

# -sometitle-

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**

**-sometitle-**

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

Supervisors:

A David Fonseca Mota

B Julian Adamek

C Francisco Antonio Villaescusa Navarro



### **Abstract**

Here come 3–6 sentences describing your thesis.

### **Sammendrag**

Here comes the abstract in a different language.



# 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	Non-linear Evolution . . . . .	9
4.5	Bispectra . . . . .	9
5	Simulation theory . . . . .	11
5.1	N-body simulations . . . . .	11
5.1.1	Describing a box of particles . . . . .	11
5.1.2	Forces and Fields . . . . .	11
5.1.3	Mass Assignment Schemes . . . . .	11
5.1.4	Validity of Box . . . . .	11
5.2	Newtonian Approach . . . . .	11
5.3	General Relativistic Approach . . . . .	11

<b>II</b>	<b>Machine Learning</b>	<b>13</b>
6	Fundamental Elements of Machine Learning . . . . .	15
6.1	Introduction . . . . .	15
6.2	Linear Algebra . . . . .	15
6.3	Probability and Information Theory . . . . .	15
6.4	Basic Machine Learning . . . . .	15
6.4.1	Estimators, Bias, Variance and Error . . . . .	15
6.4.2	Maximum Likelihood Estimation . . . . .	16
6.4.3	Bayesian Statistics . . . . .	16
6.4.4	Supervised Learning . . . . .	16
6.4.5	Unsupervised Learning . . . . .	16
7	Neural Networks. . . . .	17
7.1	Forward pass - Prediction . . . . .	17
7.1.1	Activation functions. . . . .	17
7.1.2	Loss functions. . . . .	17
7.2	Backpropagation - Training . . . . .	17
7.2.1	Gradient descent . . . . .	17
7.2.2	Optimizers . . . . .	17
7.2.3	Regularization . . . . .	17
8	Convolutional Neural Networks . . . . .	19
8.1	Convolution . . . . .	19
8.2	New Layers . . . . .	19
8.2.1	Convolutional layers . . . . .	19
8.2.2	Pooling layers . . . . .	19
8.2.3	Dropout layers . . . . .	19
<b>III</b>	<b>Acquiring Data</b>	<b>21</b>
9	Simulations. . . . .	23
10	Data Verification . . . . .	25
10.1	Slices of Datacubes. . . . .	25
10.2	Power spectra from Theory . . . . .	25
10.3	Powerspectra from Simulations . . . . .	25
10.4	Powerspectra from Datacubes. . . . .	25
11	Trainable Dataset . . . . .	29



# List of Figures

## List of Figures

# List of Tables

## List of Tables

# Preface

Here comes your preface, including acknowledgments and thanks.



# Chapter 1

## Introduction

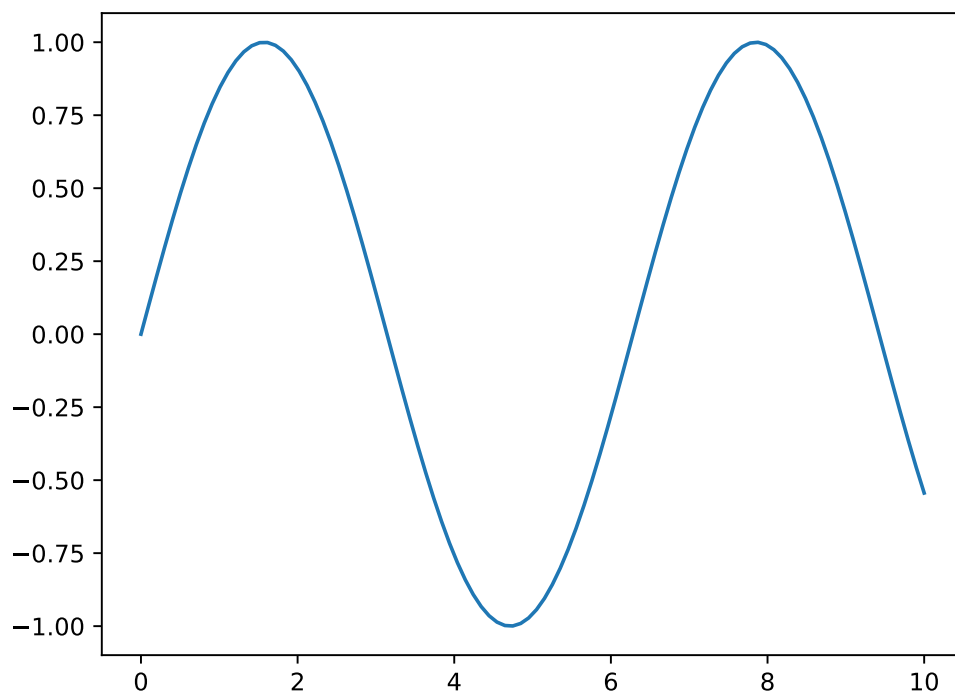
This is the introduction that will shortly be written. How fast does things change.

