



Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Designing meaningful measures to evaluate generative graph neural networks on protein datasets.

Master Thesis

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Abstract

This example thesis briefly shows the main features of our thesis style, and how to use it for your purposes.

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Chapter 1

Introduction

Background & Related Work

This chapter introduces the core concepts built upon in this thesis and surveys recent literature tackling the evaluation of generative graph neural networks and the relevance of this problem in structural biology. Section 2.1 defines core mathematical and biological concepts that will be built upon in the thesis. Section 2.2 will discuss recent advances in the design of measures used to evaluate generative graph neural networks and in structural biology.

2.1 Background

The set of methods investigated in this thesis lies at the interface of structural biology and machine learning. We start by defining some relevant biological properties of proteins, followed by a survey various graph theoretical abstractions derived from the protein structure. We then move on to define generative models and the various classes of measures used to evaluate them.

2.1.1 Proteins

Proteins are large biomolecules that are formed from a sequence of amino acids, performing their functions as determined by their three-dimensional structure, and amino acid sequence. Proteins support a vast array of functions in living organisms, such as catalysing metabolic reactions, DNA replication, providing structural support to cells, transporting molecules and sensing stimuli.

Structurally, each protein is made up of one or more chains of amino acids, each of which contain a backbone and different side chains. The atoms in the backbone include a α -Carbon,

2. BACKGROUND & RELATED WORK

2.1.2 Graphs

2.1.3 Topological Data Analysis

2.1.4 Generative models

2.1.5 Kernel methods

2.2 Related Work

2.2.1 Structural Biology

2.2.2 Metrics for Generative Graph Models

2.3 Summary

Methods

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3.1 Example Section

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3.1.1 Example Subsection

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Example Subsubsection

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Example Paragraph Dummy text.

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Results

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4.1 Example Section

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4.1.1 Example Subsection

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Example Subsubsection

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Chapter 5

Discussion

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5.1 Example Section

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5.1.1 Example Subsection

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Example Subsubsection

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Example Subparagraph Dummy text.

Conclusion

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6.1 Example Section

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6.1.1 Example Subsection

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Example Subsubsection

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Example Paragraph Dummy text.

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Appendix A

Dummy Appendix

You can defer lengthy calculations that would otherwise only interrupt the flow of your thesis to an appendix.

Bibliography



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