Guide to inferring Probability Model Ensembles (PMEs) for detrital zircon data and calculating Bayesian Population Correlation (BPC)

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1. Included files

First, download all the files by clicking 'Clone or Download' > 'Download ZIP' on Github. Then unzip the resulting folder. Included in this package are scripts necessary in order to infer PMEs, display calculated BPC values, display PME plots, and infer the shared proportions of two samples based on BPC values. In addition to being presented in their original form as MATLAB scripts, these files have been compiled into a standalone application. Installers for the application for Windows and Mac are also included. The main folder, which contains this document, contains a main menu .m file and accompanying .fig file:

'BPCmainmenu.m' – MATLAB script of the main menu for PME inference and BPC calculations, through which all included functionality can be accessed.

'BPCmainmenu.fig' – MATLAB file that contains information about the graphical user interface (GUI) for the main menu script.

The following subdirectories are also contained in this package:

'backend/' – contains scripts the user does not need to access directly. This folder also contains two third-party scripts, which are noted in the Dependencies section, below.

'sample_data/' – includes a set of sample data with which the scripts can be tested (see section Workflow, below).

The installers for the standalone applications (useful if the user lacks MATLAB or one of the required toolboxes—see Dependencies section below) are:

'BPCinstallerWin_web.exe' – this is the installer for Windows

'BPCinstallerMac_web.zip' – this is the installer for Mac, and must be manually unzipped before use

Note that these installers require an Internet connection and were compiled using the MATLAB and operating system versions listed in the Tested Hardware section below.

The package also contains a text readme file, a text license file for the set of scripts (excluding those that we did not author, which fall under pre-existing licenses included with the scripts), and this introductory document.

2. Installation versus execution from MATLAB

If the user lacks the required versions of MATLAB and the toolboxes used by the BPC scripts (see Dependencies section), then the BPC scripts can be installed as a standalone application. This requires running one of the two installers (*'BPCinstallerWin_web.exe'* for Windows machines, *'BPCinstallerMac_web.zip'* for Mac, which must be unzipped first) and clicking through the on-screen instructions. Note that *'BPCinstallerMac_web.zip'* must be unzipped manually before installation. Unzipping the file should produce a file called *'BPCinstallerMac_web.app'*, which will install the application if you double click on it. The installers were created using a built in function in MATLAB, and were compiled using the MATLAB and OS versions listed under the Tested Hardware section. An Internet connection is required for this installation because the installer downloads and installs the MATLAB runtime environment. Note that these standalone applications operate independently of the .m files contained in this package, and the directory into which you install the application shouldn't affect its functionality. The sample data that we use in the example Workflow section below will not be installed using the installer. In order to work with this data, the user must make sure to download it in addition to the installer. The BPC application will prompt the user for the location of the data they wish to model, at which time, the user can refer the application to the sample data. Finally, we have observed the Mac error sound (a short "bonk") while the script is running, and do not understand why this is happening, but it appears not to affect the result.

Note that if you run the standalone application instead of the MATLAB files, there will likely be times when you start the application or issue a command and the application appears not to do anything for several seconds. After a short delay, you should see that your command has been carried out. Please only click buttons once on the GUI and then wait for the function to execute.

On windows machines, the parallel computing performed by the scripts may cause the objection of Windows firewall. On Mac machines, note that the actual application file will be located at '*installed_directory*/application/BPC', where '*installed_directory'* is specified by the user during installation.

3. Dependencies

Note: Dependencies were assessed using the MATLAB function matlab.codetools.requiredFilesAndProducts. The user can check which toolboxes they have installed in MATLAB by typing 'ver' into the command window.

The BPC scripts require the following MATLAB toolboxes (versions shown in parentheses):

MATLAB (9.3)
Optimization Toolbox (8.0)
Statistics and Machine Learning Toolbox (11.2)
Curve Fitting Toolbox (3.5.6)
Parallel Computing Toolbox (6.11)
Global Optimization Toolbox(3.4.3)

