Deciphering a Multipeak Event in a Noncomplex Set of Detrital Zircon U–Pb Ages

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Abstract The determination of U–Pb ages from detrital zircons of sedimentary rocks using LA–ICP–MS has been widely used to develop studies of provenance analysis. A problem that frequently arises is to find a population that appears to be noncomplex despite several perceptible age peaks in their spectrum. These peaks are qualitatively defined through diagrams of relative probability (probability density function or PDF), but it is difficult to quantify their statistical significance relative to a zircon-forming multipeak event. Therefore, the question arises as to whether we can decipher and characterize a multipeak event in a noncomplex set of detrital zircon U–Pb ages. This work is an attempt to answer the above question by means of a statistical analysis. The objectives are: (1) to determine the most appropriate minimum number of zircon age populations (peaks); (2) to characterize each peak in terms of age and event duration; and (3) to compare results obtained for two datasets showing similar zircon ages. The process starts by using a cluster analysis to group zircon ages into a set of consistent clusters. A Gaussian kernel function is then fitted to each cluster and summed to obtain a theoretical PDF. At the end of the process, the best modelled PDF must coincide with the original PDF at $\geq$95 %, and the deciphered peaks can then be characterized.

Keywords Detrital zircon data · Population · Peaks · Comparisons of datasets · Gaussian kernel function

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Data

The geochronological data set selected to develop this statistical study covers two samples of greywacke from Early Carboniferous basins of southwestern Iberia recently published by Pereira et al. (2012). From the Cabrela and Mértola greywackes, 44 and 94 detrital zircon grains, respectively, were dated using U–Pb LA–ICP–MS. Cathodoluminescence images obtained from all analysed grains show that the detrital zircons are mostly simple and of magmatic origin (Pereira et al. 2012). The most salient feature of these samples is the scarcity of older zircons differing from the age spectra of detrital zircons of the oldest strata (Upper Devonian) of the South Portuguese Zone with abundant Cambrian and Neoproterozoic ages.

Problem

A global probability density function (***g***PDF) enclosing a unity area (thick line in Fig. 1) was built from the Cabrela data after summing the n = 44 zircon age U–Pb Gaussian kernel functions Kf_i (i = 1, …, n), that is,

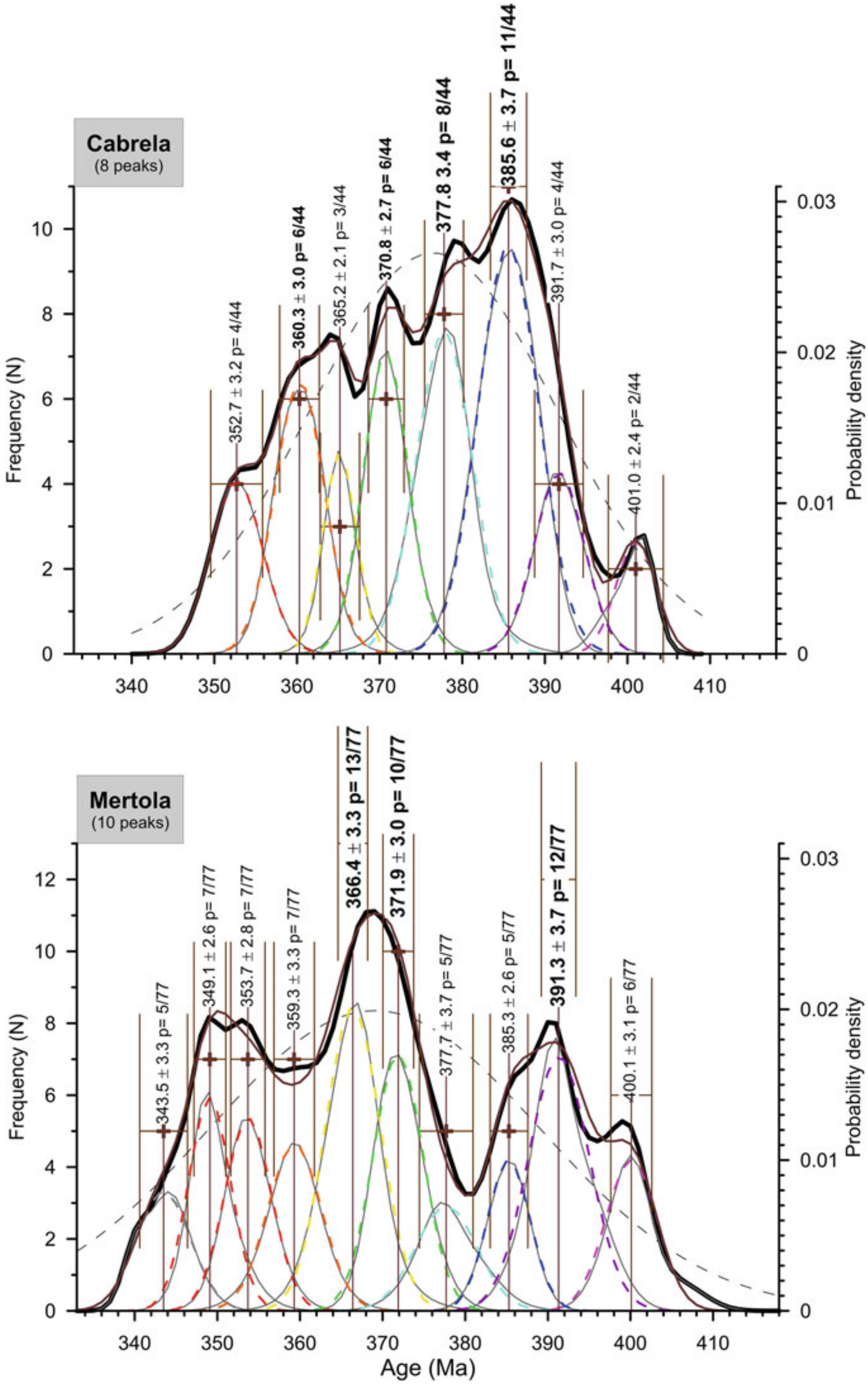
$$gPDF = \frac{1}{44}\sum_{i=1}^{n=44} Kf_i.$$

