserting these yields

$$\frac{D^2\Delta}{D^2t} + 2\frac{\dot{a}}{a} \frac{D\Delta}{Dt} = \frac{c_s^2\nabla_{\mathbf{r}}^2\Delta\rho_0}{a^2\rho_0} + 4\pi G\Delta\rho_0. \quad (2.27)$$

Now a trial solution of $\Delta \propto e^{i(\mathbf{k}_r \cdot \mathbf{r} - \omega t)}$ corresponding to a wave with comoving wavevector \mathbf{k}_c yields a wave equation

$$\frac{D^2\Delta}{D^2t} + 2\frac{\dot{a}}{a} \frac{D\Delta}{Dt} = \Delta(4\pi G\rho_0 - k^2 c_s^2). \quad (2.28)$$

Here \mathbf{k}_r has been replaced by $a\mathbf{k}$ to transform it to proper coordinates. This is a linear second-order partial differential equation that describes the evolution of perturbations. This equation represents the perturbations well if they are assumed to be spatially small compared to the observable universe at all times and that all matter behaves as non-relativistic fluid so that Newtonian physics suffice to describe the perturbation.

Whether the waves described by equation 2.28 are oscillatory or unstable depends on the sign of the right side of the equation. If $c_s^2 k^2 > 4\pi G \rho_0$ the perturbations are oscillating sound waves supported by the internal pressure of the denser regions, but if $c_s^2 k^2 < 4\pi G \rho_0$ the wave is unstable and the modes grow (Longair, 2008). In a static universe these density perturbations grow exponentially but in an expanding universe the growth is slower: e.g. in simple Einstein-de Sitter universe with $\Omega_0 = 1$ and $\Omega_{\Lambda} = 0$ the growth is only algebraically (Longair, 2008).

??? -> wave equation -> perturbations may be either oscillatory or growing
-> Jeans

Transition to later times and non-linear collapse, non-linear usually requires simulations

2.2 Local Group

2.2.1 Determining the Mass of the Local Group and Its Members

3. Simulations and Simulation Codes

Simulations are a valuable tool in astrophysical research as they bypass many major restrictions characteristic to observational astronomy such as not being able to observe the evolution of a single object with the exception of the most rapid events such as supernovae, and the observations being constrained to a single view plane. The data used in this master's thesis also originates from a cosmological N-body simulation. This section shortly introduces first some fundamental operational principles of N-body simulations and then specifics of the [insert name or other identification here] simulations from which the data used here originates from.

3.1 N-body simulations

N-body simulations are a type of computer simulations that follow a number of particles interacting with each other, often used in computational astrophysics (Binney and Tremaine, 2008). Their concept is simple: the current states of the particles are known and a physical model is used to calculate how the states of the particles should advance over a small period of time known as the time step (Binney and Tremaine, 2008). Simple dark matter only simulations might only handle gravitational interactions of the particles, but many simulation codes such as GADGET-2 (Springel, 2005) (see section 3.2.1 for more about GADGET family simulation codes)

and Enzo (Norman et al., 2007) are also able to handle hydrodynamics of baryonic matter and can include star formation, feedback and other baryonic processes.

There are multiple ways to handle both the force calculations and calculating new positions for the particles (Binney and Tremaine, 2008). For the force calculations most popular algorithms are based on either hierarchical trees or particle meshes, but for calculating the positions, a wide variety of integrators have been developed for a range of different needs (Binney and Tremaine, 2008). The [insert identification here] simulations are run using a modified GADGET-3 and thus use the TreePM method for force calculations accompanied by a leapfrog integrator. TreePM is a mix of a hierarchical tree for close range forces and a particle mesh for distant forces, the former of which is more interesting. Therefore the Barnes and Hut (1986) hierarchical tree algorithm is introduced in the following subsection, followed by a short description of the leapfrog integrator in the next one.

3.1.1 Hierarchical Tree Algorithm

In many applications of computational astrophysics the desired number of particles in a simulation is too great to allow calculating interparticle forces by direct summation as its time complexity is $\mathcal{O}(n^2)$. One of the alternatives is organizing the particles into a tree data structure, which allows distant particles residing close to each other to be approximated as single more massive particle. This approach was first introduced by Appel (1985) and Barnes and Hut (1986), the latter of which will be followed here.

Constructing the tree starts with setting the full simulation box as the root of the tree. This root cube is then subdivided into eight equally sized sub-cubes called cells. These eight cells are children of the root node. This starts a recursive process where each new cell is again divided into eight subcells recursively until each of the cells contains either no particles, one particle or eight subcells. When a new cell is

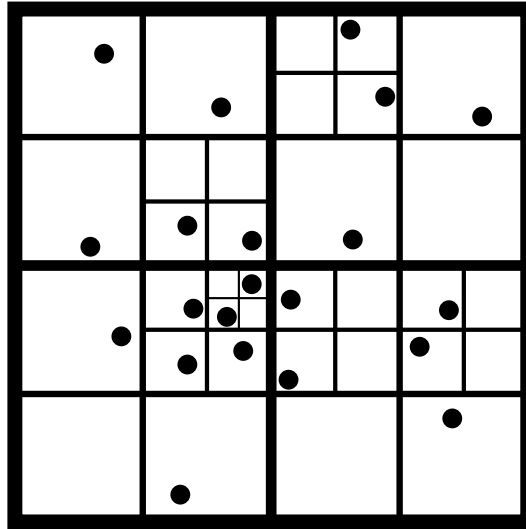


Figure 3.1: A two-dimensional example of particles (black dots) being split into cells using the Barnes-Hut algorithm (Barnes and Hut, 1986). The outermost square is the simulation box, i.e. the root of the tree, and the smaller squares with decreasing line thicknesses are its descendants. Note how each cell contains either one particle, no particles or four smaller subcells.

created, the total mass of the enclosed particles and the location of the mass centre of the particles within it is stored as a pseudoparticle to allow easy calculation of the approximate gravitational effect the particles within a cell have on a distant particle.

To aid understanding the process, a two-dimensional simplification of the simulation box after the tree has been constructed is shown in figure 3.1, together with the corresponding tree in figure 3.2. The thick outer line of the former figure is the simulation box, corresponding to the topmost node of the tree in the latter. This root cell is first divided into four (in contrast to eight in the three-dimensional case) subcells, which is shown with the second-thickest line dividing the simulation box into quarters in figure 3.1. These four cells are the four children of the root node in the tree. Each of the subcells contains more than one particle, so each of those is again split into four quarters, each quarter a child of the original node in the tree.

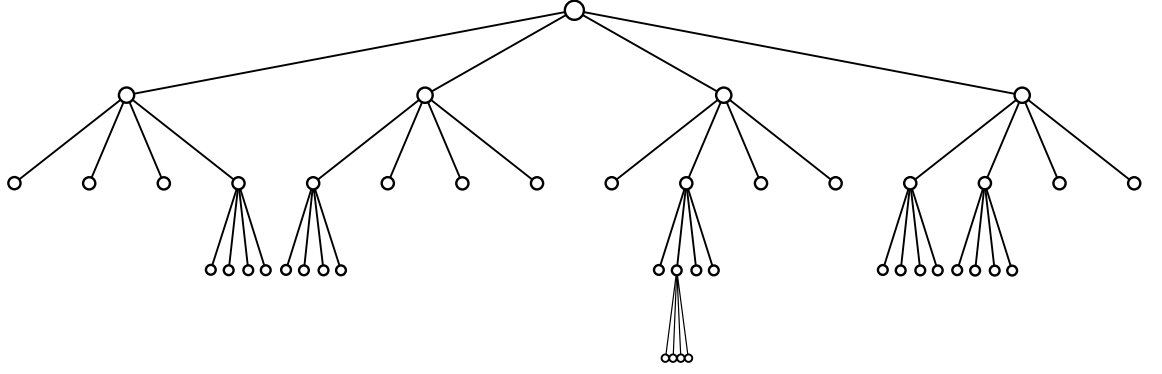


Figure 3.2: Cells of figure 3.1 shown as a tree, each level of refined cells in 3.1 traversed from left to right and up to down corresponding to each level of nodes from left to right. Cells with no particles are not used in force calculations and thus they do not need to be stored in computer memory, but they are shown here to emphasize the structure of the tree.

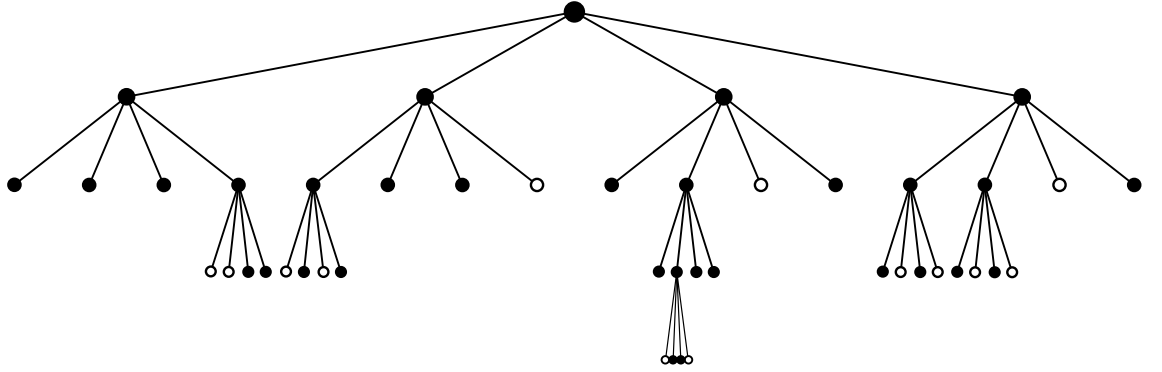


Figure 3.3: Alternative tree where cells with particles are solid, doesn't work as well as it could

These quarters of quarters form the third level of the tree in figure 3.2.

Some of these newly-created cells are empty or only have a single particle, so for them the recursion halts and the nodes of the tree are leaves. The rest are again split and a new layer of the tree is created, but as some cells were complete already the fourth layer of the tree is not full. In this case only one cell requires division beyond the fourth level, producing the last four leaves of the tree on the fifth level.

Often, as is the case in the example, some of the leaf nodes are empty. In

the case of a real simulation, these of course do not need to be saved as there is no information to store, but in this example case all are drawn to emphasize the regular structure of the tree. In the three-dimensional case where each internal cell has eight subcells the formed tree is known as an octree, whose two-dimensional analog, the quadtree, is constructed in the previous example.

The tree can then be utilized to speed up the force calculations. When calculating the gravitational acceleration felt by a single particle, the tree is traversed starting from the root. The ratio l/D of the length of a side of the cell and the distance from the particle to the pseudoparticle representing the mass within the cell is then calculated. If the ratio is smaller than a predefined accuracy parameter θ representing the opening angle of the cell, the cell is treated as if everything within it was replaced with the pseudoparticle having the combined mass of the cell. Otherwise the subcells of the cell are examined recursively in the same way until a small enough subcell is found or a leaf of the tree is reached, at which point the pseudoparticle and the real particle in the cell are equivalent and the force can be calculated with the maximum accuracy possible for the simulation.

Using the Barnes-Hut algorithm, the tree construction and the force calculations both have time complexity of $\mathcal{O}(n \log n)$. This is a significant improvement over the $\mathcal{O}(n^2)$ of the direct summation considering that the accuracy cost is fairly small: Barnes and Hut (1986) report accuracy of about 1 % when $\theta = 1$ and the accuracy can be improved by either setting a smaller θ or including multipole moments in the pseudoparticles (Barnes and Hut, 1989). Similar algorithms with even better time complexity of $\mathcal{O}(n)$ have also been introduced such as ones by Dehnen (2002) and Xue (1998).

The algorithm is also straightforward to parallelize as different branches of the tree can be assigned to their own threads, though memory management has to be done carefully when forces outside the current branch of a thread are calculated

(Binney and Tremaine, 2008). One way to circumvent the memory management issue is to use a particle mesh based integrator for long range forces as GADGET-2 does (Springel, 2005). The algorithm can also handle problems where the range of densities in the simulation box is wide which is important for applications such as galaxy mergers and cosmological simulations. This, together with their competitive time complexity, makes tree based codes an appealing tool for many astrophysical simulations (Binney and Tremaine, 2008).