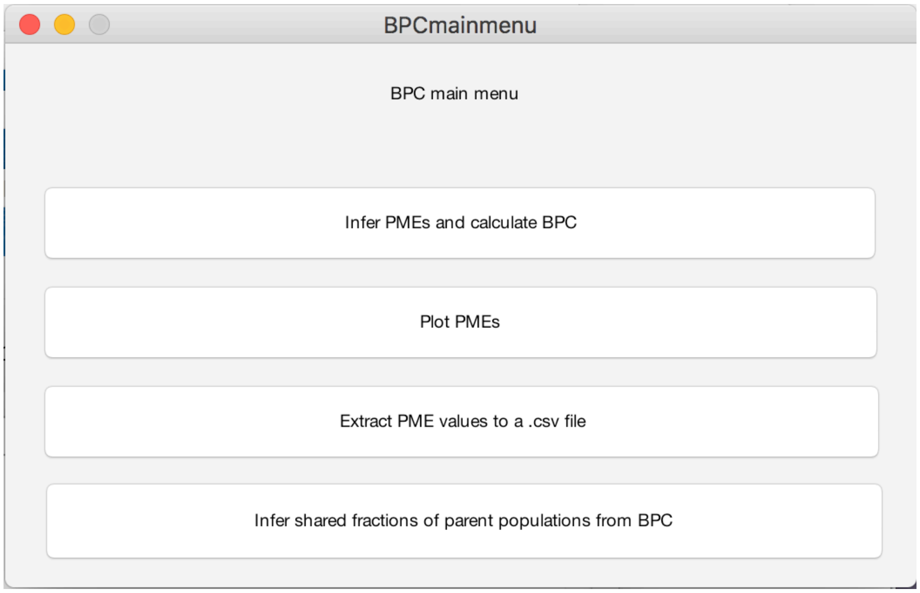
Two additional third-party scripts are required for our collection of scripts to function:

nearestSPD.m, which is copyright (c) 2013, John D'Errico, and is provided according to the license text contained in "nearestSPD_license.txt", distributed with our collection of scripts.

parfor_progressbar.m, which is copyright (c) 2016, Daniel Terry, and is provided according to the license text contained in "parfor_progressbar_license.txt".

4. Workflow

The first step of the workflow is to start the standalone application, or run the *'BPCmainmenu_GUI.m'* script from MATLAB (ensuring that your MATLAB installation meets the version and toolbox requirements shown in the Dependencies section below). Upon doing so, you should see a simple window with buttons:

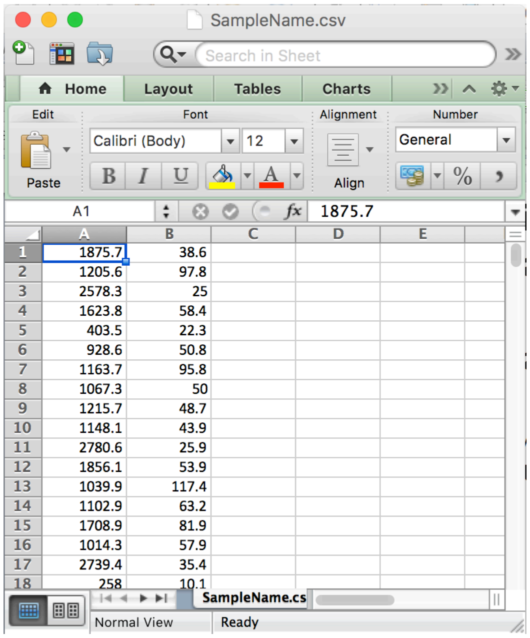

BPCmainmenu
BPC main menu
Infer PMEs and calculate BPC
Plot PMEs
Extract PME values to a .csv file
Infer shared fractions of parent populations from BPC

These four buttons allow access to the major functions included in this package by clicking the respective button. The remainder of this workflow includes 4 parts: A, B, C, and D, which correspond with the four buttons. Part A shows how to infer PMEs and calculate BPC. Part B shows how to plot PMEs. Part C shows how to extract probability values from the PMEs to a .csv file. Part D shows how to infer the shared proportions of two zircon age populations from their BPC value.

Note: For this demonstration, we run our collection of scripts on the 4 random subsamples (from data of Pullen et al., 2014, and Thomson et al., 2017), included with the scripts in the folder 'sample_data/'. Of these four random subsamples, two each are selected from the datasets of Pullen et al. (2014) and Thomson et al. (2017), and two of the samples consist of 60 grain ages each whereas the other two samples consist of 300 grain ages. The filenames indicate which subsamples are which. If the scripts are run on these data, the results should resemble those found in this document.

