

About the Book

The core idea of this book entitled "Machine Learning using Google Colab - for Chemistry & Biochemistry Applications" is to lay a foundation or stepping stone to explain the algorithmic approach for solving chemistry & biochemistry oriented research problems at the practical level. It explains various kinds of concepts, such as, classification, pre-processing techniques, datasets, packages, library files, data repository, clustering, prediction, coding, data visualization, analysis, forms, commands and case studies. The scope of this book covers a broad spectrum of people including faculty members, researchers, research scholars, students, and programmers to gain knowledge about how machine learning codes are written to construct a model for solving real-time complex problems. The entire source codes utilized in this book are available on GitHub. URL links and QR codes available to access those codes are given at the end of respective chapters.

Authors Profile

Prof. P. Subashini is working for Department of Computer Science, Avinashilingam University for Women, Tamil Nadu India, from 1994. She is the coordinator of the Centre for Machine Learning and Intelligence sanctioned by Department of Science and Technology. Her research has spanned a large number of disciplines like Image analysis, Pattern recognition, Neural networks, and Computational Intelligence. She has authored and co-authored 7 Books, 9 Book chapters, 1 Monograph, 194 research papers both at international and national levels, she received 15 sponsored research projects worth more than 5.12 crores from various government funding agencies. She also extended her contribution towards various international collaborations with universities from USA, Germany and Morocco.

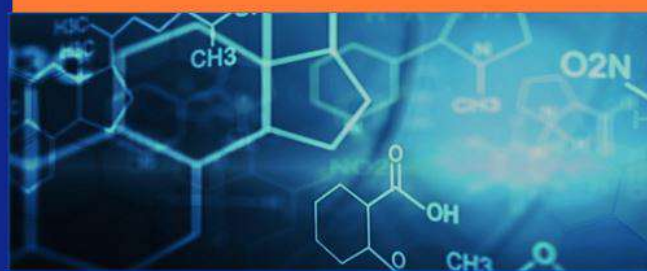
Dr. T.T. Dhivyaprabha is working as Research Associate in the "Core Research grant for Artificial Intelligence-AI" project funded by DST-CURIE-AI-PHASE-II, Centre for Machine Learning and Intelligence from May 2021 to till now. She has published 1 book, 6 journals, 5 book chapters and 21 papers in international conferences. She has 4 years of teaching experience and worked on research projects funded by DST, SERB, UGC-Startup and DRDO NPOL. Her area of interest includes Computational Intelligence, Image Processing and Analysis and Internet of Things (IoT).

Ms. M.B. Jennyfer Susan, Research Scholar in Department of Computer Science, Centre for Machine Learning and Intelligence at Avinashilingam Institute for Home Science and Higher Education for Women, Tamil Nadu India. She has published 1 International Journal, 1 National Conference, 2 International Conferences and 1 Book Chapter. The Research area of interest includes Vision AI, Medical Image Processing and Neural Networks.



MACHINE LEARNING USING GOOGLE COLAB

Prof. P. Subashini



MACHINE LEARNING USING GOOGLE COLAB

- for Chemistry & Biochemistry
Applications

Prof. P. Subashini
Dr. T.T. Dhivyaprabha
Ms. M.B. Jennyfer Susan

Table of Contents

		Page No.
CHAPTER 1	Google Colaboratory	9
	1.1 What is Google Colab?	9
	1.2 Why do we need Google Colab?	10
	1.3 Features of Google Colab	11
	1.4 GPUs and TPUs Facility on Google Colab	13
	1.5 Pre-requisites of Google Colab	13
	1.6 Colabpro and Colabpro+	19
	1.7 Organization of Chapters	20
CHAPTER 2	Basics of Google Colab	21
	2.1 Opening a New Notebook in Google Colaboratory	21
	2.2 Setting a Notebook Name	26
	2.3 Entering Code in Code Cell	27
	2.4 Adding Code Cells	27
	2.5 Adding Text Cells	29
	2.6 Executing the Code	31
	2.7 Changing Cell Order	40
	2.8 Deleting Code Cell	42
CHAPTER 3	Google Colab - Document Your Code	45
	3.1 Guide to Markdown	45
	3.2 Saving and Sharing Your Document	63
CHAPTER 4	Google Colab- System Commands	74
	4.1 Simple Commands	74
	4.2 Cloning Git Repository in Google Colab	83
	4.3 Importing the Dataset from the Github	86
	4.4 Importing the Kaggle Dataset	88
CHAPTER 5	Google Colab - Runtime	97
	5.1 Runtimes in Google Colab	97
	5.2 Enabling GPU and TPU in Colab Notebook	98
	5.3 Run CUDA C/C++ in Colab	104
	5.4 Installing Machine Learning Libraries	107
CHAPTER 6	Local Files, Drive and Sheets in the Google Colaboratory	116
	6.1 Local File Systems	116
	6.2 Google Drive	125
	6.3 Google Sheets	134

CHAPTER 7	Working with Images using Google Colab	140
	7.1 Loading an Image in Google Colab	140
	7.2 Displaying the Images using Google Colab	157
	7.3 Pre-processing	159
	7.4 Segmentation	161
	7.5 Classification	171
CHAPTER 8	Working with Data using Google Colab	187
	8.1 Loading the Data in Google Colab	187
	8.2 Displaying the Data using Google Colab	197
	8.3 Preprocessing	199
	8.4 Feature Extraction	217
	8.5 Classification	223
CHAPTER 9	Charting in Colaboratory	234
	9.1 Matplotlib	234
	9.2 Style Plots	246
	9.3 3D Graphs	248
	9.4 Seaborn	254
	9.5 Altair	256
	9.6 Bokeh	257
CHAPTER 10	Google Colab Magics	262
	10.1 Line Magic	262
	10.2 Cell Magic	284
CHAPTER 11	Forms	290
	11.1 Adding Forms	290
	11.2 Adding Forms Fields	292
	11.3 Testing Forms	297
	11.4 Hiding Code	298
	11.5 Hiding Form	299
CASE STUDIES	A Forecasting Oxidative Coupling of Methane	301
	B Visualizing 3D Structure and Predicting the Physical Property of a Molecule	326
	C Implementing Graph Neural Network for Predicting Molecular Property	341
BIBLIOGRAPHY		357