3.1.2 Leapfrog Integrator

A number of different integrators suitable for astronomical and astrophysical applications have been developed for solving different problems (Binney and Tremaine, 2008). No integrator is optimal for every task and thus factors such as the integration time, amount of memory available per particle, smoothness of the potential and the cost of a single gravitational field evaluation should be considered (Binney and Tremaine, 2008). One of the integrators that are well suited for cosmological simulations is the leapfrog integrator, which is also used by GADGET-2 simulation code among others (Springel, 2005).

When a fixed time-step is used, the leapfrog integrator conserves the energy of the system and is time reversible (Binney and Tremaine, 2008). While a variable time-step is possible and often used, it requires some modifications to the algorithm, presented in e.g. Springel (2005). Other benefits of the integrator are its second order accuracy and the fact that it doesn't require excessive amounts of memory per particle as only the current state of the system is needed in calculating the next step (Binney and Tremaine, 2008). With its second order accuracy paired with symplecticity, it rivals fourth order integrators such as the fourth order Runge-Kutta when used for long simulation runs (Binney and Tremaine, 2008).

Timestepping with the leapfrog integrator consists of two phases, the drift and

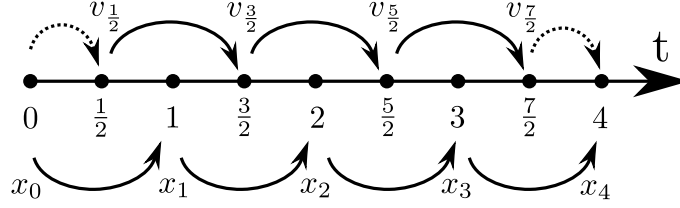


Figure 3.4: Timesteps taken by the leapfrog algorithm, positions (x) updated as indicated with lower arrows and velocities (v) as the upper arrows. It is not important for the algorithm which of the two is chosen to step through the integer times, choice of it being x in this figure is arbitrary. The dashed short arrows depict the half-steps that are needed when a synchronized output is desired.

the kick steps, which are alternated with a half-step offset as shown in figure 3.4 (Binney and Tremaine, 2008). During the kick step, the momenta of the particles are updated and during the drift step the positions of the particles are changed according to the previously calculated momenta (Binney and Tremaine, 2008). When synchronized output of both positions and velocities is desired, a half-timestep advance or backtrack to either of the variables will result in both variables being outputted at the same time. This kind of synchronization steps at the ends of the integration are indicated in figure 3.4 with dashed arrows.

3.1.3 Halo Finding

The data output by a cosmological simulation consists of individual particles tracing the underlying density field. To make comparisons to the real universe, a way of matching structures in the simulation to observable objects is needed. In a dark matter only simulation no structure would obviously be directly observable but luckily many properties of dark matter haloes from simulations can be compared with the estimated dark matter haloes of observed galaxies. Making such comparisons requires naturally such structures to be identified first, which makes structure finding a key step in the data analysis for many astrophysical and cosmological applications

(Knebe et al., 2013).

A number of different halo finders designed to read N-body data and extract locally overdense gravitationally bound systems have been developed to suit different needs, most based either on locating density peaks or collecting and linking together particles located close to each other based on some metric (Knebe et al., 2013). A pair of methods belonging to the two groups respectively, the friends-of-friends (FOF) and SUBFIND algorithms, are discussed here. Both algorithms were developed separately, FOF by Davis et al. (1985) and SUBFIND by Springel et al. (2001), but they work well when used together by inputting FOF results to SUBFIND as a starting point for the subhalo finding (Springel, 2005).

The FOF algorithm is simple and based purely on the spatial separation of the particles: pairs of particles residing closer to each other than a chosen threshold distance called linking length are marked to reside within same group by linking them together (Davis et al., 1985). When all particles have been processed, each distinct subset of particles linked to each other is defined to be a group (Davis et al., 1985). Figure 3.5 presents an example of a set of particles grouped using the FOF algorithm. Depending on the specifics of the data and its intended usage, one might want to discard the smallest groups with only a few particles both because they are more likely than bigger groups to be just realizations of the random noise instead of actual physical structures but also due to their small size as they might not be massive enough to represent the structures that are being studied.

The algorithm is made appealing by its simplicity, small number of free parameters and ability to find structures of arbitrary shape (Davis et al., 1985). However, it is prone to link unrelated structures via thin bridges that might consist of only a single chain of particles. This behaviour can be seen in figure 3.5: the leftmost group has two dense areas that could be cores of two separate groups connected by a single-particle bridge. Removal or even suitable movement of this particle

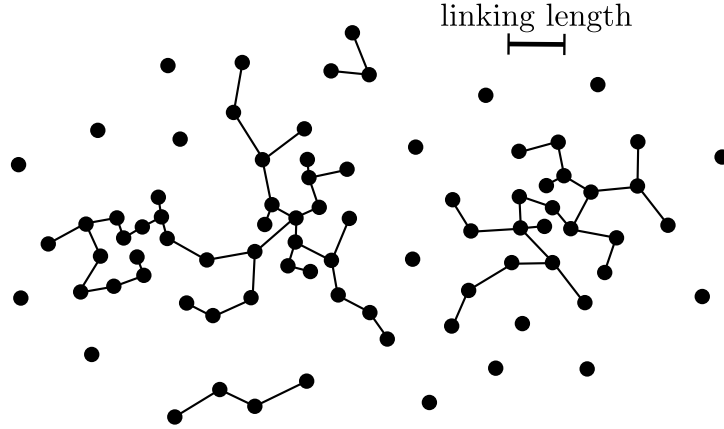


Figure 3.5: Friends-of-friends groups found from a mock data set using the length of the indicator in the upper right area of the illustration as the linking length. Particles are depicted as black dots and the links connecting particles within groups are shown with black lines.

would result in the group separating into two distinct groups. The two big groups also stretch quite close to each other in their lower parts: moving or adding one particle between the chains of particles protruding towards each other would result in the two groups merging. Also the algorithm as is cannot be used to detect substructure within larger objects, though modifications of it such as hierarchical friends-of-friends algorithm by Gottlöber et al. (1999) have been developed Springel et al. (2001).

In contrast to groups found by FOF, the SUBFIND algorithm has been developed to extract physically well-defined subhaloes that are self-bound and locally overdense from a given parent group. SUBFIND can work with an arbitrary parent group, but FOF groups are well-suited for parent groups as the algorithm is simple and with appropriately long linking lengths the FOF groups, while possible to consist of multiple independent physical structures, are unlikely to split a physical structure between FOF groups (Springel et al., 2001).

Unlike FOF, SUBFIND uses a local density estimate instead of individual par-

ticle pairs. It labels all locally overdense regions enclosed by an isodensity contour traversing a saddle point as substructure candidates (Springel et al., 2001). This is done by lowering an imaginary density threshold through the range of the density field: particles surrounding a common local density maximum are assigned to a common substructure candidate until two separate substructure regions join in a saddle point of the potential (Springel et al., 2001). When a saddle point is reached the two substructure candidates it connects are both stored individually to be processed further and the saddle point particle is added to a new substructure candidate containing the particles from both of the smaller candidates (Springel et al., 2001). Thus the algorithm is able to identify a hierarchy of substructures within each other (Springel et al., 2001).

A two-dimensional example of this substructure candidate identification is shown in figure 3.6. The algorithm starts from the particle in the most dense area of the simulation. At that point, the particle has no neighbours that would be in higher density than the particle itself, and thus it becomes the first particle of a substructure candidate. All of the particles belonging to this substructure candidate are marked with dashing in the figure. The algorithm iterates through the particles in order of decreasing density, always finding that the next particle has one neighbouring particle in higher density area than the particle itself and thus adding it to the same dashed group, until the second local density maximum is reached. At that point, a new substructure candidate marked with checkerboard pattern is created. The following particles are assigned to their respective substructure candidates based on their single higher potential neighbour until a saddle point between the two is reached, at which point the state of the substructure candidates is shown in figure 3.6. At that point the current substructure candidates are complete and will be saved. Next the particles belonging to the two structures can be joined by the saddle point particle to join a new bigger substructure candidate.

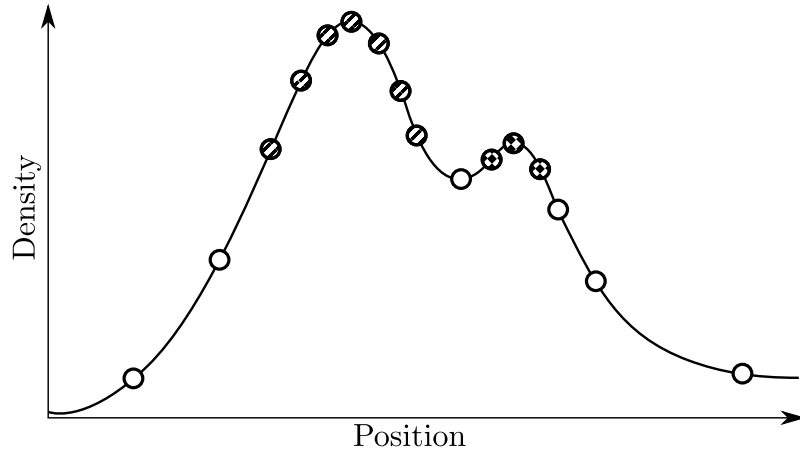


Figure 3.6: Intermediate stage of the SUBFIND algorithm, shown just before it reaches the first saddle point. Circles depict simulation particles and the line the underlying density field. Striped and checkered circles both belong to their own subhalo candidates whereas the white ones are not yet labeled.

Unfortunately, now some particles are assigned to multiple substructure candidates and it is not clear that all particles within one substructure candidate are actually part of an actual physical structure (Springel et al., 2001). It is very much possible that some particles are just passing by and if the same particles were re-examined at a later time, they would no longer be anywhere near the structure they were supposed to belong to. Hence the next step in the analysis is to eliminate unbound particles by iteratively removing particles with positive energy until all of the remaining particles are bound to each other by their mutual gravitational attraction (Springel et al., 2001). At this stage, each particle is labelled only based on the smallest structure it resides in, which solves the problem of a single particle belonging to multiple structures (Springel et al., 2001).

After the iterative pruning stage some substructure candidates can vanish completely or be left with very few members. These substructure candidates with less than some minimum number of bound particles can be discarded (Springel et al., 2001). The structures candidates surviving the pruning can then be considered to

represent physical structures and are labelled as subhaloes (Springel et al., 2001). In this work, all of the analysis is based on catalogues containing such subhaloes.

3.2 Simulation Runs

[insert some form of attribution for the simulations, e.g. some kind of "in preparation" citation?]. The simulations are cosmological zoom-in simulations, meaning that interesting regions at $z = 0$ were identified from an output from a low-resolution simulation, after which resolution of the interesting volumes was increased and the simulation was run again. In this case, the interesting regions were defined as surroundings of a pair of dark matter haloes resembling ones of the Milky Way and Andromeda galaxies, the two main galaxies of the Local Group.

The simulations contained only dark matter, and for my analysis only the dark matter halo information was needed, so instead of using the full simulation output I conducted my analysis on subhalo catalogues. The subhalo information was extracted as described in section 3.1.3. The resulting data set consists of subhalo catalogues from 448 zooms, each centered on one region resembling the Local Group in the low-resolution simulation. The following sections shortly introduce the code used to run the simulation and the parameters of the simulation for both stages of the zoom-in simulations.

3.2.1 Modified GADGET-3

The simulation code that was used to run the simulations on which all of the analysis in this master's thesis is based on was a modified version of GADGET-3, an earlier version of which is described in Springel (2005). The code is same as used in the EAGLE project, so detailed descriptions of the changes can be found in Schaye et al. (2015). However, the changes mostly affect the handling of baryonic matter

so understanding the basic GADGET-2 gives a good basis for understanding the simulations (Schaye et al., 2015).