A. Infer Probability Model Ensembles (PMEs), estimate BPC uncertainties, and display BPC values using BPConeclick_GUI.m.

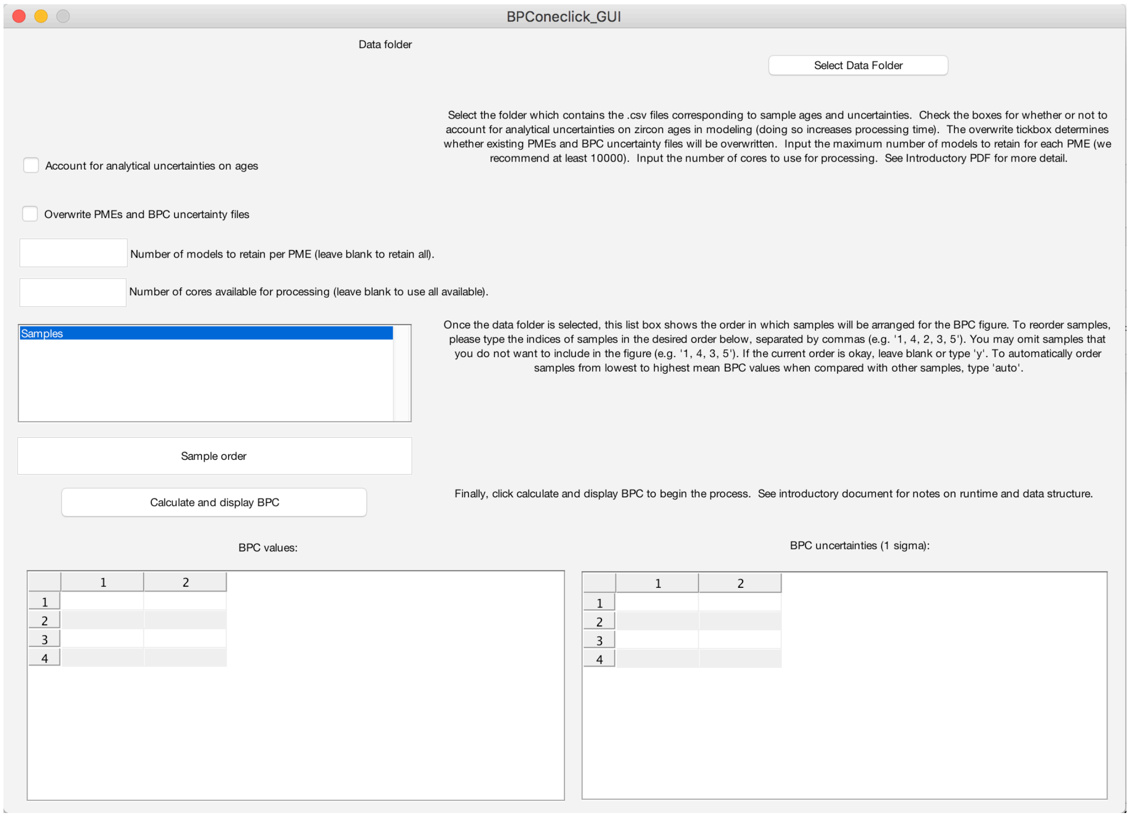
For the samples you want to model, save the best ages of these samples, along with analytical uncertainties (1σ), in two-column .csv files, as follows:



	A	B	C	D	E
1	1875.7	38.6			
2	1205.6	97.8			
3	2578.3	25			
4	1623.8	58.4			
5	403.5	22.3			
6	928.6	50.8			
7	1163.7	95.8			
8	1067.3	50			
9	1215.7	48.7			
10	1148.1	43.9			
11	2780.6	25.9			
12	1856.1	53.9			
13	1039.9	117.4			
14	1102.9	63.2			
15	1708.9	81.9			
16	1014.3	57.9			
17	2739.4	35.4			
18	258	10.1			

The first column is the preferred measured age for each analysis in millions of years and the second column is the 1σ analytical uncertainty calculated for the preferred measured age, also in millions of years.

Ensure that the .csv files corresponding to all desired samples are located in a single folder, with no other .csv files. We suggest creating a new folder. Click the *"Infer PMEs and display BPC"* button from the main menu. You should see the following window appear:



Select the folder which contains the .csv files corresponding to sample ages and uncertainties. Check the boxes for whether or not to account for analytical uncertainties on zircon ages in modeling (doing so increases processing time). The overwrite tickbox determines whether existing PMEs and BPC uncertainty files will be overwritten. Input the maximum number of models to retain for each PME (we recommend at least 10000). Input the number of cores to use for processing. See Introductory PDF for more detail.

