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Chapter 1

Preface

The use of naturally occurring radioactive isotopes to date minerals and rocks is the oldest branch of isotope geology. The foundations of these so-called isotopic or radiometric dating methods were laid shortly after the turn of the XXth century with the discovery of the laws of radioactive decay by eminent physicists such as Ernest Rutherford and Frederick Soddy rutherford1902a, rutherford1902b. The application of these principles to the field of Geology and the calibration of the geological time scale were pioneered by Arthur holmes1911, holmes1913, holmes1947. Initially, radiometric geochronology was exclusively based on uranium and its daughter products, but with the development of increasingly sensitive analytical equipment, ever more isotopic 'clocks' were added over the course of the century: Rb/Sr hahn1943, ^{14}C libby1946, K/Ar aldrich1948, ^{238}U fission tracks price1963, ^{40}Ar/^{39}Ar merrihue1966, Sm/Nd lugmair1974, etc.

The first part of these lecture notes provides a basic introduction to all these methods. Chapter **??** reviews the basic principles of radioactive decay, which form the basis of all isotopic dating techniques. It will derive the fundamental age equation and introduce the concepts of secular equilibrium, which will be revisited in later chapters. Chapter **??** provides the briefest of introductions to the world of mass spectrometry. It will sketch the basic operating principles of the instruments used to acquire the datasets that will be used for `R` programming exercises later on. Chapters **??**–**??** provide basic introductions to the radiocarbon, Rb–Sr, Sm–Nd, U–Pb, Ar–Ar, U–Th–He, fission track and Th–U methods, which will be fleshed out further in Part 2 of the notes.

Chapter **??** presents a primer in error propagation which is extremely important because, to quote K.R. Ludwig "The uncertainty of the age is as important as the age itself" ludwig2003b. Chapter **??** contains a collection of exercises that are meant to be solved by pencil on paper, whereas Chapter **??** contains a collection of practical exercises that require the `R` programming language. In these exercises, you will process some raw data files for the U–Pb, Ar–Ar and fission track methods. The purpose of these exercises is to provide a glimpse into the 'black box' data processing software that is normally used by geochronologists to turn mass spectrometer data into tables of isotopic ratios for further processing with the `IsoplotR` package that is the subject of Part 2 of this book.

The core of these notes is formed by Prof. Peter van den Haute's lecture notes (in Dutch) at the University of Ghent. This was expanded with additional material, exercises, and practicals. Some figures were modified from published sources, including allegre2008, braun2006, and galbraith2005. These books are recommended further reading material, as is the detailed textbook by dickin2005, from which both allegre2008 and van den Haute heavily borrowed. Additional lecture material, including the data files used in the programming practicals of Chapter ??, can be found at `https://github.com/pvermees/geotopes/`.

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Chapter 2

Introduction to IsoplotR

Part 1 of these notes gave a very basic introduction to geochronology. At this basic level, it is possible to write one's own data processing software, as we have done in the `R` practicals. Unfortunately this is not so easy at a more advanced level. Part 2 of the notes will introduce a plethora of more sophisticated of mathematical-statistical techniques that deal with real datasets in a rigorous and self-consistent manner. For many years, a `Microsoft Excel` add-in called `Isoplot` has served this purpose extremely well.

Developed by Kenneth R. Ludwig over a period of two decades, `Isoplot` is a user-friendly toolbox that allows geologists to calculate and visualise geochronological data within a familiar spreadsheet environment ludwig1988, ludwig1999, ludwig2003, ludwig2012. Few computer programs have been as widely used in the Earth Sciences as `Isoplot`. Written in Visual Basic for Applications (`VBA`), `Isoplot` takes isotopic data as input and produces publication-ready figures as output. Unfortunately, recent versions of `Excel` are incompatible with `Isoplot`, whose creator has retired and no longer maintains the code. These software issues are a major problem for the field of radiometric geochronology, to the point where some laboratories keep an old `Windows XP` computer with `Excel 2003` around for the sole purpose of running `Isoplot`.

`IsoplotR` is a free, open and more future proof alternative for `Isoplot` vermeesch2018c. `IsoplotR`'s software architecture uses a modular design with future proofness and extendability in mind. Chapter **??** introduces the important subject of error correlations, an shows how these are captured by `IsoplotR`'s different input formats. We will see that error correlations plays a fundamental role in all of `IsoplotR`'s methods.