GADGET uses a TreePM algorithm to compute forces, meaning that short-range forces are calculated using a tree method as described in section 3.1.1 and a particle mesh is employed for long-range forces (Springel, 2005). As the code is parallel, normal tree-construction algorithm is problematic in regards to splitting the nodes of the octree between processors (Springel, 2005). To ensure a balanced workload amongst all processors, the particles are split between processors by constructing a space-filling fractal curve known as Peano-Hilbert curve, and splitting it to segments with approximately equal number of particles on each segment (Springel, 2005). The properties of the curve ensure that particles close to each other along the curve are also near each other in the 3D space, which means that close-range forces can frequently be calculated without need to access memory belonging to other processors (Springel, 2005). In regions where an octree constructed from particles belonging to a processor should contain particles assigned to other processors, a pseudoparticle resembling in principle the pseudoparticles used when calculating forces for cells where $l/D < \theta$ is inserted instead of the full particle information (Springel, 2005).

Updating the positions of the particles is done using an integrator resembling the leapfrog integrator described in section 3.1.2, but the integrator is modified to allow using variable time-step lengths (Springel, 2005). These modifications are important, as in cosmological simulations it is not sensible to use the same time step in all parts of the simulation as there are both high-density regions and sparse void areas, first of which requiring a time-step so small that a lot of computational time is wasted while integrating the latter with more detail than is needed.

TODO: wrap up, maybe by providing the reasoning behind choosing gadget

Box size	800 Mpc/h
Number of particles	0
Particle mass	0
Softening length	0

Table 3.1: Properties of the parent simulation.

H	67.77 km/s/Mpc
Ω_m	0.307
Ω_Λ	0.693

Table 3.2: Cosmological parameters used in the simulation. TODO: planck + lensing 2013

3.2.2 Parent simulation

First step of a zoom-in simulation running process is to construct initial conditions and run a low-resolution box. A large box with 800 Mpc/h was chosen to ensure that the box is big enough to contain a reasonable sample of Local Group analogues and that the large scale structure of the universe is represented in the simulation.

TODO: simulation properties, both cosmology and resolution related, starting resolution

When the low-resolution box reached redshift $z = 0$, haloes were identified using the procedure described in section 3.1.3. From the resulting halo catalogue, halo pairs resembling the Local Group were identified. TODO: the criteria used

3.2.3 Zoom simulations

	min	mean	median	max
High resolution particles	min	mean	median	max
High resolution particle mass	min	mean	median	max
High resolution softening length	min	mean	median	max
Total particles	min	mean	median	max

Table 3.3: Properties of the zoom simulations.

4. Mathematical and statistical methods

täällä tarvittavat esitiedot ja önnönnöö, listaa mm. mitä aiot kertoa kunhan tiedät itsekkään

4.1 Statistical Background

vähän parempi Precision of the used equipment limits accuracy of all data gathered from
tässä kuin physical experiments, simulations or observations. Therefore the results are affected
aiemman otsikon by the measurement process and the results have to be presented as estimates with
alla some error, magnitude of which is affected by both number of data points and
accuracy of the measurement equipment (Bohm and Zech, 2010).

Estimating errors for measured quantities offers a way to test hypotheses and compare different experiments (Bohm and Zech, 2010). This is done using different statistical methods, of which the main methods relevant for this thesis are covered here. The methods are shortly introduced in the following sections together with basic statistical concepts that are necessary to understand the methods.

4.1.1 Hypothesis testing and p-values

A common situation in scientific research is that one has to compare a sample of data points to either a model or another sample in order to derive a conclusion from the dataset. In statistics, this is known as hypothesis testing. For example, this can mean testing hypotheses such as "these two variables are not correlated" or "this sample is from a population with a mean of 1.0" (J. V. Wall, 2003). Next paragraphs shortly introduce the basic concept of hypothesis testing and methods that can be used to test the hypothesis "these two samples are drawn from the same distribution" following the approach of (Bohm and Zech, 2010) and (J. V. Wall, 2003).

The process of hypothesis testing as described by begins with forming of a null hypothesis H_0 that is formatted such that the aim for the next steps is to either reject it or deduce that it cannot be rejected with a chosen significance level. Negation of the null hypothesis is often called research hypothesis or alternative hypothesis and denoted as H_1 . For example, this can lead to H_0 "this dataset is sampled from a normal distribution" and H_1 "this dataset is not sampled from a normal distribution". Choosing the hypothesis in this manner is done because often the research hypothesis is difficult to define otherwise.

After setting the hypothesis one must choose an appropriate test statistic. Ideally this is chosen such that the difference between cases H_0 and H_1 is as large as possible. Then one must choose the significance level α which corresponds to the probability of rejecting H_0 in the case where H_0 actually is true. This fixes the critical region i.e. the values of test statistic that lead to the rejection of the H_0 .

This kind of probability based decision making is always prone to error. It is easy to see that α corresponds to the chance of H_0 being rejected when it is true. This is known as error of the first kind. However, this is not the only kind of error possible. It might also occur that H_0 is false but it does not get rejected, which is known as error of the second kind.

kerro mikä α ja N
 käytössä
 myöhemmin
 kunhan tiedät

There is no one optimal way of choosing α , but instead one should try to find a balance between false rejections of null hypothesis and not being able to reject null hypothesis based on the dataset even if in reality it might not be true. When sample size (often denoted N) is large, smaller values of α can often be used as decisions get more accurate when N grows. For example tässä työssä α oli jokin ja N jotain muuta.

It is crucial not to look at the test results before choosing α in order to avoid intentional or unintentional fiddling with the data or changing the criterion of acceptance or rejectance to give desired results. Only after these steps should the test statistic be calculated. If the test statistic falls within the critical region, H_0 should be rejected and otherwise stated that H_0 cannot be rejected at this significance level. The critical values for different test statistics are widely found in statistical textbooks and collections of statistical tables or they can be calculated using statistical or scientific libraries available for many programming languages.

Despite statistical tests having a binary outcome " H_0 rejected" or " H_0 not rejected", a continuous output is often desired. This is what p-values are used for. The name p-value hints towards probability, but despite its name p-value is not equal to the probability that the null hypothesis is true. These p-values are functions of a test statistic and the p-value for a certain value t_{obs} of a test statistic gives the probability that under the condition that H_0 is true, the value of a test statistics for a randomly drawn sample is at least as extreme as t_{obs} . Therefore if p-value is smaller than α , H_0 is to be rejected.

4.1.2 Distribution functions

ei hyvä, harkitse
 esim
<http://puppulause-generaattori.fi/?ava-insana=jakauma-funktio>

Some statistical tests such as the Kolmogorov-Smirnov test and the Anderson-Darling test make use of distribution functions such as cumulative density function (CDF) and empirical distribution function (EDF) in determining the distribution

from which a sample is drawn.

To understand CDF and EDF, one must first be familiar with probability density function (PDF). As the name suggests, PDF is a function the value of which at some point x represents the likelihood that the value of the random variable would equal x . This is often denoted $f(x)$. Naturally for continuous functions the probability of drawing any single value from the distribution is zero, so these values should be interpreted as depicting relative likelihoods of different values. For example if $f(a) = 0.3$ and $f(b) = 0.6$ we can say that drawing value b is twice as likely as drawing value a . (Heino et al., 2012)

Another way to use the PDF is to integrate it over semi-closed interval from negative infinity to some value a to obtain the CDF, often denoted with $F(x)$:

$$F(x) = \int_{-\infty}^x f(x') dx'. \quad (4.1)$$

This gives the probability of a random value drawn from the distribution having value that is smaller than x . Relation between the PDF and the CDF is illustrated in figure 4.1, where PDFs and CDFs are shown for three different distributions. It is easy to see the integral relation between PDF and CDF and how wider distributions have wider CDFs. (Heino et al., 2012)

Both the PDF and the CDF apply to whole population or the set of all possible outcomes of a measurement. In reality the sample is almost always smaller than this. Therefore one cannot measure the actual CDF. Nevertheless, it is possible to calculate a similar measure of how big a fraction of measurements falls under a given value. This empirical counterpart of the CDF is known as empirical distribution function (EDF), often denoted $\hat{F}(x)$, and for a dataset X_1, X_2, \dots, X_n containing n samples it is defined to be

$$\hat{F}(x) = \frac{1}{n} \sum_{i=1}^n I[X_i \leq x] \quad (4.2)$$

where I is the indicator function, value of which is 1 if the condition in brackets is

PDF määritelmä
vaikea ymmärtää

esittelet nyt nolosti
EDF:n nimeltä
kahdesti, mieti
ratkaisu

lisää johonkin
selitys
normaalijakauman
parametreille

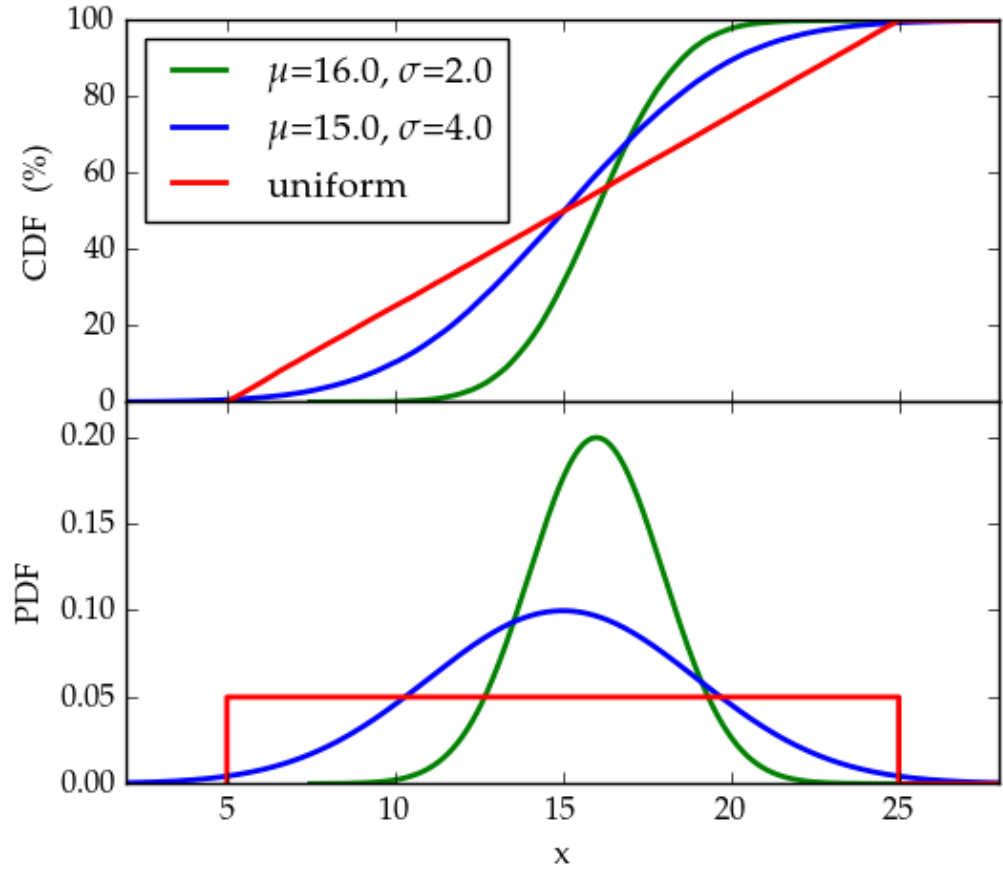


Figure 4.1: Cumulative distribution function (top panel) for three random samples (PDFs shown in the bottom panel) drawn from different distributions, two of which are normal and one is uniform. Parameters μ and σ of the normal distribution describe the mean and the spread of the distribution respectively, large values of σ resulting in wide distribution.

true, otherwise 0. (Feigelson and Babu, 2012)

harkitse laittavasi
jämpti arvo N:lle
kun muut osat
valmiita

Due to the EDF being a result of random sampling, it may deviate from the underlying CDF considerably as can be seen by comparing CDFs in figure 4.1 and corresponding EDFs in figure 4.2. This example is somewhat exaggerated with its $N=35$ as the actual dataset used in this thesis has $N>100$, but reducing the sample size makes seeing the effects of random sampling easier. The latter figure also has EDFs corresponding to two random samples drawn from the distribution of the



Figure 4.2: Empirical distribution function for four random samples ($N=35$) drawn from the same distributions as in figure 4.1. Note that both the blue and the cyan data are drawn from the same distribution.

green curve in the first figure to further illustrate the differences that can arise from random sampling. This randomness also makes determining whether two samples are drawn from the same distribution difficult.