□ Account for analytical uncertainties on ages

□ Overwrite PMEs and BPC uncertainty files

Number of models to retain per PME (leave blank to retain all).

Number of cores available for processing (leave blank to use all available).

Once the data folder is selected, this list box shows the order in which samples will be arranged for the BPC figure. To reorder samples, please type the indices of samples in the desired order below, separated by commas (e.g. '1, 4, 2, 3, 5'). You may omit samples that you do not want to include in the figure (e.g. '1, 4, 3, 5'). If the current order is okay, leave blank or type 'y'. To automatically order samples from lowest to highest mean BPC values when compared with other samples, type 'auto'.

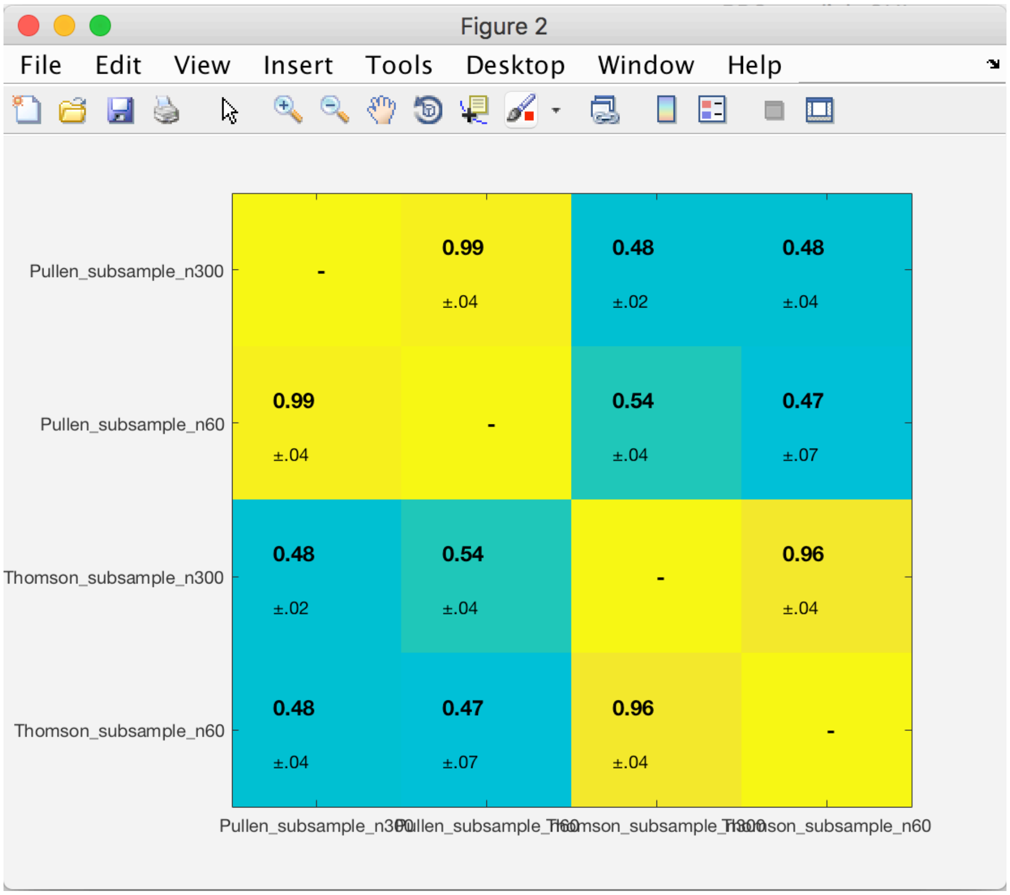
Finally, click calculate and display BPC to begin the process. See introductory document for notes on runtime and data structure.

Click the "*Select Data Folder*" button to select the folder where your .csv files are located. The path of this folder will then appear next to the button. Several options now need to be specified using the checkboxes on the left. The first option is whether to account for analytical uncertainty in zircon ages when inferring PMEs and calculating BPC. If analytical uncertainties are not being accounted for, the data files must still be in the same format discussed above, though the second column will not be used. We suggest that for final analyses, the analytical uncertainties should be modeled. Finally, there is an option to overwrite existing PME and BPC files. If this is not selected, analyses will be skipped for samples for which these files already exist. **Note:** if you have already inferred PMEs using one set of options and wish to redo the analysis with different options, you *must* check the box to overwrite previous files. Enter the number of models you wish to retain for each sample, or leave this field blank to retain all models. We recommend using a value of at least 10,000. Retaining fewer models will not improve processing time, but it will decrease the amount of disk space the outputs from the scripts occupy. Enter the number of cores you desire to be used for the BPC analysis. If this textbox is left blank, all available cores will be used.

