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Python for Scientists

Third Edition

The third edition of this practical introduction to Python has been thoroughly updated, with all code migrated to Python 3 and made available as Jupyter notebooks. The notebooks are available online with executable versions of all the book's content (and more).

The text starts with a detailed introduction to the basics of the Python language, without assuming any prior knowledge. Building upon each other, the most important Python packages for numerical math (NumPy), symbolic math (SymPy), and plotting (Matplotlib) are introduced, with brand new chapters covering numerical methods (SciPy) and data handling (Pandas). Further new material includes guidelines for writing efficient Python code and publishing code for other users.

Simple and concise code examples, revised for compatibility with Python 3, guide the reader and support the learning process throughout the book. Readers from the quantitative sciences, whatever their background, will be able to quickly acquire the skills needed for using Python effectively.

JOHN M. STEWART was Emeritus Reader in Gravitational Physics at the University of Cambridge, and a Life Fellow at King's College, Cambridge, before his death in 2016. He was the author of *Non-equilibrium Relativistic Kinetic Theory* (Springer, 1971) and *Advanced General Relativity* (Cambridge, 1991), and he translated and edited Hans Stephani's *General Relativity* (Cambridge, 1990).

MICHAEL MOMMERT is Assistant Professor for Computer Vision at the University of St. Gallen, Switzerland, where he combines computer vision and Earth observation to implement efficient learning methods for a wide range of use cases. Before, he was a solar system astronomer and actively wrote scientific open-source code for this community.

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Third Edition

JOHN M. STEWART University of Cambridge

MICHAEL MOMMERT University of St. Gallen, Switzerland



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Shaftesbury Road, Cambridge CB2 8EA, United Kingdom

One Liberty Plaza, 20th Floor, New York, NY 10006, USA

477 Williamstown Road, Port Melbourne, VIC 3207, Australia

314-321, 3rd Floor, Plot 3, Splendor Forum, Jasola District Centre, New Delhi - 110025, India

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Preface

I bought a copy of *Python for Scientists* at a conference booth in 2016, looking for an affordable and easily readable textbook for a Python course I was teaching at that time. I was intrigued by how straightforwardly even complex things were explained in this book. It was a perfect match for my course and my students, despite my impression that the book was rather heavily focused on mathematical applications.

It has been five years since the second edition of *Python for Scientists* was released. This is a long time in the life cycle of a programming language that is still under active development. It was definitely time for an update.

Unfortunately, John is no longer with us to provide this update himself. Instead, I was honored that this task was offered to me, and I could not decline.

Besides updating the Python code examples shown in the book, I took the opportunity to also update the content of the book with the goal of making it accessible to a broader audience of scientists, especially those with a quantitative focus in their work. This includes a more in-depth discussion of numerical mathematics with NumPy (Chapter 4) and SciPy (Chapter 5), plotting capabilities with Matplotlib (Chapter 6), and, for the first time, data handling with Pandas (Chapter 8), performance computing with Python (Chapter 9), and an outline of software development techniques that are useful to scientists (Chapter 10). However, in order to keep the book reasonably short and affordable, other content, such as the detailed treatment of ordinary and partial differential equations, had to be significantly shortened or removed altogether – Python packages for dealing with such problems exist, but their discussion is beyond the scope of this beginner book.

I sincerely hope the third edition of *Python for Scientists* will be a useful companion on your long journey to becoming a scientific programmer.

Michael Mommert St. Gallen, November 2022