4.2 Linear Regression

Regression analysis is a set of statistical analysis processes that are used to estimate functional relationships between a response variable (denoted with y) and one or more predictor variables (denoted with x in case of single predictor or $x_1 \dots x_i$ if there are multiple predictor variables) (Feigelson and Babu, 2012). In this section, we will cover both simple regression where there is only one response variable and multiple linear regression where there are more than one response variables. The models also contain ε term that represents the scatter of measured points around

the fit. One of the models used is linear regression model, which can be used to fit any relationship where the response variable is a linear function of the model parameters (Montgomery, 2012). In addition to the widely known and used models where the relationship is a straight line, such as

$$y = \beta_0 x + \varepsilon \quad (4.3)$$

all models where relationship is linear in unknown parameters β_i are linear (Montgomery, 2012). Thus for example the following are linear models

$$y = \beta_0 x^2 + \varepsilon \quad (4.4)$$

$$y = \beta_0 e^x + \beta_1 \tan x + \varepsilon \quad (4.5)$$

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \varepsilon \quad (4.6)$$

On the other hand, all models where the relationship is not linear and therefore

$$y = x_0^\beta + \varepsilon \quad (4.7)$$

$$y = \beta_0 x + \cos(\beta_1 x) + \varepsilon \quad (4.8)$$

are nonlinear.

4.2.1 Simple linear regression

onko otsikko Simple linear regression is a model with a single predictor variable and a single
järkevä kun response variable with a straight line relationship, i.e.

$$y = \beta_0 + \beta_1 x + \varepsilon \quad (4.9)$$

where parameter β_0 represents the y axis intercept of the line and β_1 is the slope of the line (Montgomery, 2012). The parameters can be estimated using method of least squares, where such values are found for the parameters that the sum of squared differences between the data points and the fitted line is minimized (Montgomery, 2012).

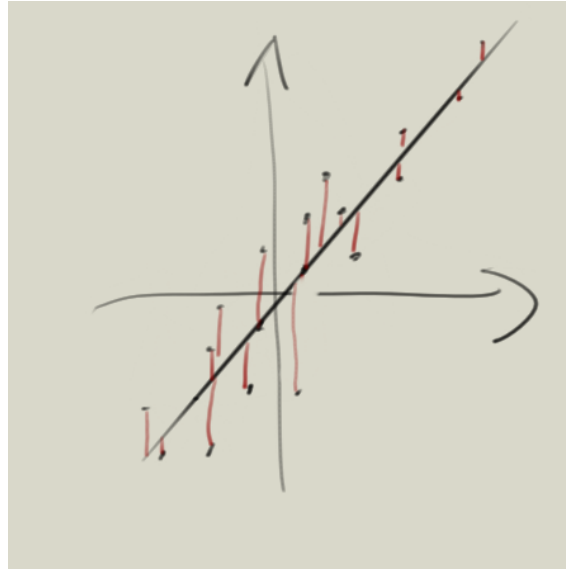


Figure 4.3

toisiko jotain lisää The best-known method of minimizing the sum of squared error is the ordinary
 jos olisi β_1 ja β_2 least-squares (OLS) estimator. The OLS method uses distances measured vertically
 lausekkeet? as shown in figure 4.3 and thus the minimized sum is

$$\sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2 \quad (4.10)$$

where x_1 and y_i are single values of the measured quantities (Feigelson and Babu, 2012). This approach requires that the values of the predictor variable are known exactly without error and all uncertainty is in the values of the response variable (Feigelson and Babu, 2012). In those situations where this assumption is not valid, results acquired using OLS may be counterintuitive. This can be seen for example in figure 4.4 where OLS is used to calculate two linear fits: one where x is used and predictor variable and y as response variable and another where y is the predictor and x the response.

HF: OLS/TLS? When dividing the variables to the independent variable with no error and a
 Sido PCA:han response variable with possible measurement error is not a justifiable choice OLS
 should not be used. One alternative for OLS is total least squares (TLS, also known as orthogonal least squares in some sources such as (Feigelson and Babu, 2012))

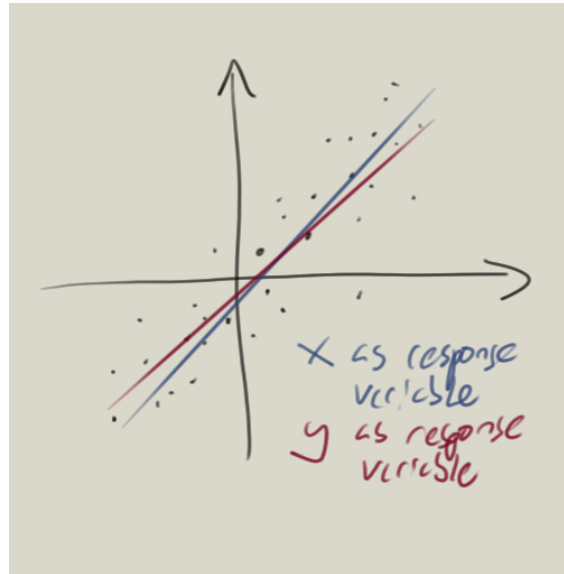


Figure 4.4

regression can be used instead of OLS (Markovsky and Huffel, 2007). The major difference between OLS and TLS is that instead of vertical distance, the minimized squared distance is measured between a point and its projection to the fitted line, thus providing minimum of the sum of the squared orthogonal distances from the line (Feigelson and Babu, 2012).

4.2.2 Multiple linear regression

gradun sovellus: ongelman kuvailu, esim OLS:lle yleistys, jälleen liittyy PCA
 onko PCR
 relevantti?

4.3 Principal Component Analysis

orthogonal vs uncorrelated: Principal component analysis (PCA) is a statistical procedure first introduced by Pearson (1901) to aid physical, statistical and biological investigations where fitting a line or a plane to n -dimensional dataset is desired. When performing PCA, one transforms a data set to new set of uncorrelated variables i.e. ones represented by orthogonal basis vectors. These variables are called principal components (PCs)



Figure 4.5

(Jolliffe, 2002). This approach also solves the problem of sometimes arbitrary choice of division of the data to dependent and independent variables introduced in section 4.2.something Pearson (1901).

PCA can be used to both reduce and interpret data (Johnson, 2007). Often PCA alone does not produce the desired result, but instead PCs are used as a starting point for other analysis methods such as factor analysis or multiple regression (Johnson, 2007). These applications are introduced in the following subsections together with a short description of performing PCA and interpreting its results. In addition to these applications, PCA is also used in image compression, face recognition and other fields (Smith, 2002).

4.3.1 Extracting Principal Components

In order to understand the process of obtaining principal components of a data set let us follow the procedure on a two-dimensional data set shown in the top panel of figure 4.6 with black dots. First step of finding the PCs is to locate the centroid of the dataset i.e. the mean of the data along every axis (Smith, 2002). This is marked

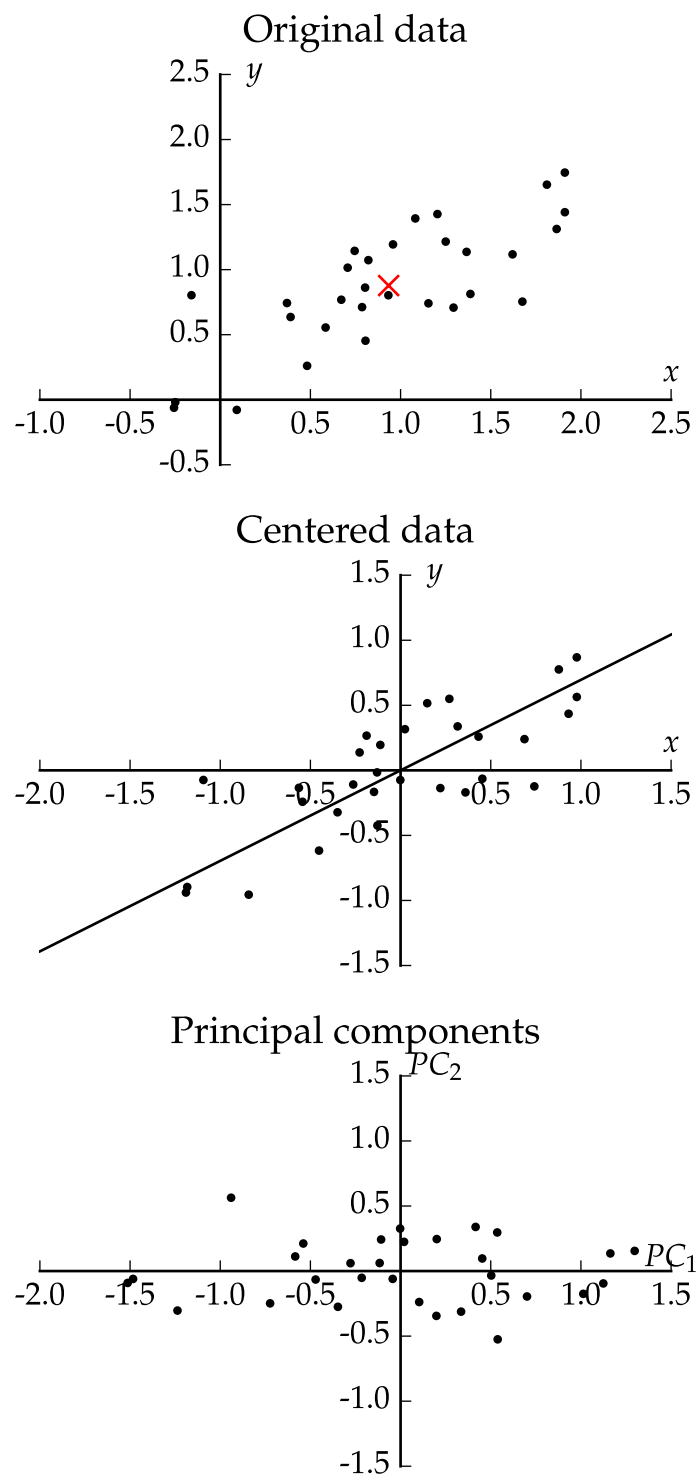


Figure 4.6: .

with a red x in the top panel of figure 4.6.

jos päädyt The best-fit line and therefore the PCs always pass through the centroid of the
puhumaan system (Pearson, 1901), so subtracting the location of the centroid from the data
eigenvektoreista tai is a natural next step, as this ensures that in the next step only the slope has to
kovarianssimatrii- be optimized. This is done in the middle panel of the figure 4.6. If the variables
seista, selitä ne have different units, each variable should be scaled to have equal standard devia-
täällä tions (James et al., 2013) unless the linear algebra based approach with correlation
matrices, as explained in e.g. (Jolliffe, 2002), is used.

If this scaling is not performed, the choice of units can arbitrarily skew the principal components. This is easy to see when considering for example a case where one has distances to galaxies in megaparsecs and their masses in units of $10^{12} M_{\odot}$, both of which might result in standard deviations being of the order of unity and PCA might thus yield principal components that are not dominated by neither variable alone. Now, say another astronomer has a similar data set, but distances are given in meters. In this case, most of the variation is in the distances, so distances will also dominate the PCs. If all variables are measured in the same units, scaling can be omitted in some cases (James et al., 2013).

Now the first PC can be located by finding the line that passes through the origin and has the maximum variance of the projected data points (Jolliffe, 2002), shown with a black line in the middle panel of figure 4.6 for our data set. PCs are always orthogonal and intersect at the origin, so in the two-dimensional example case the second and final PC is fully determined. The data set can now be represented using the PCs as is shown in the bottom panel of the figure 4.6.

Had the data set had more than two dimensions, the second PC would have been chosen such that it and the first PC are orthogonal and that variance along the new PC is again maximised (Jolliffe, 2002). This can be repeated for each dimension of the data set or, if dimensionality reduction is desired, only for a smaller number

of dimensions.

mieti mitä This level of understanding is often enough to successfully apply PCA to a
monospeissillä ja problem, because PCA has ready-made implementations for many programming lan-
ole konsistentti guages such as `prcomp` in R (James et al., 2013) and `sklearn.decomposition.PCA`
in scikit-learn library (Pedregosa et al., 2011) for Python. If a more mathematical
approach is desired, Smith (2002) explains PCA together with covariance matrices,
eigenvectors and eigenvalues required to understand the process very clearly. Jolliffe
(2002) also includes a very thorough description of PCA.