If a folder has been selected, the filenames of the sample .csv files will be shown in the listbox on the left side of the window. The BPC values, once calculated, will be shown in an NxN matrix, where N is the number of compared samples. The "*Sample order*" textbox allows you to change the order in which the samples will appear in this matrix. To specify the order, type the indices of the sample filenames (shown in the listbox) in the desired order, separated by commas (e.g. '1, 3, 4, 2, 5'). See the text in the window for further instructions. You can also leave "*Sample order*" blank or enter "y" to use the default order shown in the listbox, or you can type "auto" to automatically order the samples in terms of lowest to highest mean BPC value calculated with all other samples.

Click *"Calculate and display BPC"* to begin the process of inferring PMEs and calculating BPC values. First, the script will infer PMEs for the samples in the referenced folder. During this time, a progress bar will appear that says "Inferring PMEs…". Inferring PMEs takes significant time, as discussed in the General Notes section, but *progress is saved* (ticking 'Overwrite PMEs and BPC uncertainty files' will overwrite previously saved progress). If the script is interrupted, restart it in the same way as is described here, and the portions of the process that were already completed will not be run again. If a recalculation is desired, check the 'Overwrite PMEs and BPC uncertainty files' box, or manually delete the files created by the program. The directory structure of these saved files is described in the File Architecture section.

While the script is running, MATLAB may appear not to be busy, causing confusion (see further discussion in the General Notes section). After the required calculations are complete, you should see a color-coded table output to a new figure:



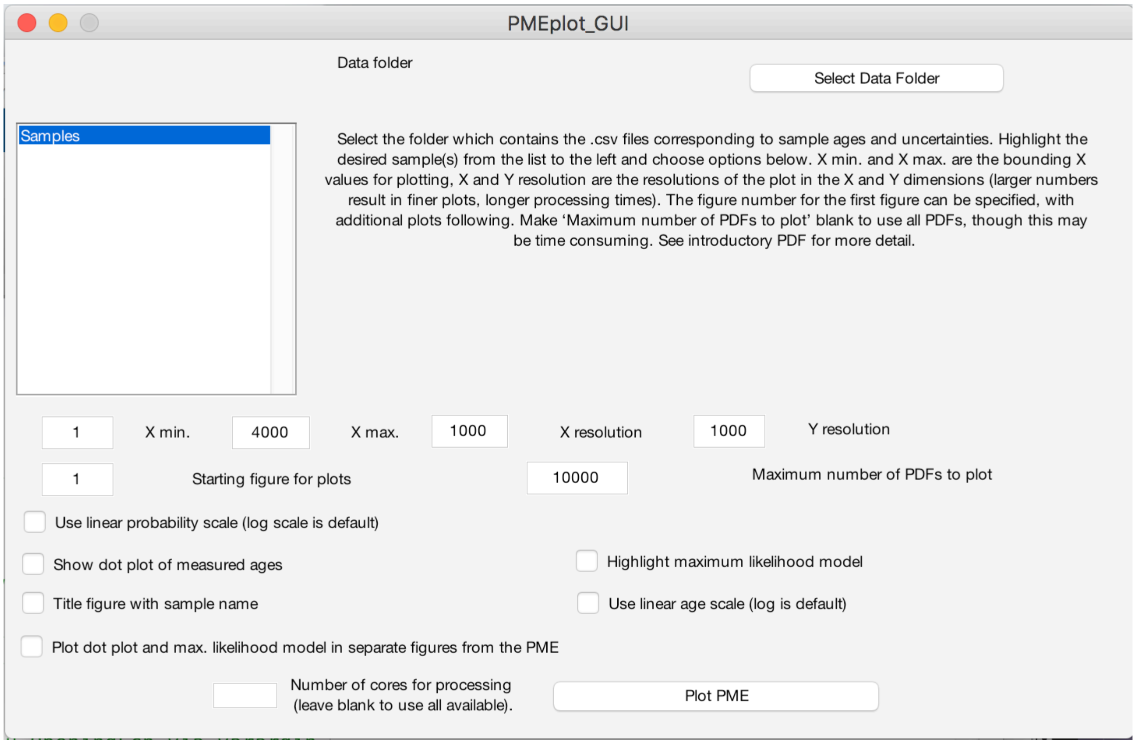
	Pullen_subsample_n300	Pullen_subsample_n60	Thomson_subsample_n300	Thomson_subsample_n60
Pullen_subsample_n300	-	0.99 ±.04	0.48 ±.02	0.48 ±.04
Pullen_subsample_n60	0.99 ±.04	-	0.54 ±.04	0.47 ±.07
Thomson_subsample_n300	0.48 ±.02	0.54 ±.04	-	0.96 ±.04
Thomson_subsample_n60	0.48 ±.04	0.47 ±.07	0.96 ±.04	-