### 1.1 Motivation

### 1.2 Outline

### 1.3 Aim

### 1.4 Nomenclature





# **Part I**

## **Cosmological Structure Formation**



## Chapter 2

# Preliminaries

### 2.1 General Relativity

#### 2.1.1 Einstein's Field Equations

$$G_{\mu\nu} = 8\pi GT_{\mu\nu} \quad (2.1)$$

$$G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R \quad (2.2)$$

$$R = g^{\mu\nu}R_{\mu\nu} \quad (2.3)$$

$$R_{\mu\nu} = \partial_\rho \Gamma_{\mu\nu}^\rho - \partial_\nu \Gamma_{\mu\rho}^\rho + \Gamma_{\mu\nu}^\rho \Gamma_{\rho\sigma}^\sigma - \Gamma_{\mu\sigma}^\rho \Gamma_{\nu\rho}^\sigma \quad (2.4)$$

#### 2.1.2 Riemann Connection and Covariant Derivatives

$$\Gamma_{\mu\nu}^\rho = \frac{1}{2}g^{\rho\sigma}(\partial_\mu g_{\nu\sigma} + \partial_\nu g_{\mu\sigma} - \partial_\sigma g_{\mu\nu}) \quad (2.5)$$

$$\nabla_\mu T_\nu^\mu = \partial_\mu T_\nu^\mu + \Gamma_{\mu\alpha}^\mu T_\nu^\alpha - \Gamma_{\mu\nu}^\alpha T_\alpha^\mu \quad (2.6)$$

#### 2.1.3 Geodesic Equation

$$\frac{d^2 x^\mu}{d\tau^2} + \Gamma_{\alpha\beta}^\mu \frac{dx^\alpha}{d\tau} \frac{dx^\beta}{d\tau} = 0 \quad (2.7)$$

#### 2.1.4 The Stress-Energy Tensor

$$T_{\mu\nu} = (\rho + p)u_\mu u_\nu + pg_{\mu\nu} \quad (2.8)$$

### 2.2 Useful Relations



## Chapter 3

# Background Cosmology

### 3.1 The homogeneous Universe

In this chapter I will focus on explaining the background cosmology in light of a homogeneous universe. A natural place to start is the cosmological principle, followed by a description of the geometry of space itself. If not otherwise stated, the development of this chapter is based on Dodelson and Schmidt 2020, Weinberg 2008 and [TODO: cite Baumann](#)

#### 3.1.1 The Cosmological Principle

#### 3.1.2 The Robertson-Walker Metric

$$ds^2 = -dt^2 + a^2(t) \left[ \frac{dr^2}{1 - kr^2} + r^2 d\Omega^2 \right] \quad (3.1)$$

#### 3.1.3 The Friedmann Equations

### 3.2 My Universe is loaded with...

### 3.3 Thermal History of the Universe



## Chapter 4

# Perturbation Theory

### 4.1 Initial Conditions

### 4.2 Transfer Functions

### 4.3 Power Spectra

### 4.4 Non-linear Evolution

### 4.5 Bispectra

The bispectra are powerful tools for studying the non-linear evolution of the density field. The bispectrum is defined as the Fourier transform of the three-point correlation function, and is given by:

$$\langle \delta(\mathbf{k}_1)\delta(\mathbf{k}_2)\delta(\mathbf{k}_3) \rangle = (2\pi)^3 \delta_D(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3) B(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) \quad (4.1)$$

Well this is rather awkward. Adamek et al. 2016 or (Falck et al. 2017)





## **Chapter 5**

# **Simulation theory**

Some theory and history as to how to conduct N-body simulations.