Each Kf_i was computed by introducing the respective age (***a***) and standard deviation (***s***) in the Gaussian kernel equation

$$Kf_i = \frac{1}{s_i\sqrt{2\pi}} e^{\left[-\frac{(x-a_i)^2}{2s_i^2}\right]},$$

adapted from Silverman (1986). An age (***x*** values) step (standard increment) of 1 Ma together with a time range from 340 to 409 Ma was used. The chosen range encloses the minimum ($\boldsymbol{a}_i - 4{*}\boldsymbol{s}_i$) and the maximum ($\boldsymbol{a}_i + 4{*}\boldsymbol{s}_i$) found in the dataset, while the chosen step is recommended (Sircombe 2004) because geochronological results are typically reported in rounded Ma values. Also, using the step of 1 is very practical since the PDF value computed for each ***x*** directly gives the area beneath.

From the Cabrela ***g***PDF, a set of ***m*** minor peak events (zircon age populations) is apparent. Our purpose is to decipher them and to statistically validate and characterize them using the age and duration. The procedure used is based on a statistical analysis performed on the ***n*** = 44 $\boldsymbol{Kf_i}$, aiming to answer the following questions:


Cabrela
(8 peaks)
352.7 ± 3.2 p= 4/44
360.3 ± 3.0 p= 6/44
365.2 ± 2.1 p= 3/44
370.8 ± 2.7 p= 6/44
377.8 3.4 p= 8/44
385.6 ± 3.7 p= 11/44
391.7 ± 3.0 p= 4/44
401.0 ± 2.4 p= 2/44
Frequency (N)
Probability density
Mertola
(10 peaks)
343.5 ± 3.3 p= 5/77
349.1 ± 2.6 p= 7/77
353.7 ± 2.8 p= 7/77
359.3 ± 3.3 p= 7/77
366.4 ± 3.3 p= 13/77
371.9 ± 3.0 p= 10/77
377.7 ± 3.7 p= 5/77
385.3 ± 2.6 p= 5/77
391.3 ± 3.7 p= 12/77
400.1 ± 3.1 p= 6/77
Frequency (N)
Probability density
Age (Ma)

◀ **Fig. 1** Global probability density function (gPDF: *thick black line*) for Cabrela (*top*) and Mértola (*bottom*). Peaks (*coloured dashed lines*) were deciphered from the Cabrela (*top*) and Mértola (*bottom*) datasets after determination of the best minimum number of peaks. Colours are used to highlight the comparison between the two sets

(1) How many (***m***) peaks (zircon age populations, ***j***) can be deciphered from the global PDF?
(2) In a set of ***m*** (***j*** = 1,…, m) peaks, how can we decide to which ***j*** each Kf_i (individual zircon spot) most likely "belongs"? Or, how can we separate the available ***n*** Kf_i into a set of ***m*** coherent groups (zircon age populations)?
(3) How can we trust and check the results obtained?