This figure shows the BPC value and uncertainty for each pair of compared samples. The colors illustrate the BPC value on the MATLAB parula colormap stretched from 0 to 1. In addition, the "*BPC value*" and "*BPC uncertainties (1 sigma)*" fields in the window are populated with values that can be copied to the clipboard.

To re-display BPC values after the analysis is complete, simply re-run BPConeclick_GUI.m by clicking on the *"Infer PMEs and display BPC"* button from the main menu (without selecting the option to overwrite existing files). Because completed analyses won't be re-done, the function will quickly display BPC values.

B. Displaying Probability Model Ensembles (PMEs) using PMEplot_GUI.m

Plotting a PME can be done only after PMEs have been inferred using 'BPConeclick_GUI.m' above. Click the *"Plot PMEs"* button on the main menu. You should see the following window:



Select the folder which contains the .csv files corresponding to sample ages and uncertainties. Highlight the desired sample(s) from the list to the left and choose options below. X min. and X max. are the bounding X values for plotting, X and Y resolution are the resolutions of the plot in the X and Y dimensions (larger numbers result in finer plots, longer processing times). The figure number for the first figure can be specified, with additional plots following. Make 'Maximum number of PDFs to plot' blank to use all PDFs, though this may be time consuming. See introductory PDF for more detail.

1 X min. 4000 X max. 1000 X resolution 1000 Y resolution

1 Starting figure for plots 10000 Maximum number of PDFs to plot

□ Use linear probability scale (log scale is default)

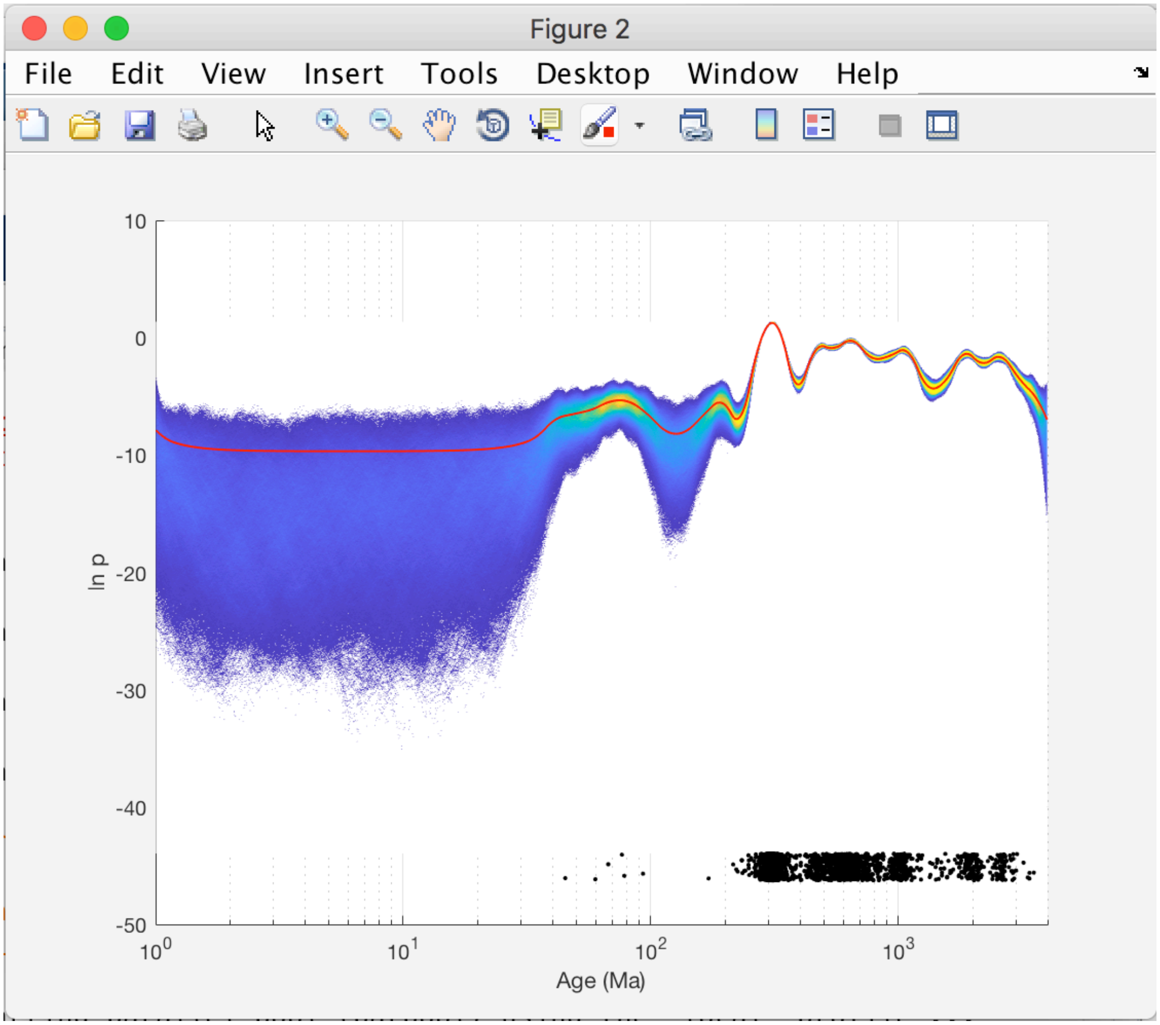
□ Show dot plot of measured ages □ Highlight maximum likelihood model