Section **??** reviews the subject of linear regression, which underpins the construction of isochrons. `IsoplotR` currently implements three different types of error weighted linear regression algorithms that account for error correlations between variables and between aliquots in two or three dimensions. Chapter **??**

explains how these three methods represent different approaches of dealing with overdispersion. Chapter ?? introduces a weighted mean plot to visualise multiple age estimates and proposes a heuristic method to detect outliers. Chapter ?? presents three approaches to construct confidence intervals for isochron ages, weighted means and so forth. It introduces a profile log-likelihood method for the calculation of asymmetric confidence intervals.

Chapter ?? discusses three further methods to visualise multi-aliquot collections of ages. Cumulative age distributions (CADs) and kernel density estimates (KDEs) show the frequency distribution of the age measurements but do not explicitly take into account the analytical uncertainties. The radial plot is introduced as a more appropriate data visualisation tool for 'heteroscedastic' data (i.e. data with unequal measurements uncertainties). The radial plot provides a good vehicle to assess the dispersion of multi-aliquot datasets. Overdispersed datasets require further processing with continuous or discrete mixture models that are discussed in Chapter ??.

With these basic statistical building blocks in place, the remainder of the notes cover issues that are specific to individual geochronometers and their geological applications. Chapter ?? provides specific details about the Rb–Sr, Sm–Nd, Lu–Hf, Re–Os and K–Ca, Ar–Ar, Th–Pb and Pb–Pb chronometers. Chapter ?? provides an in-depth discussion of `IsoplotR`'s U–Pb functionality. This includes an overview of the various input formats, concordia ages, discordia regression, common-Pb correction methods and initial disequilibrium corrections. Chapter ?? covers the subject of detrital U–Pb geochronology, which includes a discussion of discordance filters, maximum depositional age estimation and multidimensional scaling analysis. Chapter ?? covers U–Th dating and Chapter ?? thermochronology, including both the traditional external detector method and the new LA-ICP-MS based approach.

Finally, Section ?? sets out a roadmap for future developments to improve the accuracy and precision of geochronological data, and to provide closer integration of `IsoplotR` with earlier steps of the data processing chain.

2.1 Software architecture

There are three ways to use `IsoplotR`: online, offline and from the command line.

The online version[1] is convenient in several ways. First, it requires no software installation. Second, the `IsoplotR` website is perfectly platform-independent. It renders on any modern HTML-5 compatible web browser, including those installed on smartphones and tablet computers. Third, by using the online version, the user is guaranteed to have accessed the most up-to-date version of the

[1] `http://isoplotr.london-geochron.com/`

software.

An offline version of the GUI is provided for use on computers that are not (permanently) connected to the internet. This is often the case for machines that are connected to mass spectrometers, as a safety precaution. The offline version of the GUI works by emulating a web server within the default browser on the user's system. Installation instructions are provided on the `IsoplotR` website and on `GitHub`[2].

The third way to access the full functionality of `IsoplotR` is through the command line within the `R` programming environment. The command line offers the greatest flexibility to automate, modify and extend `IsoplotR`'s functionality.

The code base for the GUI and the core data processing algorithms are surgically separated. The command-line functionality is grouped in a lightweight package called `IsoplotR` that may be installed from CRAN as instructed in Section **??**. The `IsoplotR` package has minimal dependencies and should work on a basic `R` installation. In contrast, the GUI is written in `HTML` and `Javascript` and interacts with `IsoplotR` via an interface package. It is provided in a second `R` package called `IsoplotRgui` that is available from CRAN as well:

```
install.packages('IsoplotRgui')
```

`IsoplotRgui` is separate from but depends on `IsoplotR`. The clean separation between the two programs allows `IsoplotR` to remain light and easy to install. This is important for any future `R` packages that may wish to incorporate `IsoplotR` functions. `IsoplotR` and `IsoplotRgui` are free and open software. The computer code for both programs is made available under the GPL license, which permits re-use and modification provided that any derived code is released under the same conditions.

[2] `https://github.com/pvermees/IsoplotRgui/`

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