Temporal explosion: the need for new approaches in interpreting and managing geochronology data

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Abstract

Recent analytical improvements have provided a new wave of geochronology data, but developments in understanding of the analytical process and the application of statistically robust interpretative/visualisation tools have lagged. Some tools are emerging, but there is a strong need for further development. A fundamental concern is simply how to manage the volumes of data now being acquired. Work has begun on developing a standard for the exchange of geochronology data using XML technology within the framework of other standard developments in Australian geosciences. However, a caveat in both the development of tools and standards is that they must be usable and must be accompanied by sufficient education to enable regular use.

Keywords: geochronology, statistics, analytical tools, data management.

Introduction

Geology is a four dimensional science: When did this volcano last erupt? What is the rate of crustal uplift in this area? Are the deformation and mineralising events at gold prospect A the same age as at gold mine B? Does the age of these dune fields fit the known climate record?

Geochronology – the sub-discipline that measures the age of earth materials – provides the temporal framework in which other geoscience data can be interpreted in an evolutionary context. The integration of data across geoscience sub-disciplines is increasingly an important feature of geological research, thus it is important that the strategies and tools are available to make the most effective use of these data.

This paper will focus on the radiometric geochronology methods that provide absolute ages of earth materials using the radioactive decay of isotopes. Traditionally, radiometric geochronology involves a laboratory intense procedure known as Thermal Ionisation Mass Spectrometry (TIMS) that required the meticulous dissolution, separation and measurement of individual elements and/or isotopes from suitable minerals phases such as zircon, monazite, and biotite. A single analysis can take days from start to finish. The specialist facilities required and laborious process naturally limited the amounts of geochronological data that could be produced.

Like much of geoscience, geochronology has experienced a rapid evolution in analytical capability in the last decade and also faces a data explosion. The development of methods such as Secondary Ionisation Mass Spectrometry (SIMS) and Laser Ablation Inductive Coupled Plasma Mass Spectrometry (LA-ICPMS) that can measure isotopes from areas within individual mineral grains within minutes has created this wave of data. Many facilities have become geochronology production lines that have provided a wealth of new information, but the tools for data management and interpretation – and even the analytical approach – have not evolved as rapidly.

Analysis

A geochronology workflow will typically analyse several to hundreds of individual mineral grains depending on the aims of the project, the methods being applied and the type of equipment used. An individual analysis will measure a variety of isotopic ratios (e.g. lead and uranium) from which an age can be calculated. Depending on the method there can be considerable mathematical processing of the 'raw' data via a variety of regressions and statistical tests. The calculated age is typically in millions of years and is reported with an associated uncertainty based on uncertainties propagated from analytical counting statistics and calibrations. TIMS analyses are typically have much greater precision than SIMS or LA-ICPMS analyses. A determined age for a sample (e.g. the age of volcanic rock) is based on a statistical assessment of the analyses such as a weighted mean or a linear regression, and is reported as age ± uncertainty at 95% confidence. An illustration of this is provided in Figure 1.

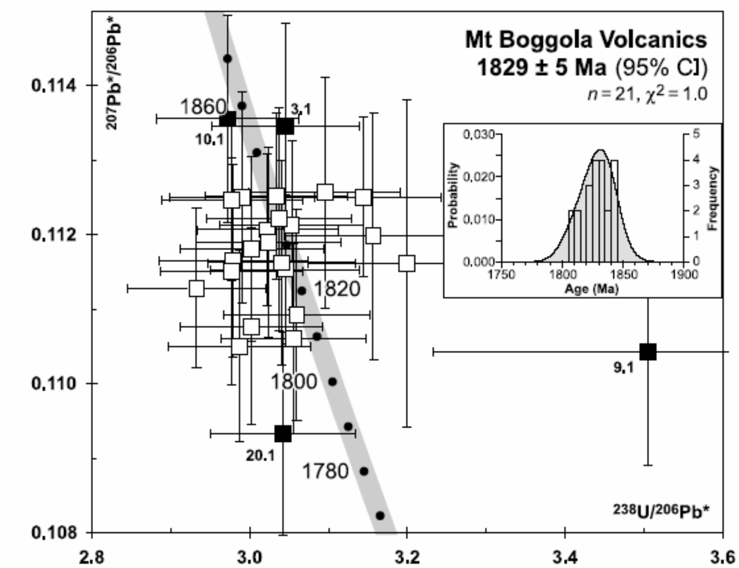

Figure 1. A typical illustration of geochronological data - in this case uranium-lead isotopic data acquired using a SIMS instrument. The main diagram illustrates the interaction of two isotopic systems while the inset diagram provides a univariate probability density distribution of the ages derived from the plotted data. The determined age of the sample, in this case a weighted mean of the all the analyses except those excluded for analytical and geological reasons (solid squares), is provided in the top right. (From Sircombe, 2003).

