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Episodic zircon age spectra of orogenic granitoids: The supercontinent connection and continental growth

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ABSTRACT

To identify age peaks and other features in an isotopic age distribution, it is common to perform a kernel density estimation or similar analysis. A key aspect of this estimation process is the choice of an age resolution bandwidth that best reflects the random variable and other assumptions on the data. Probabilistic kernel density analysis of large databases (up to nearly 40,000 samples) of U/Pb zircon ages suggests an optimum bandwidth of 25–30 My for many key features, which yields approximately 40 peaks with confidence levels of $c \geq 0.9$. Because of natural redistribution processes, geographic sample bias may be minimized by jointly analyzing isotopic ages from both orogenic granitoids and from detrital zircons. We show that the relative heights of age peaks are commonly controlled by the local geographic distribution of samples and are not necessarily correlated with total geographic extent. Eight peaks with $c \geq 0.9$ occur on five or more cratons or orogens (at 750, 850, 1760, 1870, 2100, 2650, 2700, and 2930 Ma). Results suggest that orogenic plutonism age peaks principally reflect subduction system episodicity on local or regional scales, but not on continental or supercontinental scales. In contrast, peak clusters that are jointly defined by granitoid and detrital ages may be more representative of the general age distribution of the continental crustal record.

Five major peak clusters are closely tied to supercontinent formation at 2700, 1870, 1000, 600, and 300 Ma and minima in age spectra correspond to supercontinent stasis or breakup (2200–2100, 1300–1200, 750–650, and ≤200 Ma). Age clusters also show a decrease in cycle duration beginning at 1000 Ma. A new histogram of continental preservation rate shows that approximately one-third of the extant continental crust formed during the Archean, about 20% during the Paleoproterozoic, and only 14% during the last 400 My. Peak clusters are probably related chiefly to preservation of juvenile crust in orogens during supercontinent assembly, although locally, continental crustal production rate may be enhanced during actual collisions.

1. Introduction

The episodic nature of terrestrial magmatism is widely recognized, but only in the last few years has it been well documented by high-precision U/Pb and Hf isotopic studies of zircons (Rino et al., 2008; Pietranik et al., 2008; Condie et al., 2009a; Wang et al., 2009a,b; Yang et al., 2009). Yet we still face two major interpretive problems: robust statistical estimation and identification of age peaks and troughs, and the geographic extent of peaks and troughs. Published age spectra commonly use histograms or density probability estimates. In such analyses, the age bandwidth used in smoothing data controls the tradeoff between resolution and statistical robustness of spectral features. Age peaks occurring on several different continents are often interpreted as global events, yet the term "global" is ambiguous because of sampling and preservation biases. For rocks older than 100 Ma almost all age data come from the continents, yet continents have never covered the complete surface of the Earth. For this reason, we avoid the term "global" for the ages of continental magmatism, and refer to geographic distributions as local, regional, or widespread on the continents based on the best presently available data.

Here, we analyze a large database of concordant and near-concordant U/Pb zircon ages (8928 igneous and 28,027 detrital ages) using combined Monte Carlo simulations and kernel density analysis with varying bandwidths to explore the optimal resolution and statistical inferences permitted by the data (e.g., Rudge, 2008). A summary of the U/Pb ages is given in Appendix 1. The age database of single zircon ages with uncertainties (with minor updates for this paper) is given in Condie et al. (2009a), and the ε_{Nd}(T) data for whole rocks from which the zircon ages were determined are given in Condie et al. (2009b). Although most of the igneous data are high-precision TIMS (thermal ionization mass spectrometry) results, most of the detrital ages are from lower precision SHRIMP (sensitive high-resolution ion microprobe) and LAM ICP-MS (laser

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ablation microprobe inductively coupled plasma mass spectrometry). From these results, we discuss the identification of age peaks and age peak clusters, possible geographic biases, and the significance of U/Pb age distributions in terms of the supercontinent cycle. This paper expands on Condie et al. (2009a,b) in that it introduces a new statistical method to identify meaningful age peaks, discusses the interpretation of age peaks and age peak clusters, presents revised peak clusters based on a greater number of ages and new statistical analysis of data, discusses both granitoid and detrital ages (from both modern and ancient sediments) in terms of the supercontinent cycle, and presents a new comprehensive estimate for the preservation rate of continental crust with time.

2. Monte Carlo kernel density estimation

Estimating probability density from sample data is a fundamental problem in many fields that has been approached with a variety of methods (e.g., Silverman, 1986; Brandon, 1996; Chaudhuri and Marron, 1999, 2000; McLachlan and Peel, 2000; Rudge, 2008). The basic challenge is to estimate the unknown probability density of a random variable (here, the probability of occurrence for an isotopic date of a particular age range) given a finite sample (a finite set of realizations of the random variable). This estimation process is subject to data errors and commonly unknown sampling biases. Here, age errors in the samples reflect uncertainties in individual U/Pb ages arising from measurement uncertainties (e.g., Chang et al., 2006), and the sampling bias reflects non-uniform geological exposure, preservation, and collection. An additional source of uncertainly can arise from sparse sampling in particular data sets or within particular age ranges. Once a density function is estimated, it is important to assess its characteristics in a statistically meaningful way, which is sometimes referred to as the problem of feature significance (Rudge, 2008). Key features in the context of age studies are the time localization, significance, and precise location of peaks and troughs in age spectra.