4.3.2 Excluding Less Interesting Principal Components

maininta Even though a data set has as many principal components as there are mea-
bootstrappingista sured variables, one is often not interested in all of them as the last principal com-
(loppuun?) ja siitä, ponents might explain only a tiny fraction of the total variation in the data (James
että maistuu et al., 2013). Reducing the dimensionality of the problem also greatly eases visual-
koneoppiminen? izing and interpreting the data. Thus one might want to retain only first few of the
PCs when PCA is used to for example compress, visualize or just interpret the data
set at hand (James et al., 2013; Johnson, 2007). Unfortunately, many of the rules
and methods used to determine the number of PCs to retain are largely without a
formal basis or require assuming a certain distribution which is often not justifiable
with the data (Jolliffe, 2002). With careful consideration these methods can never-
theless aid a researcher in making informed decisions and reasoned conclusions, so
some rules are introduced in this section.

If the PCA is performed to aid visualizing the data set, retaining only the two
first PCs can be a justified choice as two is the maximum number of dimensions
that are easy to visualize on two-dimensional media such as paper and the two first
PCs determine the best-fit plane for the data (Jolliffe, 2002). Of course the question
whether the two PCs are sufficient to describe the data reasonably well still remains

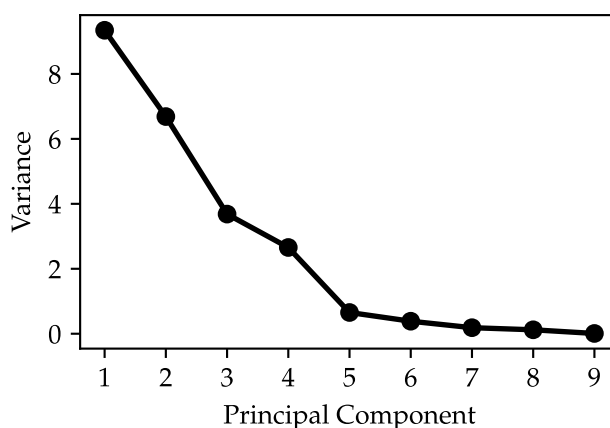


Figure 4.7: Example of a scree plot of randomly generated normally distributed data. In this case the plot has a clear elbow at fifth PC with the PCs 5-9 appearing roughly on a line. Thus the last five PCs could be a good number of PCs to be omitted if dimensionality reduction is desired.

unanswered in this case. Fortunately it can be addressed using some of the following methods used in general case of determining how many PCs to retain.

One widely used technique was introduced by Cattell (1966) to be used in factor analysis, but is also very much applicable to PCA (Jolliffe, 2002). This so called Cattell scree test involves plotting the variance of the data points along each PC versus the index of the PC. These plots tend to look similar to what is shown in figure 4.7, resembling a steep cliff with eroded material accumulated at the base, which is why these plots are known as scree plots and the nearly linear section of the plot is called the scree.

When the scree plot has two clearly different areas, the steep slope corresponding to the first PCs and a more gently sloping scree for the latter PCs, locating this elbow in the plot connecting the two areas will give the number of PCs that should be included (Jolliffe, 2002), which in case of figure 4.7 would yield five PCs. Some sources such as (Cattell, 1966) suggest that in some cases the PC corresponding to

the elbow should be discarded, which will result in one less PC.

Unfortunately, as Cattell also acknowledges in his paper, all cases are not as easy to analyze as the one in figure 4.7 and may prove difficult to discern for an inexperienced researcher. This problem might arise from for example noise in the linear part of the plot or scree line consisting of two separate linear segments with different slopes. The first case has no easy solution, but in the latter case Cattell suggests using the smaller number of PCs.

joku kiva lopetus
tämän jälkeen?

Another straightforward method for choosing how many PCs to retain is to examine how much of the total variation in data is explained by first PCs and including components only up to a point where pre-defined percentage of the total variance is explained (Jolliffe, 2002). Whereas the previous method posed a challenge in determining which PC best matches the exclusion criteria, when using this approach the problem arises from choosing the threshold for including PCs. Jolliffe (2002) suggests that a value between 70 % and 90 % of the total variation is often a reasonable choice, but admits that the properties of the data set may justify values outside this range. Unfortunately, the suggested range is quite wide, so it may contain multiple PCs and therefore it is up to the researcher to determine the best number of PCs, while the criterion again acts as only an aid in the process.

4.3.3 Principal Component Regression

4.4 Error analysis

TODO: oispa
parempi otsikko.
mieti, onko tämä
muutenkaan hyvä
nyt kun on siirretty
yksi otsikkotasoa
ylöspäin

4.5 Comparing two samples drawn from unknown distributions

A common question in multiple fields of science is whether two or more samples are drawn from the same distribution. The most relevant methods that can be used to address this problem are introduced here following (Bohm and Zech, 2010) and (Feigelson and Babu, 2012) apart from introducing the χ^2 test which is mostly based on the approach of (Corder, 2014).

Questions related to comparing samples can emerge for example when comparing effectiveness of two procedures, determining if the instrument has changed over time or whether observed data is compatible with simulations. There are multiple two-sample tests that can address this kind of questions, e.g. χ^2 , Kolmogorov-Smirnov, Cramér-von Mises and Anderson-Darling tests.

In addition to comparing two samples, these tests can be used as one-sample tests to determine whether it is expected that the sample is from a particular distribution. However, some restrictions apply when using the one-sample variants. Some of these tests use categorical data, i.e. data where variables fall in pre-defined categories, and compares numbers of samples in different categories, whereas the others are applied to numerical data and compare empirical distribution functions (EDF) of the datasets.. Examples of such categories might be for example "galaxies that are active" or "data points between values 1.5 and 1.6".

4.5.1 χ^2 test

keksi paremmat

esimerkit koko

kappaleeseen,

jotain relevanttia

myöhempää

tutkimusta

ajatellen. katso

kommentit

paperista sen

jälkeen, kaikkia ei

täällä vielä

Astronomical data often involves classifying objects into categories such as "stars with exoplanets" and "stars without exoplanets" or the spectral classes of stars (Feigelson and Babu, 2012). One tool for analyzing such categorical data is χ^2 test, which can be used both to determine whether a sample can be drawn from a certain distribution and to test whether two samples can originate from a single distribution.

The method described here is sometimes referred to as Pearson's χ^2 test due

Stellar class	Number of observed planetary systems
A	6
F	38
G	39
K	134

Table 4.1: Example of categorical data.

to existence of other tests where χ^2 distribution is used. In some cases, such as with small 2×2 contingency tables and when expected cell counts are small, other variants of χ^2 test should be used. For example the Yates's χ^2 test or the Fisher exact test work better in these cases than the χ^2 test.

For one-sample test, the χ^2 test uses the number of measurements in each bin together with a theoretical estimate calculated from the null hypothesis. For example one might have observed exoplanets and tabulated the number of planet-hosting stars of different spectral class as is shown in table 4.1 and now wants to test the observations against null hypothesis "Distribution of stellar classes for observed exoplanet-hosting stars is equal to that of main sequence stars in solar neighbourhood as given by Ledrew (2001)" using significance level $\alpha = 0.01$. The data is categorical, so now χ^2 test is a justified choice.

In this case the first step would be to calculate the expected observation counts for each bin according to the null hypothesis. Table 4.2 contains these expected counts (f_e) together with the observations (f_o). These observed and expected values are then used to calculate the χ^2 test statistic, defined as

$$\chi^2 = \sum_i \frac{(f_o - f_e)^2}{f_e}. \quad (4.11)$$

With the data given above this results in $\chi^2 \approx 23.6$. The data has four bins, so the degree of freedom is $4 - 1 = 3$. Next one can compare the calculated χ^2 value

Stellar class	Observations (f_o)	Theory (f_e)
A	6	6
F	38	28
G	39	71
K	134	112
total	217	217

Table 4.2: Data of table 4.1 together with expected values if null hypothesis was true.

to a tabulated critical value for our significance level $\alpha = 0.01$. These tabulated values can be widely found in statistics textbooks and books specifically dedicated to statistical tables.

In this case according to Corder (2014) the critical value is 11.34, which means that as $23.6 > 11.34$ one can reject the null hypothesis and conclude that at 1% significance level the distribution of stellar classes for observed exoplanet-hosting stars is not equal to that of main sequence stars in solar neighbourhood. This of course can either be due to exoplanets being more numerous around some stellar classes than others or arise from some observational effect such as the observer observing more of the later type stars and thus arbitrarily skewing the distribution of the exoplanet finds.

The χ^2 test can also be used to test for independence of two or more samples. The data is again tabulated and now the χ^2 test statistic is calculated as

$$\chi^2 = \sum_i \sum_j \frac{(f_{oij} - f_{eij})^2}{f_{eij}} \quad (4.12)$$

where f_{oij} denotes the observed frequency in cell (i, j) and f_{eij} is the expected frequency for that cell. The expected frequency can be calculated using the following

formula

$$f_{eij} = \frac{R_i C_j}{N} \quad (4.13)$$

where R_i is the number of samples in row i , C_j is the number of samples in column j and N is the total sample size.

According to Corder (2014), the degrees of freedom is $(R-1)(C-1)$ where R is the number of rows and C is the number of columns in tabulated data. This is true in many if not most cases, but the way of collecting data can affect the degrees of freedom in both one-sample and multi-sample cases, as Press et al. (2007) explains. For example, if the one-sample model is not renormalized to fit the total number of observed events or, in two-sample case, the sample sizes differ, the degrees of freedom equal to number of bins N_b instead of $N_b - 1$.

Before performing the χ^2 test on a dataset, it is important to confirm that the data meets the assumptions for χ^2 test, given for example in (Bock et al., 2014) and (Heino et al., 2012). First of all, the data has to consist of counts i.e. not for example percentages or fractions. These counts should be independent of each other and there has to be enough of them, generally > 50 is sufficient. Bins should also be chosen such that all bins have at least five counts according to the null hypothesis. If the last condition is not met, one can consider combining bins.

4.5.2 Kolmogorov-Smirnov test

For astronomers one of the most well-known statistical test is the Kolmogorov-Smirnov test, also known as the KS test. It is computationally inexpensive to calculate, easy to understand and does not require binning of data. It is also a nonparametric test i.e. the data does not have to be drawn from a particular distribution.

In the astrophysical context this is often important because astrophysical models usually do not fix a specific statistical distribution for observables and it is com-

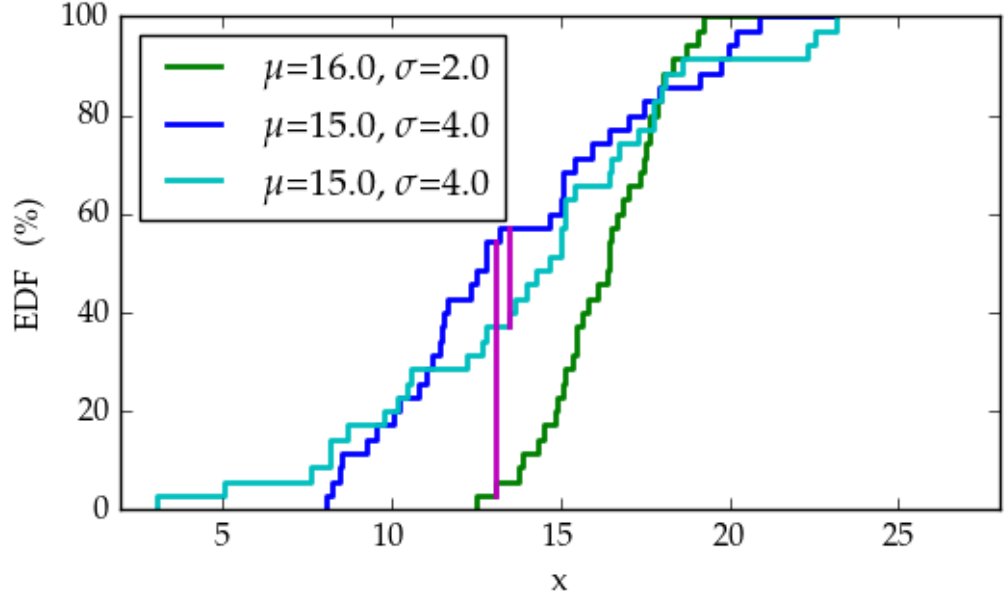


Figure 4.8: KS test parameter values (magenta vertical lines) shown graphically for three samples from figure 4.2.

mon to carry out calculations with logarithms of observables, after which the originally possibly normally distributed residuals will no longer follow a normal distribution. When using the KS test, the values on the x-axis can be freely reparametrized: for example using $2x$ or $\log x$ on x-axis will result in same value of the test statistic as using just x (Press et al., 2007).