### **5.1 N-body simulations**

#### **5.1.1 Describing a box of particles**

#### **5.1.2 Forces and Fields**

#### **5.1.3 Mass Assignment Schemes**

#### **5.1.4 Validity of Box**

### **5.2 Newtonian Approach**

### **5.3 General Relativistic Approach**



# **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 Gradient descent**

#### **7.2.2 Optimizers**

#### **7.2.3 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**



# **Part III**

## **Acquiring Data**



## **Chapter 9**

# **Simulations**



## Chapter 10

# Data Verification

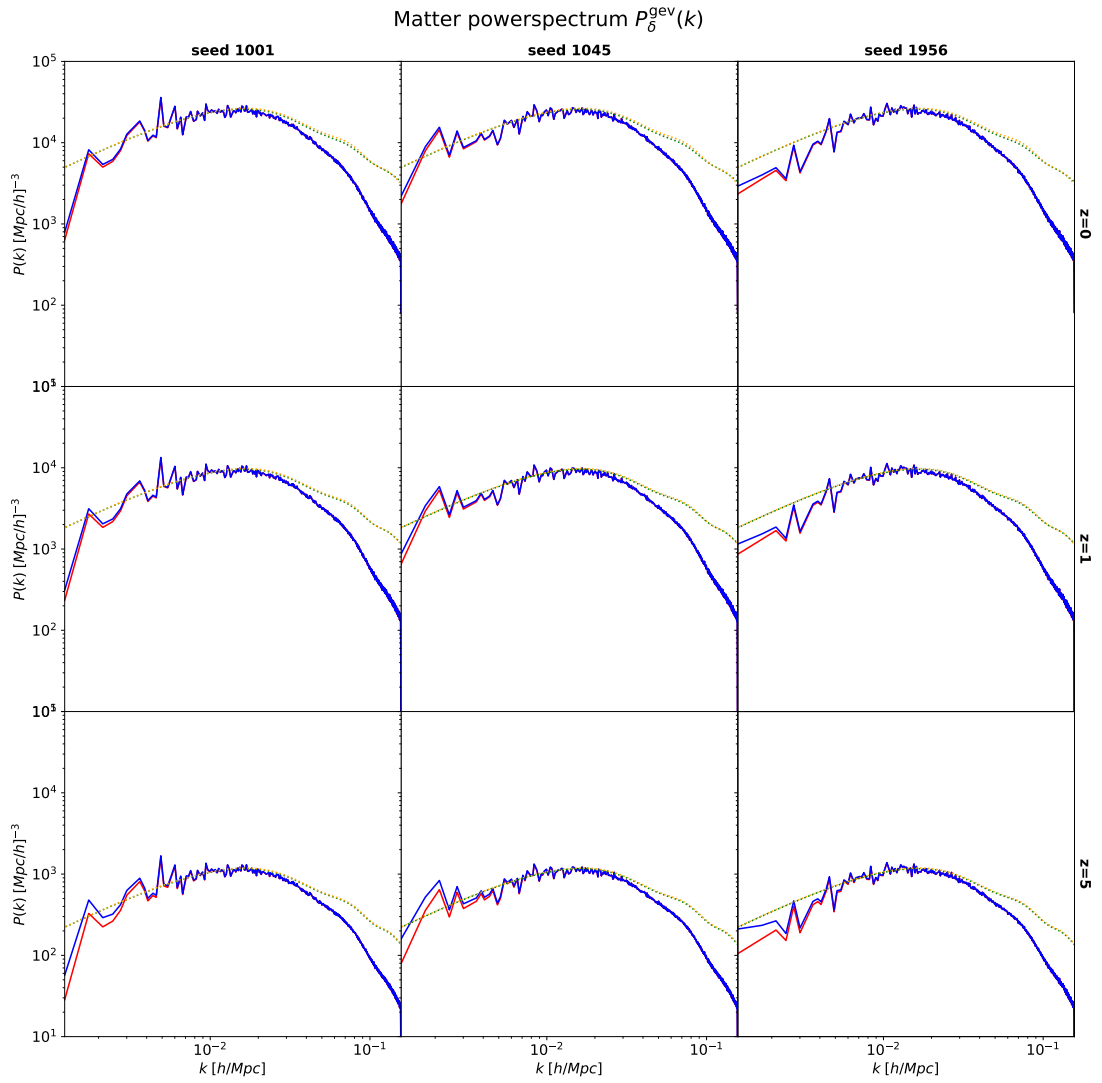
### 10.1 Slices of Datacubes

### 10.2 Power spectra from Theory

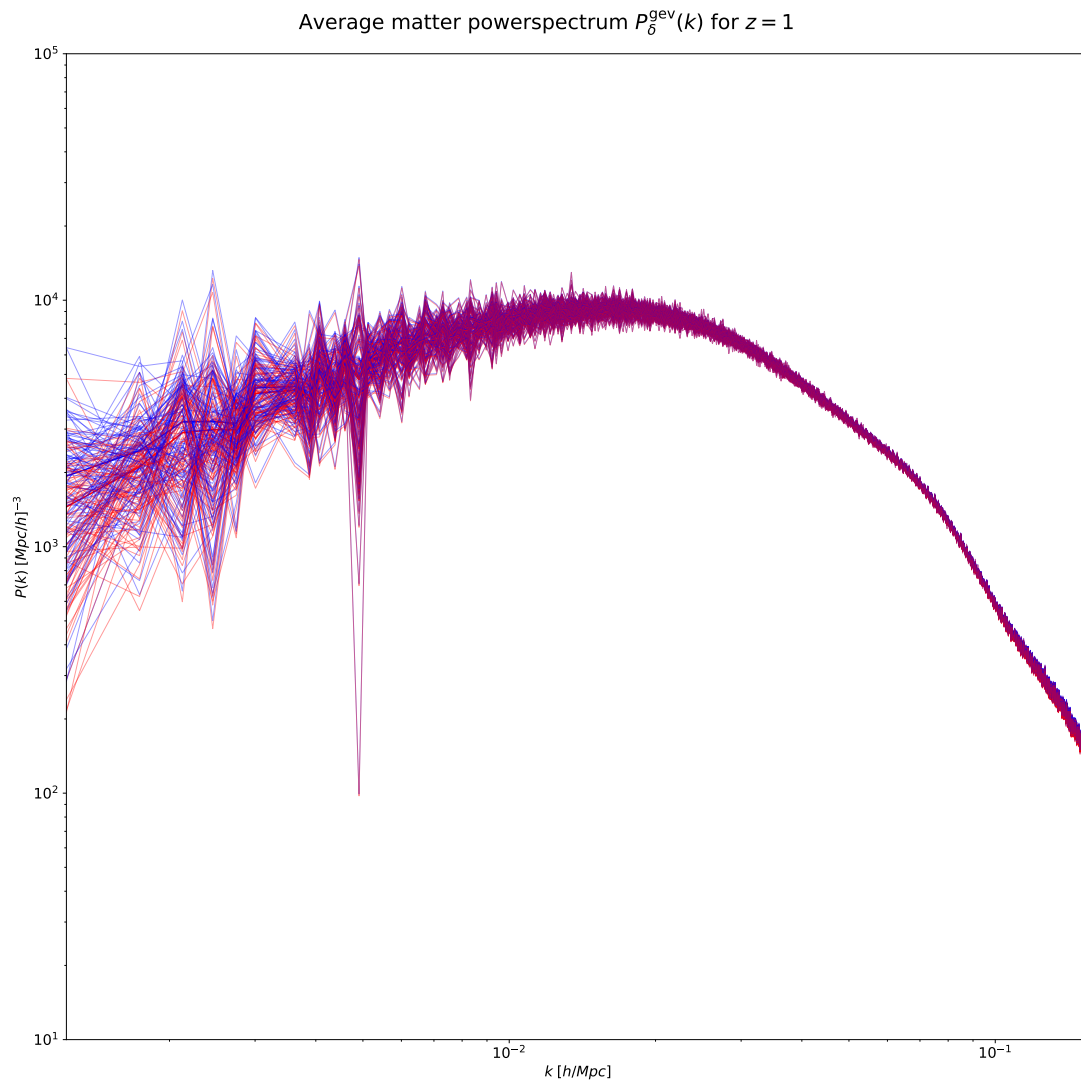
TODO: Provide some camb and class power spectra here.

### 10.3 Powerspectra from Simulations

### 10.4 Powerspectra from Datacubes









## **Chapter 11**

# **Trainable Dataset**



# Bibliography

- Adamek, Julian et al. (29th July 2016). ‘gevolution: a cosmological N-body code based on General Relativity’. In: *Journal of Cosmology and Astroparticle Physics* 2016.7, pp. 053–053. ISSN: 1475-7516. DOI: 10.1088/1475-7516/2016/07/053. arXiv: 1604.06065[astro-ph,physics:gr-qc,physics:physics]. URL: <http://arxiv.org/abs/1604.06065> (visited on 23/08/2023).
- Dodelson, S. and F. Schmidt (2020). *Modern Cosmology*. Elsevier Science. ISBN: 9780128159484. URL: <https://books.google.no/books?id=GGjfywEACAAJ>.
- Falck, B. et al. (16th Mar. 2017). ‘The Effect of Corner Modes in the Initial Conditions of Cosmological Simulations’. In: *The Astrophysical Journal* 837.2, p. 181. ISSN: 1538-4357. DOI: 10.3847/1538-4357/aa60c7. arXiv: 1610.04862[astro-ph]. URL: <http://arxiv.org/abs/1610.04862> (visited on 20/09/2023).
- Goodfellow, Ian, Yoshua Bengio and Aaron Courville (2016). *Deep Learning*. <http://www.deeplearningbook.org>. MIT Press.
- Hastie, T., R. Tibshirani and J.H. Friedman (2009). *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*. Springer series in statistics. Springer. ISBN: 9780387848846. URL: <https://books.google.no/books?id=eBSgoAEACAAJ>.
- Weinberg, S. (2008). *Cosmology*. Cosmology. OUP Oxford. ISBN: 9780191523601. URL: <https://books.google.no/books?id=nqQZdg020fsC>.