A key parameter in any distribution estimation is the bandwidth, which is the width of time averaging in the estimation algorithm (Silverman, 1986). A short bandwidth will typically produce numerous low-confidence peaks (i.e., the estimate is under-smoothed), while a long bandwidth will not resolve shorter time features that may be significant (i.e., the estimate is over-smoothed). In this sense, the bandwidth choice and the methodology of implementation can be generally viewed as a regularization process applied to the inverse problem of estimating a density function from sample data (e.g., Aster et al., 2004). In its most basic implementation, kernel analysis estimates are obtained by convolving the age sample distribution, parameterized as a superposition of delta functions, with a kernel function (chosen to be Gaussian). The use of delta functions for characterizing sample age determinations is appropriate if individual age errors are small relative to width of this convolving kernel. The bandwidth of the estimate in this case can be generically specified in terms of the standard deviation for the normal convolving kernel.

Because the bandwidth is typically an ad hoc parameter that is difficult to constrain in advance, a reasonable way to explore regularization tradeoffs is to estimate the unknown distribution using a range of convolving kernel bandwidths and assess feature significance as a function of bandwidth. One example of this general approach is the SiZer (Significant Zero crossings of the derivative) method of Chaudhuri and Marron (1999), which approximates slopes in distribution estimates evaluated for a range of bandwidths to determine significant peaks. Alternatively, optimal bandwidths may be estimated from the data for specific (e.g., Gaussian) kernel types (e.g., Brandon, 1996). In this study we evaluate estimates calculated by the convolution approach for Gaussian kernels corresponding across a scale range of (3σ) bandwidths, w (i.e., the $\pm 1\sigma$ width of the applied Gaussian function is $2w/3$).

Individual sample age errors from isotopic datasets are not necessarily small relative to kernel bandwidths of interest (the mean age error standard deviation for the complete dataset examined here is 18.7 My). We thus incorporate the effect of data and errors into our probability density estimates using a Monte Carlo approach, where each U/Pb age in an n-sample data set is modeled as a statistically independent normally distributed random variable specified by its age estimate and standard deviation. This approach age-widens the influence of each sample into a standard deviation-consistent Gaussian function.

To incorporate Monte Carlo methods into the probability density analysis, we generate M independent realizations of the data set by selecting n individual sample age estimates from the dataset, choosing M to be a large enough number (e.g., 1000) to adequately characterize the associated statistical variation in the kernel density estimate of the probably density for the dataset. During this realization process, we bootstrap resample the data (with replacement) using a random index drawn from an independent uniform distribution to incorporate the influence of finite sampling. This random index approach has a negligible effect on densely sampled age regions, but will decrease the certainty of features associated with small numbers of samples in isolated age regions. As an end-member example, this reduces the effect of a single age-isolated sample from producing a significant peak.

Performing this procedure for a range of kernel bandwidth (i.e., applying multi-scale analysis) we produce a bandwidth-dependent suite of probabilistic kernel density function estimates, with mean and standard deviation envelopes calculated from the underlying M realizations. These realizations reflect the uncertainties of the constituent age data, small sampling effects, and the smoothing effects of the particular Gaussian convolving kernel.

A more general feature of these bootstrapped Monte Carlo probability density function estimates is that probabilistic assessments of feature significance, such as the time localization and significance of peaks, can also be readily estimated from the population of M realizations. For example, given a kernel bandwidth w, the probability of a peak occurring within a particular time interval (as defined by its estimated value being significantly above those of adjoining time intervals within a time region of width w) can be assessed from the M-normalized proportion of times that the count within that region exceeds that of its neighbors. In this evaluation, we utilize a peak detection algorithm successively applied to each of the M realizations. We use the Matlab *findpeaks* function, which is summarized in Appendix 2 with an example. This procedure produces a statistical confidence measure for the reliability of a peak as a function of bandwidth that is consistent with the statistical data assumptions that the individual sample dates are normally distributed and independent. This peak detection algorithm has the desirable feature that it provides a local feature significance measure that is unaffected by sample density variations with age across large data sets. Error bars on peak time estimates determined by this method are estimated by least-squares fitting of a Gaussian function to the kernel-smoothed peak detection region and evaluating its standard deviation.

Multi-scale kernel density analysis of the complete zircon database (37,830 samples) discussed in this paper is shown in Fig. 1 for 3σ Gaussian kernel widths between 1 and 100 My. Fig. 1a shows Monte Carlo bootstrapped estimates of sample counts (log color scale) as a function of Gaussian kernel bandwidth (w). The general trend, not surprisingly, is for numerous short-time-scale features to be resolved at small w and for a few long-time-scale features to be resolved at large w. Fig. 1b shows peak detection confidence results, similarly plotted. Three representative age spectra (w = 10, 30 and 90 My) are shown in Fig. 2.