The test can be used as either one-sample or two-sample test, both of which are very similar. For two-sample variate the test statistic for the KS test is calculated based on empirical distribution functions \hat{F}_1 and \hat{F}_2 derived from two samples and the test statistic

$$D = \sup_x |\hat{F}_1(x) - \hat{F}_2(x)| \quad (4.14)$$

uses the maximum vertical distance of the EDFs. This test statistic is then used to determine the p-value and thus decide whether the null hypothesis can be rejected. For one-sample variate the procedure is similar, but EDF \hat{F}_2 is substituted with the CDF that corresponds to the null hypothesis.

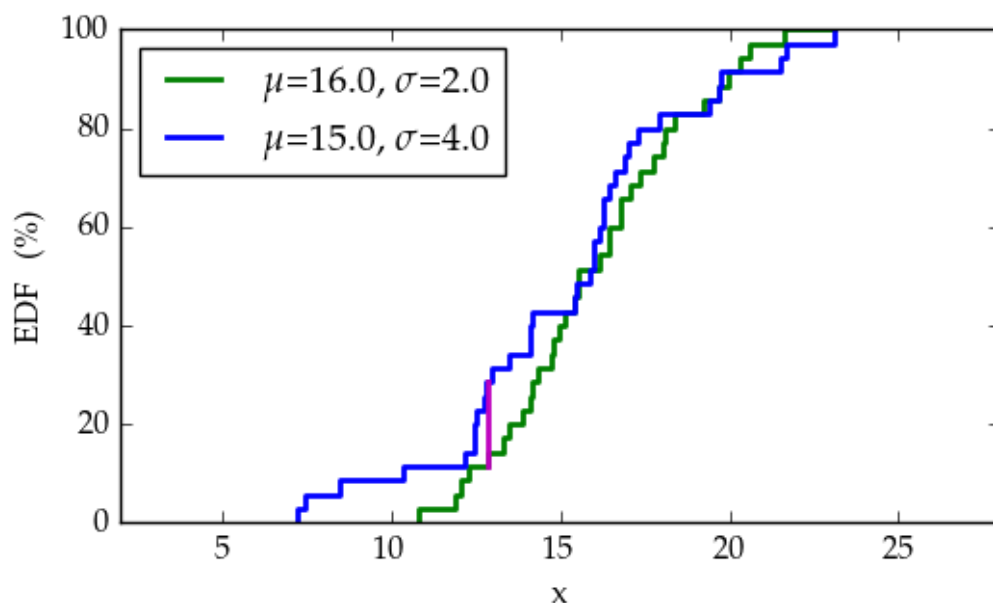


Figure 4.9: KS test ran on another pair of samples drawn from blue and green distributions in figure 4.1.

As an example, let us consider two pairs of samples from figure 4.2: green and blue (two samples drawn from different normal distributions) and blue and cyan (two samples drawn from same normal distribution). We can formulate the test and null hypotheses for both pairs as H_0 ="the two samples are drawn from the same distribution" and H_1 ="the two samples are not drawn from the same distribution" and choose a significance level of for example $\alpha = 0.05$ or $\alpha = 0.01$.

mistä p-value
saadaan, kerro taas
aiemmin (tai
täällä)

The test statistic is then calculated and for these samples we get $D = 0.51$ for the green-blue pair and $D = 0.20$ for the blue-cyan pair. Test statistics are illustrated in figure 4.8 where the test statistics D are shown as vertical magenta lines. According to Python function `scipy.stats.ks_2samp`, these values of D correspond to p-values 9.9×10^{-5} and 0.44 respectively, which means that the null hypothesis "green and blue samples are drawn from the same distribution" is rejected at both 0.05 and 0.01 significance levels but the null hypothesis "blue and cyan samples are drawn from the same distribution" cannot be rejected.

In this case the KS test produced result that matches the actual distributions from which the samples were drawn. Using a different random realization might have resulted in a different conclusion, for example one shown in figure 4.9 results in $D = 0.17$ that corresponds to a p-value of 0.64 i.e. null hypothesis could not have been rejected using the α specified earlier. In a similar manner there can be cases where two samples from one distribution are erroneously determined not to come from the same distribution if the samples differ from each other enough due to random effects.

The latter example case also illustrates one major shortcoming of the KS test: it is not very sensitive to small-scale differences near the tails of the distribution. For example in figure 4.9 the blue sample goes much further left, but because EDF is always zero at the lowest allowed value and one at the highest one the vertical distances near the tails are small and the test is most sensitive to differences near the median value of the distribution. On the other hand, the test performs quite well when the samples differ globally or have different means. (Feigelson and Babu, 2012)

The KS test is also subject to some limitations and it is important to be aware of them in order to avoid misusing it. First of all, the KS test is not distribution free if the model parameters, e.g. mean and standard deviation for normal distribution, are estimated from the dataset that is tested. Thus the tabulated critical values can be used only if model parameters are determined from some other source such as a simulation, theoretical model or another dataset.

Another severe limitation of KS test is that it is only applicable to one-dimensional data. If the dataset has two or more dimensions, there is no unique way of ordering the points to plot EDF and therefore if KS test is used, it is no longer distribution free. Some variants that can handle two or more dimensions have been invented, such as ones by Peacock (1983) and Fasano and Franceschini

"explain better"

(1987), but the authors do not provide formal proof of validity of these tests. Despite this, the authors claim that Monte Carlo simulations suggest that the methods work adequately well for most applications.

4.5.3 Other tests based on EDFs

ehkä vähän lyhyenpuoleisia kappaleita Unsatisfactory sensitivity of the KS test motivates the use of other more complex tests. Such tests are for example the Cramér-von Mises test (CvM) and Anderson-Darling (AD) test, both of which have their strengths. Similar to KS test, both of these can be used as one-sample or two-sample variants.

First of these tests integrates over the squared difference between the EDF of the sample and CDF from the model or two EDFs in case of two-sample test. The test statistic W^2 for one-sample case can be expressed formally as

$$W^2 = \int_{-\infty}^{\infty} [\hat{F}_1(x) - F_0(x)]^2 dF_0(x) \quad (4.15)$$

For two-sample version, the theoretical CDF F_0 has to be replaced with another empirical distribution function \hat{F}_2 .

Due to integration, the CvM test is able to differentiate distributions based on both local and global differences, which causes it to often perform better than the KS test. Similar to the KS test, the CvM test also suffers from EDFs or an EDF and a CDF being equal at the ends of the data range, which again makes the test less sensitive to differences near the tails of the distribution.

In order to achieve constant sensitivity over the entire range of values, the statistic has to be weighted according to the proximity of the ends of the distribution. The AD test does this with its test statistic defined as

$$A^2 = N \int_{-\infty}^{\infty} \frac{[\hat{F}_1(x) - F_0(x)]^2}{F_0(x)[1 - F_0(x)]} dF_0(x) \quad (4.16)$$

where N is the number of data points in sample. This weighing makes the test more powerful than the KS and CvM tests in many cases. (Bohm and Zech, 2010;

Feigelson and Babu, 2012)

hnnngh Also other more specific tests exist, such as the Kuiper test which is well suited for cyclic measurements. The test should always be chosen to match the dataset such that it best differentiates between the null and research hypotheses.

4.6 Cluster Analysis

DBSCAN

5. Findings from DMO Halo Catalogue Analysis

5.1 Selection of Local Group analogues

criteria, how many found, what are like (some plots maybe? distributions of masses, separations, velocity components, number of subhaloes within some radius or correlations between two of those?). Some of this might be part of previous chapter too (relevant to resimulation)?

TODO: selitykset
sille, miten osa on
keskittynyt
tiettyihin arvoihin
sallitulla välillä ja
osa jakautunut
tasaisemmin.

Figure 5.1 shows how different features of the found LG analogues are distributed. TODO: selitykset
sille, miten osa on keskittynyt tiettyihin arvoihin sallitulla välillä ja osa jakautunut tasaisemmin.

5.2 Hubble Flow Measurements

Mieti, pitäisikö
kolme viimeistä
esittää esim
scatterplottina
combined mass vs
mass in more
massive

HF, local H_0 , H_0 within shells, zero-point, are previous consistent with what went into the simulation

Figure 5.2: two different simulations, MW-centered, huom obs nb how different they are: scatter, number of haloes, changes in scatter (bound structures)

Figure 5.3 shows haloes included and excluded in fitting, how is the process done

Figure 5.4 shows H_0 at different radii. First bump is clear, latter ones not,

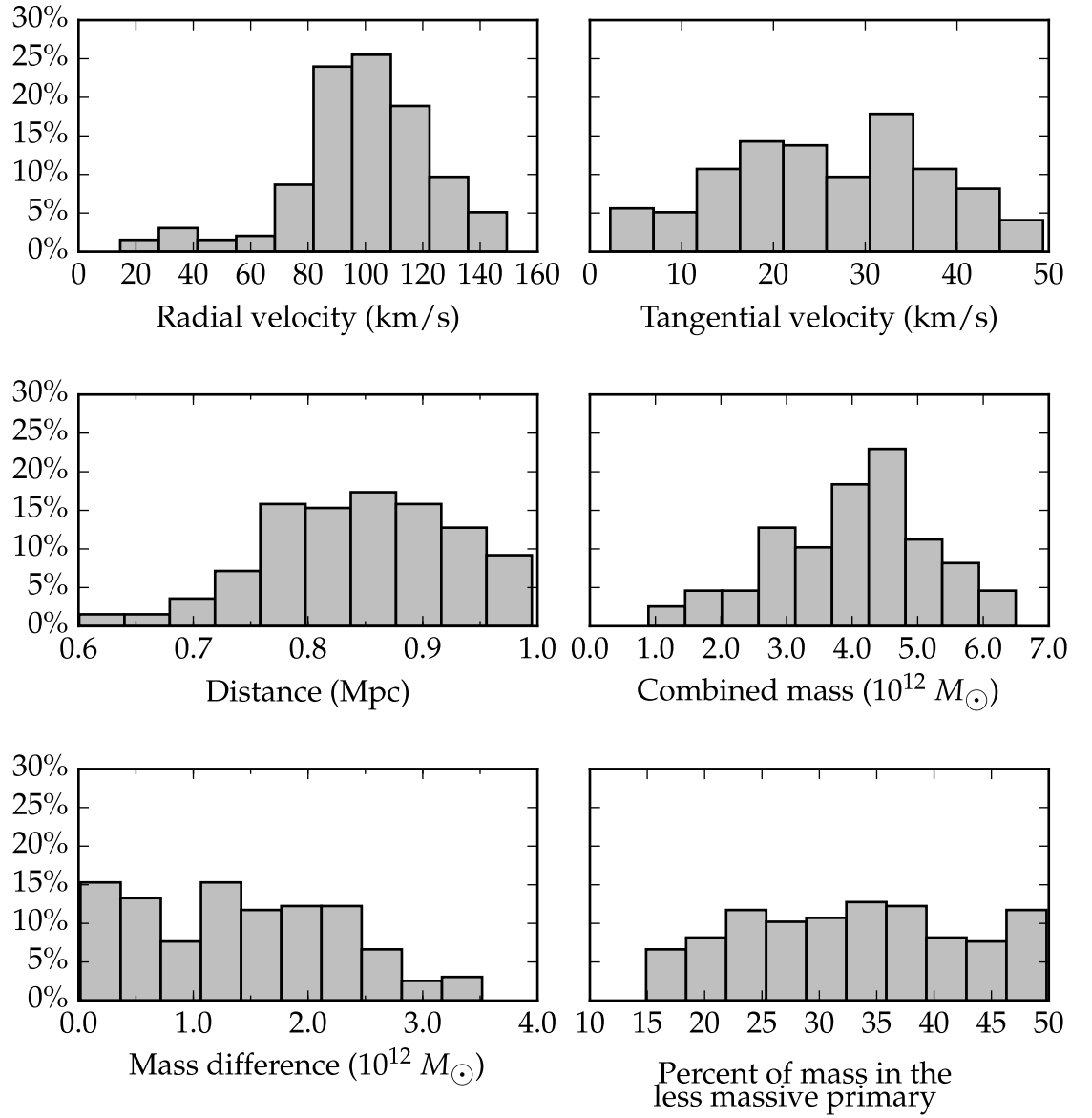


Figure 5.1: Distributions of LG analogue properties. TODO: selitä, mieti miten y-akselin label, binien rajat pitäisi pakottaa suurimpaan ja pienimpään sallittuun arvoon



Figure 5.2: Hubble Flows around Milky Way in two simulations.