A set of six or seven peaks can be observed in the gPDF (thick line in Fig. 1), but any number chosen by simple visual inspection is subjective and may lead to misleading results. Assuming that a major geological event (a noncomplex gPDF) can be subdivided into a set of ***m*** bell-shaped, minor geological events ***j***, a theoretical PDF with ***m*** zircon age populations can be built after adjusting a kernel function p_jKf_j to a group n_j of Kf_i endorsed to a certain theoretical peak ***j***, followed by the sum of all p_jKf_j (j = 1, 2, …, ***m*** and $p_j = n_j/n$). As limiting examples, a theoretical PDF with the lowest possible number of peaks ***m*** = ***j*** = 1 can be built (dashed grey line in Fig. 1), whereas the highest possible number of peaks ***m*** = 44 is the ***g***PDF itself. For all the other possible cases (***m*** = 2, 3, …, 43), some Kf_i must be grouped, posing the problem of choosing the way to join them. Assuming that each Kf_i is related to only one ***j*** of the ***m*** "hidden" peaks of the ***g***PDF, we need to determine to which peak ***j*** each Kf_i most likely belongs.

Methodology

A cluster analysis was computed with the 44 Kf_i of the Cabrela dataset (44 variables and 70 cases). The cluster analysis was performed to separate the 44 Kf_i into ***m*** (1, …, ***j***, …, ***m***) coherent clusters.

A phenon line was drawn in the tree diagram slightly above the merging cost necessary to merge the 44 $\boldsymbol{Kf_i}$ into ***m*** (1 to 12) clusters. For a certain level of merging cost, a unique number ***m*** of clusters ***j*** is obtained and each $\boldsymbol{Kf_i}$ is assigned to a unique cluster ***j***. This allows its partial PDF to be built, followed by the respective age ***a*** and standard deviation ***s***. Finally, a theoretical PDF_m can be obtained by summing the ***m*** adjusted p_jKf_j.

To check the results, the misfit area between PDF_m and gPDF is computed. This allows finding the best minimum number of clusters set as the lowest number of ***m*** for which the PDF_m reaches a certain level of proximity (95 %) to the ***g***PDF.

Results

For the Cabrela dataset, the best minimum number of peaks deciphered is 8 (Fig. 1 (top), together with PDF_8 (brown thick line)). This was obtained after results for Pearson r and area misfit between gPDF and $PDF_{\boldsymbol{m}}$ dropped to values of $\leq$0.995 and $\leq$5 %, respectively. Also, no superposition is observed for the 95 % confidence interval (1.96*standard error of $\boldsymbol{a}$) of the eight $p_j Kf_j$ curves (Fig. 1).

Cabrela Versus Mértola Formations

A similar procedure was performed for the Mértola dataset (77 Kf_i). The time range is 333–418 Ma. The best minimum $\boldsymbol{m}$ achieved is 10 (Fig. 1 (bottom)).

Each one of the 8 peaks of Cabrela coincides with one of the 10 peaks from Mértola (Fig. 1). The age difference varies from 0.1 to 1.2 Ma, which is inside the estimated standard deviation (minimum standard deviation = 2.1 Ma for the third peak of Cabrela) of any peak computed.

Conclusions

The curves highlight that both greywackes result from the dismantling of magmatic sources, which reproduce a long period of active magmatism ranging from ca. 400–340 Ma. Part of this time spectrum coincides with the ages obtained for the magmatism of the South Portuguese Zone (Rosa et al. 2009: Cercal ca. 369–374 Ma, Azinheira dos Barros ca. 362 Ma, Aljustrel ca. 354–357 Ma, Serra Branca ca. 357–355 Ma, Chança, 354–349 Ma). However, both curves reflect the influence of a 380–390–400 Ma magmatism, which so far has not been identified in the South Portuguese Zone or in the Ossa–Morena Zone, which was interpreted by Pereira et al. (2012) as representative of missing Rheic Ocean magmatic arcs.

The multiple discriminated peaks repeat in both samples, but the two youngest peaks of Mértola of age <350 Ma have no corresponding peaks in Cabrela, suggesting that the production of zircons supplied to the Cabrela Basin stopped some 9 Myr before those supplied to Mértola. These results can also be used to achieve the maximum depositional age (352.7 ± 3.2 Ma with p = 4/44 for Cabrela and 343.5 ± 3.3 Ma with p = 5/77 for Mértola).

The age interchange of the major peaks observed in both datasets (Mértola 391.3 Ma—Cabrela 385.6—Mértola 366.4—Cabrela 360.3—Mértola 349.1) suggests some type of cyclic palaeogeographical change.

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