Geochronological analyses of single mineral grains can follow two strategies (Fedo et al., 2003). The first, qualitative analysis, involves the analyst specifically selecting grains on the basis of colour, morphology, internal compositional zoning or other properties. The purpose is to identify and date all components that make up the sample, for instance a small proportion of grains with convolute internal zoning may be a different age to the majority of grains with internal oscillatory zoning. This strategy is principally employed to date material where a relatively single age or a simple collection of ages are expected such as in igneous or some metamorphic rocks.

The second strategy is quantitative analysis which involves analysing a random selection of grains from the sample. The aim is to sample an accurate representation of the total population. This strategy is principally employed to date detrital material from sedimentary rocks where a mixture of ages can be expected and the proportions of various components themselves provide information.

In quantitative analyses statistical concerns become paramount. How many analyses are enough to be sure that the ages are an accurate representation of the total population? This question was originally approached by Dodson et al (1988) which calculated a “magic” number of ~60 as producing a sample where there was a less than 5% probability that a component compromising 1 in 20 of the total would be missed. These calculations have recently been revived by Vermeesch (2004) and Andersen (2005), to much produce much larger values for statistical adequacy (typically 100+). However, a truly rigourous adequate sample size may need to be judged on the heterogeneity of the population and further work is required.

Often the purpose of analysing sedimentary rocks using a quantitative approach is to gain an idea of the age of the deposition. To this end, the youngest age in a suite of analysed grains is often treated as the proxy for the maximum of deposition for that sedimentary rock. These types of analyses have become vital in broad homogeneous sedimentary sequences where there is little other suitable material to date. However, these data sets frequently provide mathematical conundrums on how to define the youngest age in the data. Is it the solitary analysis that in a strict statistical sense is an outlier? Is it the weighted mean of the youngest *n* grains that can provide a statistically valid grouping? Can it be calculated via deconvolution methods (e.g. Sambridge and Compston, 1994)? Again further work is required to develop a statistically rigourous and practically acceptable method.

Interpretation and visualisation

In geologically simple samples, such as a single phase igneous rock with no isotopic inheritance from older rocks, interpretation and comparison of geochronology data can be equally simple. Determined ages for samples are calculated from the analyses and can be compared using t-tests. However, the large volumes of data produced by quantitative style analyses often pose interpretative problems, particularly if they are complex, heterogeneous samples. The problem can be further compounded when attempting to compare results produced by different methods that can have widely ranging individual analytical precisions and methods for illustrating the data. The description below will focus on the display of univariate age data in probability density distributions, although there are also recent efforts to develop tools that enable visualisation to provide more ‘multi-dimensional’ information from the original data.

The traditional approach has been to simply eye-ball plots of the data to ‘see’ if there were common components or patterns in the age distributions between samples (e.g. the left-hand column of Figure 2). While this is a practical first-pass approach, it is obviously subjective and quickly become impractical beyond a few samples (some studies such as regional synthesis projects can potentially have hundreds of samples to compare). Attempts have been made to develop statistical methods for comparing and contrasting these distributions (Sircombe, 2000; Berry et al., 2001) and the most recent approach is to use kernel functional estimation (Sircombe and Hazelton, 2004).

These developments are still in their emergent phase and considerable testing and refinement of mathematical techniques are required. However, a crucial element of any such development is not mathematical, but psychological. Many geological practitioners are uncomfortable with mathematics and are particularly discouraged by complex processes with cumbersome interfaces. In such an environment an otherwise perfectly robust and valuable process can simply sink from the collective scientific consciousness if it, or rather its authors, do not provide sufficient usability and user education.