Figure 5.3: HF slope: 86.9929348817



Figure 5.4: Mean H_0 in different 2 Mpc bins, grey curves show standard error.

$H_0 > 67.7$ km/s, why. First ones have 350 samples, last ones only seven, remember to explain standard error. Figure 5.5 has bigger bins and shows zero points. Think whether both should use same plot type and which is better (line vs boxplot). If boxplot stays, change colours to all-black? At least explain what is what in plot.

X

5.3 Anisotropy of Hubble flow

isotropy + randomness or anisotropy? esittele konsepti. plots: see notebook last pages

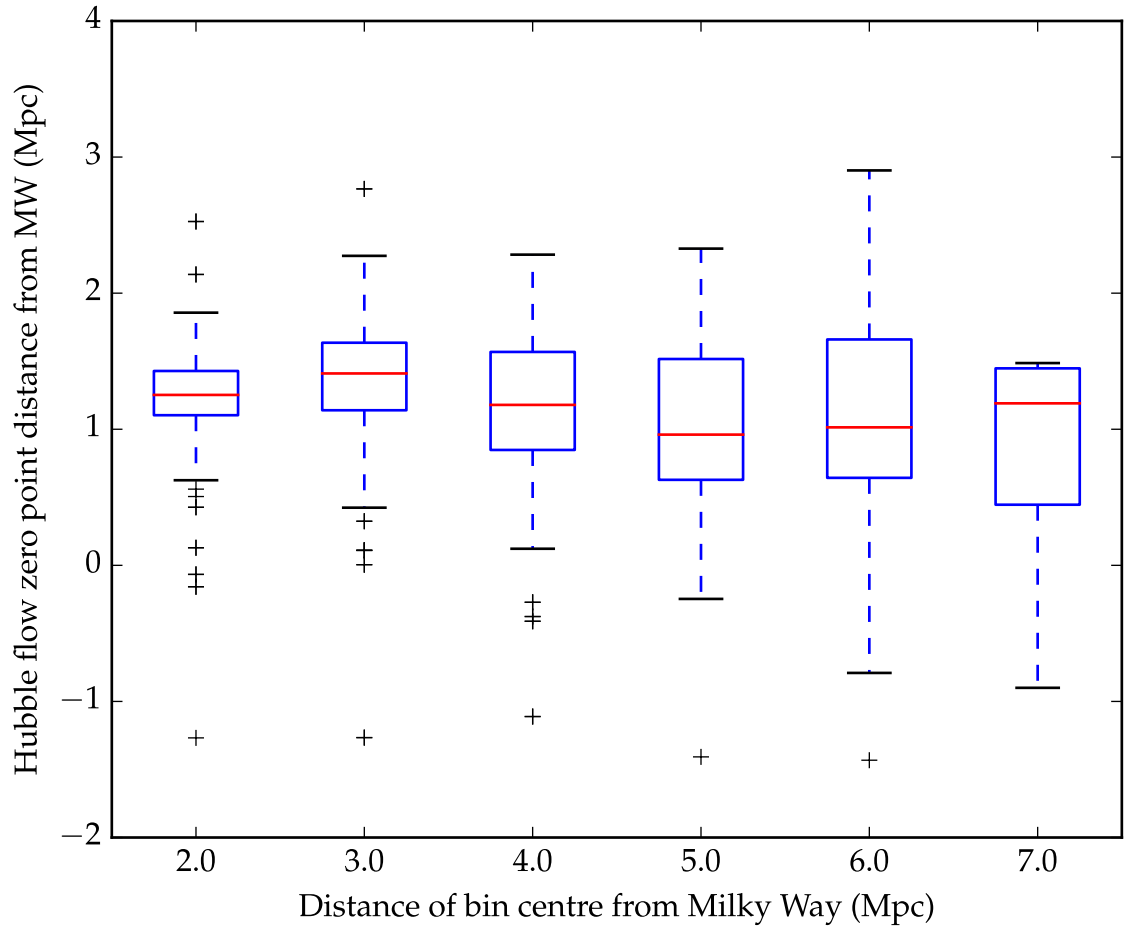


Figure 5.5: HF zero point in different 4 Mpc bins. specify one outlier outside the plot

Simulaatio 97,
esittele jo tässä
näkyvät klöntit
joissa paljon samaa
väriä, näytä myös
klusterointi ja
vertaa löytöjä
siihen

Figure 5.6 shows distribution of haloes around Milky Way analogue from one simulation with haloes closer than 1.5 Mpc away from center excluded to avoid cluttering the view with Andromeda counterpart and its satellites.

5.3.1 Clustering

Used DBSCAN introduced in [earlier chapter], angular distances of projections on sky as seen from MW.

Figure 5.8 shows the effect of varying minsamples and ϵ on number of clusters found in each simulation ($1.5 \text{ Mpc} < r < 5.0 \text{ Mpc}$ again). Regions where there are

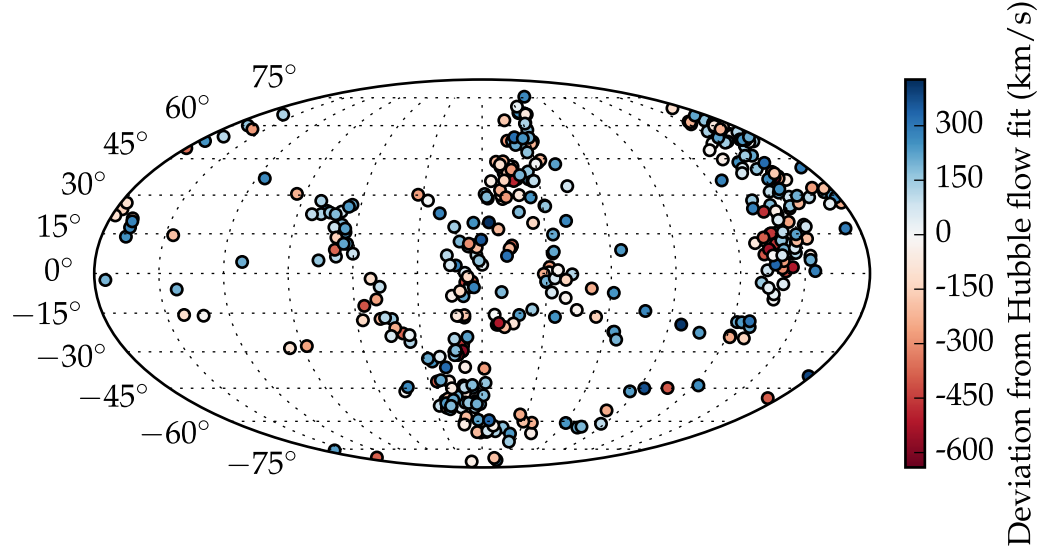


Figure 5.6: Projections of haloes around the less massive LG primary with distances ranging from 1.5 Mpc to 5.0 Mpc.

ridiculously many clusters and ones where there are one or zero, relevant region in between, some areas have similar number of clusters but do the clusters look the same, see plots that don't exist yet

TODO: mieti Figure 5.9 shows the change in mean diameter (supremum of angular distance
laitatko samaan between haloes) in cluster when ε and minsamples are varied. White areas where
figureen, vertaile no clusters are found in any simulation.
kuitenkin, selitä
Ehkä vähän Figures 5.10 and 5.11 show how the clustering results vary when clustering
vasemmanpuolim- parameters are varied.
vähemmän tilaa
mainen
plottien välissä
Massaliskat
vaakasunnassa? Figure 5.12 shows how derived values of slope and zero-point for the Hubble
Kaksi eri flow change when the Hubble flow fitting is carried out on partial data chosen based
Keltaiset vähän on the cluster membership of the haloes.
kynnystä? Liian
turhan samanlaisia.
kapea ja
epätasapainoinen,
laita päällekkäin?

5.4 Statistical Estimate of the Local Group Mass

Analysis similar to Fattahi et al 2016 paper

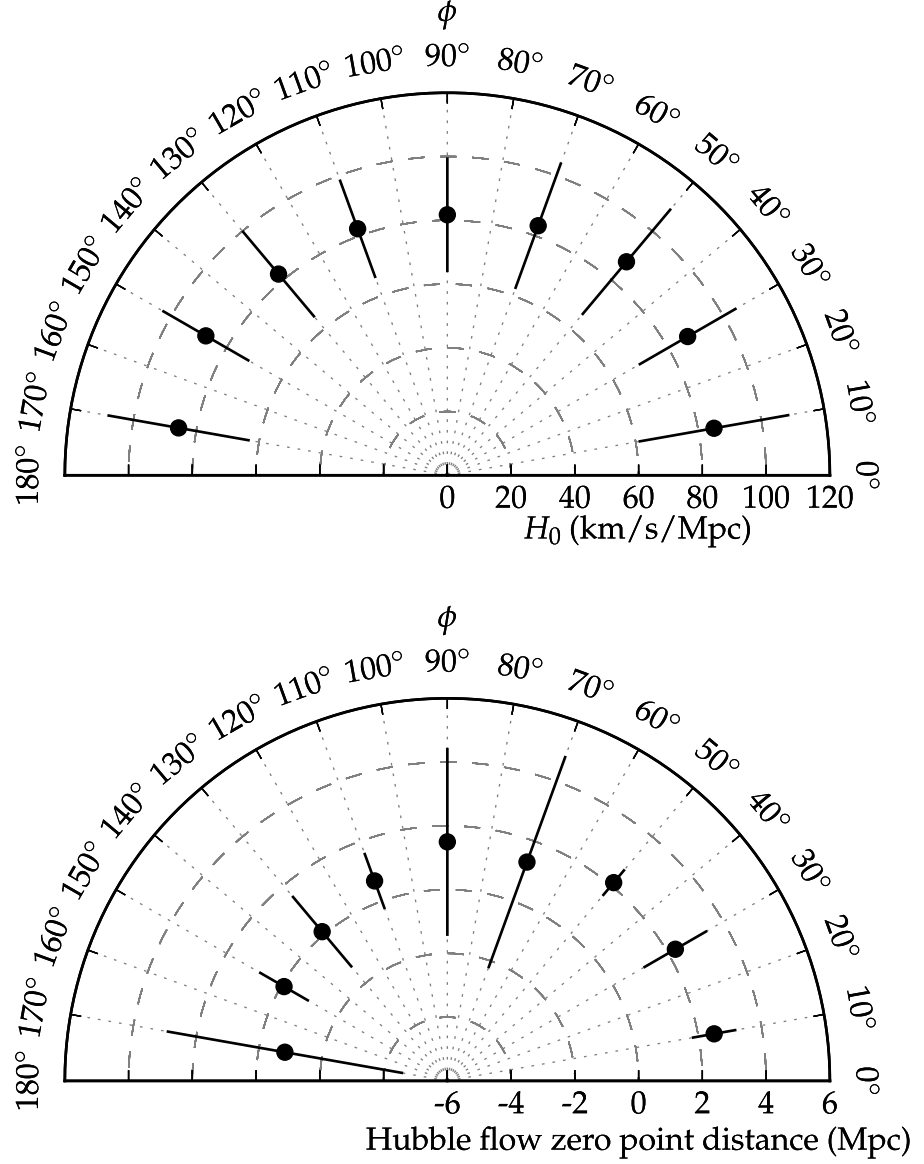


Figure 5.7: Mean Hubble flow slope and zero point as seen from Milky Way analogue in different 20° bins as measured from line connecting Milky Way and Andromeda analogues, direction 0° being towards Andromeda.



