Investigation of Bond Strain Effects on XANES Structure Spectra by Supervised Machine Learning

by
Jeremy K. Thaller

Professor Anatoly Frenkel, Advisor

A thesis submitted in partial fulfillment
of the requirements for the
Erasmus Mundus Joint Master Degrees:
Masters in Materials Science Exploring Large Scale Facilities

Brookhaven National Labs
Brookhaven, New York
February 17, 2021

Abstract

Your abstract will summarize your thesis in one or two paragraphs. This brief summary should emphasize methods and results, not introductory material.

Executive Summary

Your executive summary will give a detailed summary of your thesis, hitting the high points and perhaps including a figure or two. This should have all of the important take-home messages; though details will of course be left for the thesis itself, here you should give enough detail for a reader to have a good idea of the content of the full document. Importantly, this summary should be able to stand alone, separate from the rest of the document, so although you will be emphasizing the key results of your work, you will probably also want to include a sentence or two of introduction and context for the work you have done.

Acknowledgments

The acknowledgment section is optional, but most theses will include one. Feel free to thank anyone who contributed to your effort if the mood strikes you. Inside jokes and small pieces of humor are fairly common here ...

Contents

List of Figures

Chapter 1

Introduction

The introduction is one of the most important pieces of your thesis. Here is a place for you to introduce the problem(s) on which you have worked and place them in the larger context of your field. You should aim to ensure that this section is completely understandable to virtually anyone - and certainly anyone with a sophomore-level grasp of physics. Presumably this will include references to the literature.

In addition to setting your work into context, a second good idea for your introduction is to give a short outline for what the rest of your thesis will discuss. This is often done in the closing paragraph(s) of the introduction with sentences like "In the following chapters ..." and "Chapter 2 discusses ..." Tremendous detail is not required in this outline, but rather just a brief road map for the rest of the document.

1.1 Traditional XANES

The `\section` tag will create a new section within a chapter. Sections will be sequenced with digits following a decimal point in the table of contents, i.e. this is section 1.1.

This is an example to-do

1.2 Machine Learning in Science

Probably want to talk about these papers in this section [1] [2].

Chapter 2

Machine Learning Approach

Here is a second mock chapter. As far as the LaTeX is concerned, it is in no way different from the introduction excepting that it appears after it in the main .tex file. As before, it can be populated with sections, subsections, figures, etc. as you see fit.

In fact, you will probably write perhaps three to six chapters for your thesis depending on how your work is most effectively organized. Most theses will contain an introduction, at least one 'body' chapter, and some sort of conclusions/future directions chapter. Most theses will also include an appendix or two ...

2.1 Autoencoders

Talk about how autoencoders work. Give a nice broad explanation and really go into the math. Include some nice diagrams

Here's [3] a good source to read and model off of. Here [**?**] is another paper that might be interesting to read. It's about getting noise free data from the original data using an autoencoder. Neat idea, and could actually be very relevant because they're using geophysical data.

Chapter 3

Results

I think results and discussion of results should go here

Appendix A

An appendix

Appendices are a good idea for almost any thesis. Your main thesis body will likely contain perhaps 40-60 pages of text and figures. You may well write a larger document than this, but chances are that some of the information contained therein, while important, does *not* merit a place in the main body of the document. This sort of content - peripheral clarifying details, computer code, information of use to future students but not critical to understanding your work . . . - should be allocated to one or several appendices.

Bibliography

[1] J. Timoshenko, A. Anspoks, A. Cintins, A. Kuzmin, J. Purans, and A. I. Frenkel, Physical review letters **120**, 225502 (2018).

[2] J. Timoshenko, D. Lu, Y. Lin, and A. I. Frenkel, The Journal of Physical Chemistry Letters **8**, 5091 (2017).

[3] A. Ng et al., CS294A Lecture notes **72**, 1 (2011).