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

**Johan Mylius Kroken**

Computational Science: Astrophysics  
60 ECTS study points

Institute of Theoretical Astrophysics  
Faculty of Mathematics and Natural Sciences



**Johan Mylius Kroken**

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Supervisors:

A David Fonseca Mota

B Julian Adamek

C Francisco Antonio Villaescusa Navarro



## 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  $\Phi$ . This is a good choice for comparison as  $\Phi$  is gauge invariant and the Newtonian and relativistic simulations are performed in different gauges.

The investigation is done by running 2000 simulations using identical  $\Lambda$ CDM 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  $\Phi$ . 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  $\Phi$ . 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.



# Contents

1	Introduction . . . . .	1
1.1	Motivation . . . . .	1
1.2	Outline . . . . .	1
1.3	Aim . . . . .	1
1.4	Nomenclature . . . . .	1
<b>I</b>	<b>Cosmological Structure Formation</b>	<b>3</b>
2	Preliminaries . . . . .	5
2.1	General Relativity . . . . .	5
2.1.1	Einstein's Field Equations . . . . .	5
2.1.2	Riemann Connection and Covariant Derivatives . . . . .	5
2.1.3	Geodesic Equation . . . . .	5
2.1.4	The Stress-Energy Tensor . . . . .	5
2.2	Useful Relations . . . . .	5
3	Background Cosmology . . . . .	7
3.1	The homogeneous Universe . . . . .	7
3.1.1	The Cosmological Principle . . . . .	7
3.1.2	The Robertson-Walker Metric . . . . .	7
3.1.3	The Friedmann Equations . . . . .	7
3.2	My Universe is loaded with... . . . .	7
3.3	Thermal History of the Universe . . . . .	7
4	Perturbation Theory . . . . .	9
4.1	Initial Conditions . . . . .	9
4.2	Transfer Functions . . . . .	9
4.3	Power Spectra . . . . .	9
4.4	Linear Evolution . . . . .	9
4.5	Non-linear Evolution . . . . .	9
4.6	Bispectra . . . . .	9
4.6.1	Analytical Bispectrum . . . . .	9
5	Simulation theory . . . . .	13
5.1	N-body simulations . . . . .	13
5.1.1	Describing a box of particles . . . . .	13
5.1.2	Forces and Fields . . . . .	13
5.1.3	Mass Assignment Schemes . . . . .	13
5.1.4	Validity of Box . . . . .	13
5.2	Newtonian Approach . . . . .	13
5.3	General Relativistic Approach . . . . .	13

<b>II</b>	<b>Machine Learning</b>	<b>15</b>
6	Fundamental Elements of Machine Learning . . . . .	17
6.1	Introduction . . . . .	17
6.2	Linear Algebra . . . . .	17
6.3	Probability and Information Theory . . . . .	17
6.4	Basic Machine Learning . . . . .	17
6.4.1	Estimators, Bias, Variance and Error . . . . .	17
6.4.2	Maximum Likelihood Estimation . . . . .	18
6.4.3	Bayesian Statistics . . . . .	18
6.4.4	Supervised Learning . . . . .	18
6.4.5	Unsupervised Learning . . . . .	18
7	Neural Networks. . . . .	19
7.1	Forward pass - Prediction . . . . .	19
7.1.1	Activation functions. . . . .	19
7.1.2	Loss functions. . . . .	19
7.2	Backpropagation - Training . . . . .	19
7.2.1	Chain rule . . . . .	19
7.2.2	Gradient descent . . . . .	19
7.2.3	Optimizers . . . . .	19
7.2.4	Regularization . . . . .	19
8	Convolutional Neural Networks . . . . .	21
8.1	Convolution . . . . .	21
8.2	New Layers . . . . .	21
8.2.1	Convolutional layers . . . . .	21
8.2.2	Pooling layers . . . . .	21
8.2.3	Dropout layers . . . . .	21
<b>III</b>	<b>Acquiring Data</b>	<b>23</b>
9	Simulations. . . . .	25
9.1	Parameters . . . . .	25
9.1.1	Cosmological parameters . . . . .	25
9.1.2	Primordial power spectrum . . . . .	25
9.1.3	Box parameters . . . . .	26
9.1.4	Seeds and gravity theories . . . . .	26
9.2	Output. . . . .	26
9.2.1	Datacubes . . . . .	26
9.2.2	Redshift problem. . . . .	27
9.2.3	Statistics of dataset. . . . .	27
9.2.4	Normalisation . . . . .	27
10	Data Verification . . . . .	29
10.1	Slices of Datacubes. . . . .	29
10.2	Powerspectra from Simulations . . . . .	29
10.3	Powerspectra from Datacubes . . . . .	29
10.4	Analytical Bispectra . . . . .	29
10.5	Bispectra from Cube . . . . .	29
10.5.1	Binning . . . . .	29
10.5.2	Bispectra . . . . .	29



11	Trainable Dataset . . . . .	37
11.1	Gathering the cubes . . . . .	37
11.2	Find image from index . . . . .	37

## Contents

# List of Figures

4.1	Angles in arbitrary bispectrum triangle configuration where $\sum_i \mathbf{k}_i = 0$ . . . .	10
10.1	Slice 0 . . . . .	30
10.2	Average matter power spectra at different redshifts. . . . .	31
10.3	Average potential power spectra at different redshifts. . . . .	32
11.1	Outline of data structure. . . . .	38

## List of Figures

# List of Tables

9.1	Cosmological parameters . . . . .	25
9.2	Primordial power spectra parameters . . . . .	25
9.3	Box parameters . . . . .	26

## List of Tables

# 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)  $\theta$  which remain unknown,<sup>1</sup> 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  $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m\}$  drawn from the same probability distribution  $p(\mathbf{x})$ . An *estimator* of the true values  $\theta$  is any function of the data such that  $\hat{\theta}_m = g(\mathbf{x}_1, \dots, \mathbf{x}_m)$ , where  $\hat{\theta}$  is the estimate of  $\theta$ . 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  $\hat{\theta}_m$  that is close to the true value  $\theta$ .

---

<sup>1</sup>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 approximation  $f(\mathbf{x})$  plus some error  $\epsilon$ :  $\mathbf{y} = f(\mathbf{x}) + \epsilon$ . 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  $\hat{\theta}_m$  is defined as the difference between the expected value of the estimator and the true value of the parameter:  $\text{bias}(\hat{\theta}_m) = \mathbb{E}[\hat{\theta}_m] - \theta$ . An unbiased estimator has zero bias, i.e.  $\mathbb{E}[\hat{\theta}_m] = \theta$ . An estimator is asymptotically unbiased if its bias approaches zero as the number of data points  $m$  approaches infinity, i.e.  $\lim_{m \rightarrow \infty} \mathbb{E}[\hat{\theta}_m] = \theta$ .

**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  $x$ :

$$\frac{df}{dx} = \frac{dg}{dh} \frac{dh}{dx}. \quad (7.1)$$

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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