Figure 5.8: Mean number of clusters found for all simulations in dataset with different DBSCAN parameters. In all simulations ε is scaled using the mean distance between closest neighbours.



Figure 5.9: Mean diameter of clusters found for all simulations in dataset with different DBSCAN parameters. In all simulations ε is scaled using the mean distance between closest neighbours.

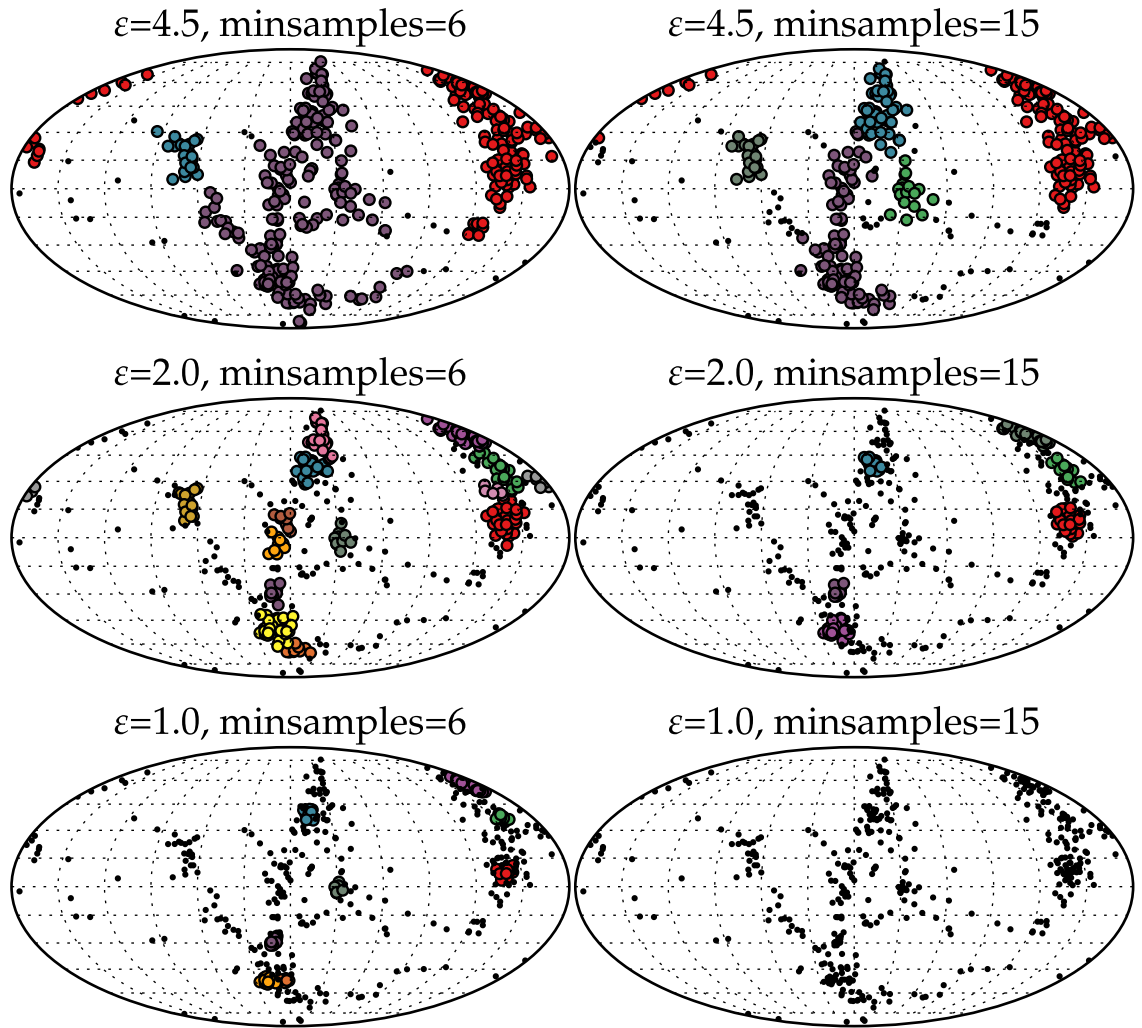


Figure 5.10: Results of DBSCAN clustering on same simulation output with different clustering parameters. TODO: mieti, kuuluuko tämäntyyppinen DBSCANin yleisiä ominaisuuksia esittelevä kuva enemmänkin teoriaosaan. Toisaalta selvästi dataspesifejä juttuja.

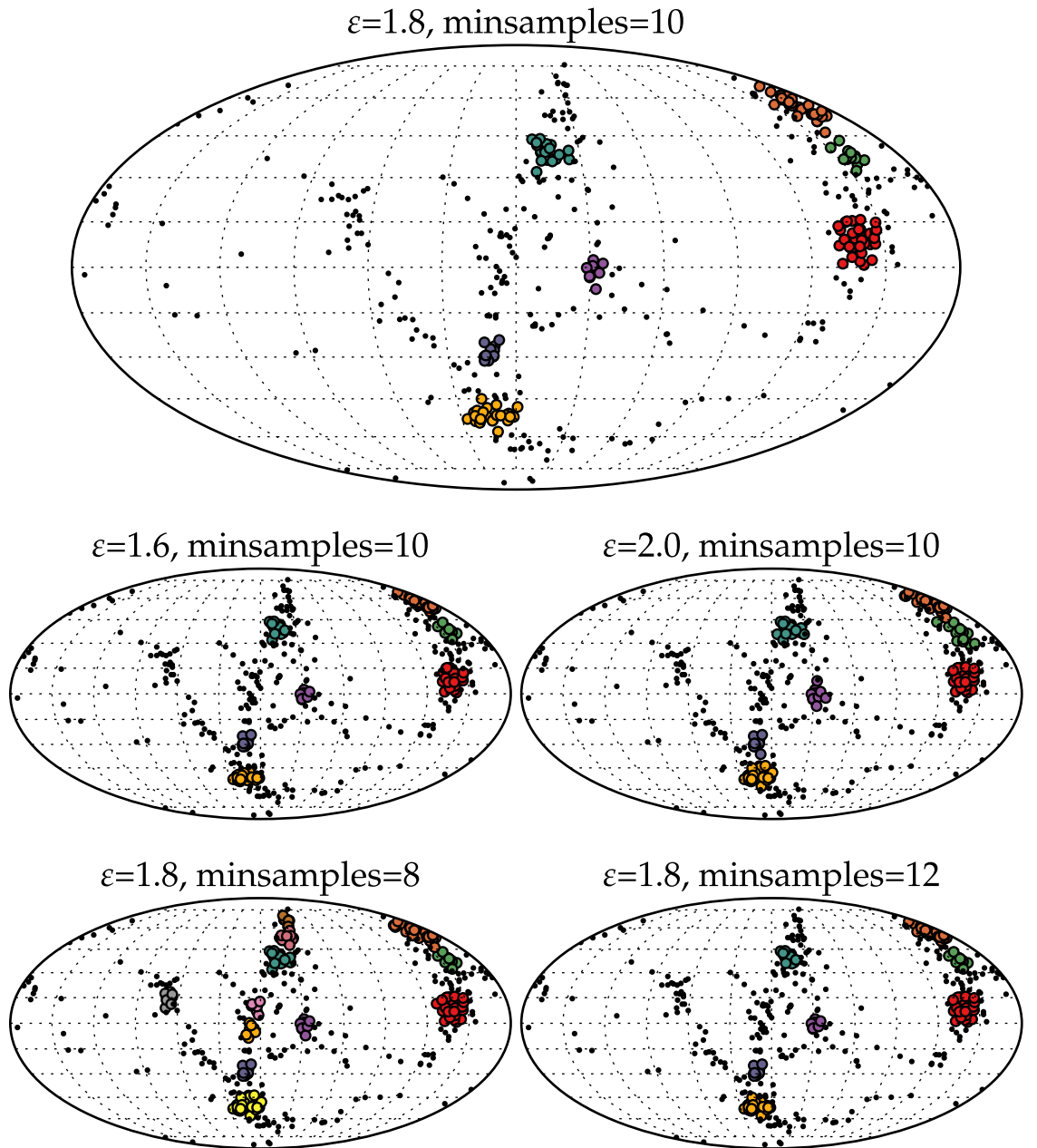


Figure 5.11: The effect of slightly varying the clustering parameters around the values $\varepsilon=1.8$ and $\text{minsamples}=10$ used when analyzing clustered data.

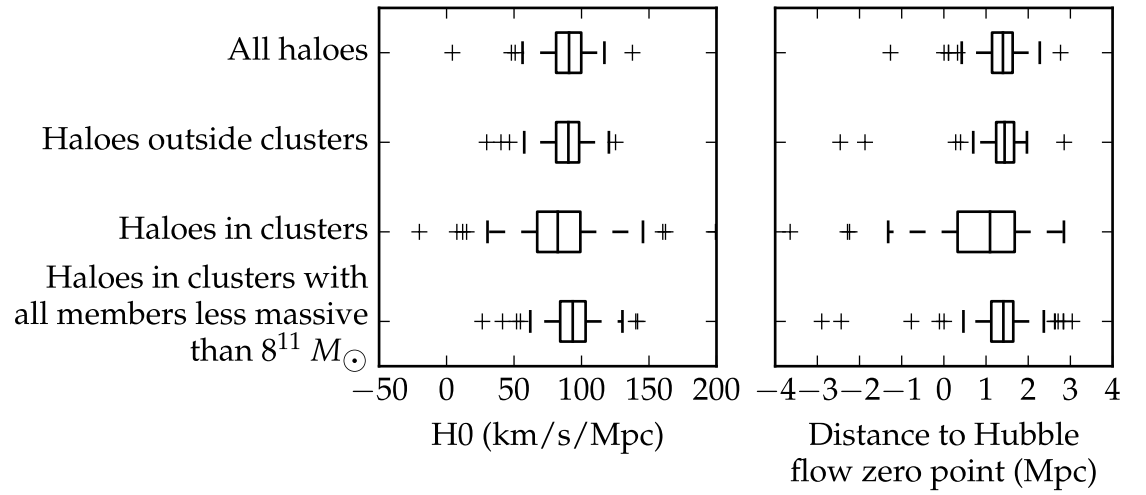


Figure 5.12: Hubble constant and distance to the point at which velocity due to the fitted Hubble flow is zero calculated from different samples. HUOM OBS NB erittele plotin ulkopuolelle jääneet kaukaiset outlierit

6. Conclusions

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A. Principal Components

PC	H_0	HF zero (clustered)	HF zero (not clustered)	σ_{radvel} (clustered)	σ_{radvel} (not clustered)	$v_{r,LG}$	$v_{t,LG}$	r_{LG}	
1	-0.386	-0.449	-0.324	-0.393	-0.211	-0.384	-0.211	0.097	0.013
2	0.147	0.221	0.248	-0.064	-0.599	-0.056	-0.599	-0.103	0.332
3	0.287	0.145	0.186	-0.531	0.258	-0.535	0.258	0.115	0.313
4	0.009	0.020	-0.152	0.151	-0.047	0.136	-0.047	0.934	0.221
5	-0.024	-0.171	-0.273	0.140	0.134	0.227	0.134	-0.270	0.840
6	0.015	-0.092	0.706	0.049	0.065	0.072	0.065	0.147	0.127
7	-0.848	0.156	0.323	-0.074	0.071	0.060	0.071	-0.001	0.128
8	-0.162	0.582	-0.206	0.456	0.024	-0.529	0.024	-0.018	0.061
9	0.041	-0.572	0.239	0.549	-0.008	-0.452	-0.008	-0.016	0.031
10	0.000	-0.000	0.000	-0.000	0.707	-0.000	-0.707	0.000	-0.000

Table A.1: component H_0 s zeropoints inClusterZeros outClusterZeros allDispersions clusterDispersions unclusteredDispersions radialVelocities tangentialVelocities LGdistances