

Development of an R Toolbox for Near-Infrared Spectroscopy Data Processing and Analysis of Plant Metabolic Phenotypes

DEGGENDORF INSTITUTE OF TECHNOLOGY

MSC. LIFE SCIENCE INFORMATICS

Methun George

Supervised by
PD Dr. habil. rer. nat. Steffen Neumann
Prof. Dr. Melanie Kappelmann-Fenzl

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Chapter 1

Introduction

Scientific curiosity often begins with a simple question of, how can meaningful insights be extracted from the vast amount of scientific data.

1.1 Related Work

The related work include, the followings

Chapter 2

Background

The background of this study include

2.1 Near Infrared Spectroscopy (NIRS)

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2.1.1 Introduction

2.2 Metabolomics

2.2.1 Introduction

2.2.2 Mass Spectrometry

2.3 Machine Learning

2.3.1 Introduction

2.3.2 Partial Least Square Regression (PLS)

2.3.3 Random Forest (RF)

2.3.4 Convolutional Neural Network (CNN)

Chapter 3

Methods and Implementation

3.1 MSNovelist

3.1.1 Basic Idea of the Software

3.1.2 Deep Learning Architecture

3.1.3 Preparation of Data

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3.2.1 Data Records

3.2.2 File Formats

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3.7 Hardware

Chapter 4

Results and Discussion

4.1 Baseline Model

4.1.1 Termination Criterion

4.1.2 Impact of the Amount of Data

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4.2 Alternative Tokenization of SMILES Sequences

4.2.1 QBMG Tokenization