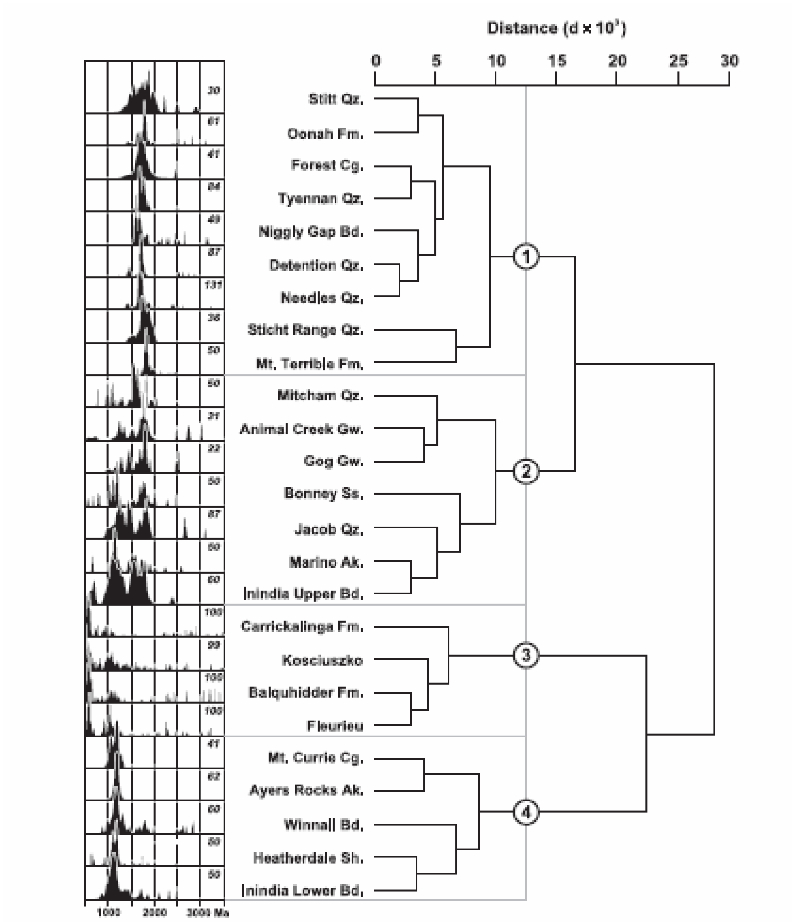

Figure 2. Illustration of statistical comparison techniques being applied in the interpretation of large sets of geochronological data. This case involves 25 sets of quantitative data from sedimentary rocks across central, southeast Australia and Tasmania. A more traditional approach would have been simply to eye-ball the probability density distributions illustrated in the left-hand column. (From Sircombe and Hazelton, 2004).

Data management

The explosion of geochronology data has created data management issues because it has highlighted the lack of adequate standards in managing and exchanging data at all phases from acquisition to end-user. These issues are not unique to geochronology, but form part of the greater challenge of developing the technology, user processes and culture that will enable the full potential of interoperable scientific research networks to be realised. The impetus for the development of these networks within Australian geoscience is enormous as many of the major questions now facing academic, government and industry geoscientists can only be answered via the efficient and effective integration of data across many disciplines. The development of these systems has been highlighted as being of national importance (Department of Industry, Tourism and Resources, 2004; Department of Education, Science and Training, 2005).

As a contribution to the broader efforts, Geoscience Australia has initiated a project to develop a standard data format for the exchange of geochronology data based on XML (eXtensible Markup Language) technology and strongly linked to other related developments in geosciences (e.g. XMML, eXploration & Mining Markup Language, https://www.seegrid.csiro.au/twiki/bin/view/Xmml/WebHome) and similar international efforts related to the management and usage of spatial information. This project is currently in the early phases of development and is concentrated on gathering user requirements in order to begin the development of data models. Feedback from geochronology specialists to basic users is sought in order to ensure that the user requirements are robust and widely applicable. Given the wide variety of geochronology methods and usages available developing the data models to express the relationships among the required data fields will be a complex task and any contributors will be welcome.

The ultimate aim of the project is to ensure that users of geochronological data within Australia can quickly find the data they require via an Internet portal and download it in such a format that they – or their application – can readily translate the information and make effective use of it. Again, there is a strong need to note that simply providing the technology is often not enough. Systems must have a high usability and be accompanied by sufficient education and motivation to encourage regular use beyond a small huddle of specialists.

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