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Master's thesis

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Classifying N-body simulations with and without relativistic corrections
using machine learning techniques

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Classifying N-body simulations with and without relativistic corrections using machine learning techniques

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Abstract

On large scales, comparable to the horizon, relativistic effects will affect the cosmological observables. In order to solve for these effects, one need to consistently solve for the metric, velocities and densities in a particular gauge. When simulating large-scale structures we use N-body simulations, which are usually performed in the Newtonian limit. However, it is not obvious that Newtonian gravity yield a good global description of an inhomogeneous cosmology across all scales (Jeong, Schmidt and Hirata 2012). However, literature suggest that Newtonian simulations are still solving the dynamics correctly, even on large scales close to the horizon where relativistic effects are important but may be corrected for (Chisari and Zaldarriaga 2011) (Green and Wald 2012).

Recently, Adamek et al. 2016 developed a relativistic N-body code, `gevolution`, which evolves large scales structures based on the weak field expansion in GR. I investigate the differences in the gravitational dynamics between structures evolved with and without relativistic effects, with focus on the gravitational potential Φ. This is a good choice for comparison as Φ is gauge invariant and the Newtonian and relativistic simulations are performed in different gauges.

The investigation is done by running 2000 simulations using identical ΛCDM cosmologies for the two gravity theories. The simulations are run using 64^4 particles on a 256^3 grid each with dimension 5120 Mpc/h which is a compromise in order to include both large and nonlinear scales. The data analysis consist of a preliminary analysis using conventional summary statistics, with focus on the bispectrum of Φ. There is a difference in the two cases for low redshifts in the equilateral and squeezed configurations. However, the main idea is to train a Convolutional Neural Network (CNN) to classify the two cases, given snapshots of Φ. The main analysis then involves interpretability of the CNN, which may be done by considering for instance saliency maps (Alqaraawi et al. 2020) or Grad-CAM (Selvaraju et al. 2020). In either case, revealing the features separating the two cases may help us understand the differences in the gravitational dynamics between the two theories. I expect that such a network is able to find relativistic corrections to the Newtonian snapshots that are of higher order than those obtained from power spectra and bispectra analysis. Further, it may also reveal which configurations of Fourier modes $\mathbf{k}$ yield the highest bispectral power, which for now is mainly trial and error.

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Preface

Here comes your preface, including acknowledgments and thanks.

Part II

Machine Learning

Chapter 6

Fundamental Elements of Machine Learning

6.1 Introduction

In this chapter I will give a brief introduction into machine learning. This includes a mathematical description of some fundamental concepts common across numerous machine learning models. The more advanced models will be dealt with at a later stage. If not otherwise stated, the following chapter is based on Goodfellow, Bengio and Courville 2016 and Hastie, Tibshirani and Friedman 2009.

6.2 Linear Algebra

maybe

6.3 Probability and Information Theory

maybe

6.4 Basic Machine Learning

TODO: Fill more here

6.4.1 Estimators, Bias, Variance and Error

Estimators Based on the assumption that there exists some true parameter(s) $\boldsymbol{\theta}$ which remain unknown,[1] we are able to make predictions and estimations of such parameter(s). Let's say we have m independent and identically distributed (i.i.d.) random variables $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_m\}$ drawn from the same probability distribution $p(\mathbf{x})$. An *estimator* of the true values $\boldsymbol{\theta}$ is any function of the data such that $\hat{\boldsymbol{\theta}}_m = g(\mathbf{x}_1, \ldots, \mathbf{x}_m)$, where $\hat{\boldsymbol{\theta}}$ is the estimate of $\boldsymbol{\theta}$. This is known as point estimation, as we are estimating a single value. This definition does not pose any restrictions on the function g. However, a good estimator would yield an estimate $\hat{\boldsymbol{\theta}}_m$ that is close to the true value $\boldsymbol{\theta}$.

[1] This is the frequentist perspective of statistics

Function estimators Say we want to predict a variable $\mathbf{y}$ given some vector $\mathbf{x}$. We assume the true variable $\mathbf{y}$ is given by some function approxiamation $f(\mathbf{x})$ plus some error $\boldsymbol{\epsilon}$: $\mathbf{y} = f(\mathbf{x}) + \boldsymbol{\epsilon}$. The aim is then to estimate the function f with the estimator $\hat{f}$. If we then realise that $\hat{f}$ is really just a point estimator in function space, the two above concepts are equivalent.

Bias The bias of the estimator $\hat{\boldsymbol{\theta}}_m$ is defined as the difference between the expected value of the estimator and the true value of the parameter: $\text{bias}(\hat{\boldsymbol{\theta}}_m) = \mathbb{E}[\hat{\boldsymbol{\theta}}_m] - \boldsymbol{\theta}$. An unbiased estimator has zero bias, i.e. $\mathbb{E}[\hat{\boldsymbol{\theta}}_m] = \boldsymbol{\theta}$. An estimator is asymptotically unbiased if its bias approaches zero as the number of data points m approaches infinity, i.e. $\lim_{m\to\infty} \mathbb{E}[\hat{\boldsymbol{\theta}}_m] = \boldsymbol{\theta}$.

Variance

Standard Error

Mean Squared Error

6.4.2 Maximum Likelihood Estimation

6.4.3 Bayesian Statistics

6.4.4 Supervised Learning

6.4.5 Unsupervised Learning

Chapter 7

Neural Networks

7.1 Forward pass - Prediction

7.1.1 Activation functions

7.1.2 Loss functions

7.2 Backpropagation - Training

7.2.1 Chain rule

Basics Lets say we have a function $f(x)$ that is composed of two functions $g(x)$ and $h(x)$, such that $f(x) = g(h(x))$. The chain rule states that the derivative of $f(x)$ with respect to x is the product of the derivative of $g(x)$ with respect to $h(x)$ and the derivative of $h(x)$ with respect to x:

$$\frac{df}{dx} = \frac{dg}{dh}\frac{dh}{dx}. \tag{7.1}$$

This can be generalised into the vector case where $f(\mathbf{x}) = g(h(\mathbf{x}))$ and $\mathbf{x} \in \mathbb{R}^n$ and TODO: write more ahaha

7.2.2 Gradient descent

7.2.3 Optimizers

7.2.4 Regularization

Chapter 8

Convolutional Neural Networks

8.1 Convolution

8.2 New Layers

8.2.1 Convolutional layers

8.2.2 Pooling layers

8.2.3 Dropout layers

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