□ Title figure with sample name □ Use linear age scale (log is default)

□ Plot dot plot and max. likelihood model in separate figures from the PME

Number of cores for processing (leave blank to use all available).

Again use "*Select Data Folder*" to select the folder where the sample .csv files are stored. As with evalBPC_GUI.m, the folder path will be shown next to the button and the samples contained in the folder will be shown in a listbox on the left. Highlight the desired sample(s) in the listbox and specify options using the text boxes and check boxes. Options that can be specified in textboxes include the minimum and maximum x values for plotting, and x and y resolution for the plot, and the number of the figure for output. If more than one figure is plotted, then subsequent figures will be plotted in sequentially numbered plots. In addition, checkboxes allow you to specify whether to highlight the maximum likelihood probability model in the PME plot, whether to title the plot with the sample name, whether to use a linear or logarithmic probability scale, whether to use a linear or logarithmic age scale, and whether to include a dotplot of measured ages in the figure. The dotplot appears in a thin band beneath the probability models, similar to plots shown in Pullen et al. (2014). The dotplot and maximum likelihood model can be plotted in their own figure windows, as well, which can be useful if further processing of the figures is intended in graphics software. The number of cores for the operation can also be specified. Once the desired options are specified, click "*Plot PME*". A progress bar should appear. Once reading and processing the data is complete, the resulting plot(s) will appear:

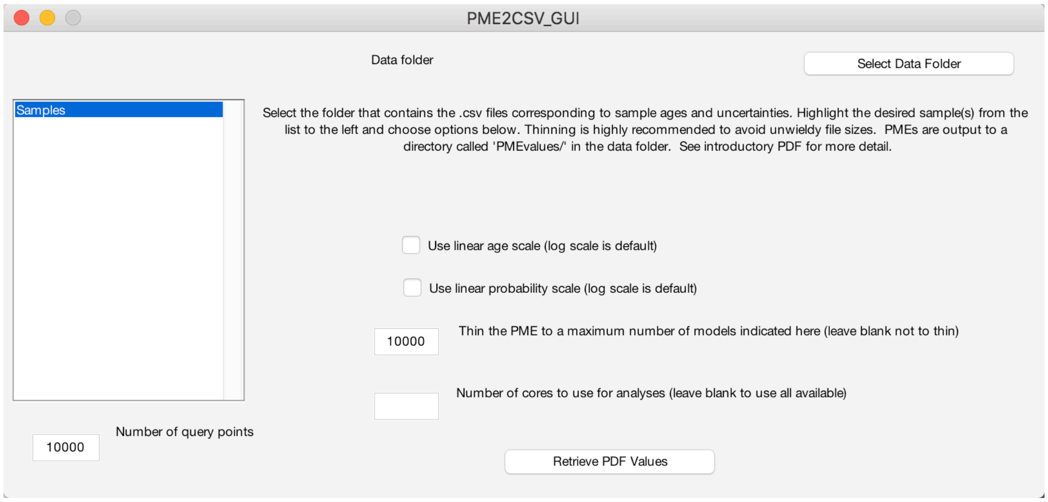


In this example, “Highlight maximum likelihood model” was selected, along with “Show dot plot of measured ages”, and all other check boxes were left blank. The x and y resolutions were set to 1000. This figure shows a natural logarithmic age scale and probability scale. In this script, the area covered by the probability models of the PME is discretized into cells in the x and y directions with the number of cells in one dimension equal to the resolution input into the GUI. Then, the cells that have probability models that pass through them are colored according to the number of models that pass through them, using the MATLAB parula colormap.

If more than one sample was selected in the listbox in the main window, the PME plots for each selected sample will appear sequentially.

C. Extract probability values from PMEs using PME2CSV_GUI.m

A PME consists of many probability density functions (PDFs), and their values can be queried at a given set of x values using PME2CSV_GUI.m. This is the way to obtain the function values of a PME for further processing. First, click *"Extract PME values to a .csv file"* in the main menu. You should see the following window:



Select the folder that contains the .csv files corresponding to sample ages and uncertainties. Highlight the desired sample(s) from the list to the left and choose options below. Thinning is highly recommended to avoid unwieldy file sizes. PMEs are output to a directory called 'PMEvalues/' in the data folder. See introductory PDF for more detail.

□ Use linear age scale (log scale is default)

□ Use linear probability scale (log scale is default)

10000 Thin the PME to a maximum number of models indicated here (leave blank not to thin)

Number of cores to use for analyses (leave blank to use all available)

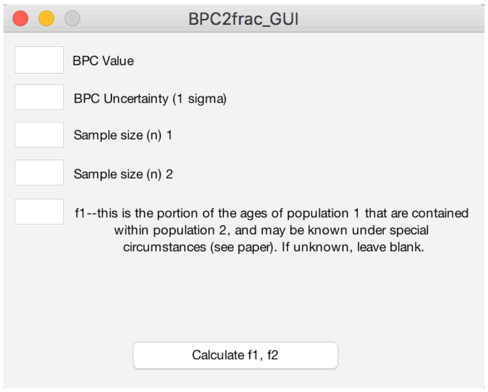
Number of query points 10000

First, click *"Select Data Folder"*, which will open a directory selection dialog. The selected directory should contain the .csv files that correspond to each modeled sample—this is the same data folder that BPConeclick_GUI.m uses. The listbox will then show the names of samples with .csv files saved in the data folder. Select the sample(s) for which you want to extract values, then choose options. Input the number of points for which you want to output PDF values. Two checkboxes control whether the output uses linear or logarithmic age and probability scales. Some notes on the use of logarithmic versus linear age scales are included in Section S4 of the text. Enter the maximum number of probability models from which you wish to extract values—a default value of 10000 is listed. Remove this default and leave the space blank to use all the probability models in a PME, but this may result in a very large output that takes a long time to write to disk. Optionally enter a number of cores to use for processing (leave blank to use all cores available). In the lower left corner, enter the number of points for which you want probability values returned. These points will be evenly distributed over the range of x values used for modeling on either a linear or logarithmic scale, depending on options chosen. A progress bar should appear which says *"Evaluating PDFs…"*, and a message box will appear when the process is complete.

The script creates a new subdirectory within the data folder you specified called 'PMEvalues/' and writes .csv files containing PDF values at the queried ages in that subdirectory. Output .csv files are named according to the sample name, followed by 'PMEvals.csv'. In these output .csv files, there is a header line that describes what information is in the file. One line shows the integral of each PDF at the resolution you selected, approximated by the Riemann summation method. The resolution ('Number of points' field) can be increased to make integral values closer to 1. Below, the first column lists the queried ages. Then, each successive column displays the probability density values of one PDF at each of the queried age values. Each column (except the first) contains values from a single PDF. **Note that if a log age scale was requested in the GUI**, the first column of the output file will contain ln age values (e.g. the first column will contain values from 0, which equals ln 1, to ~8.3, which equals ln 4000).

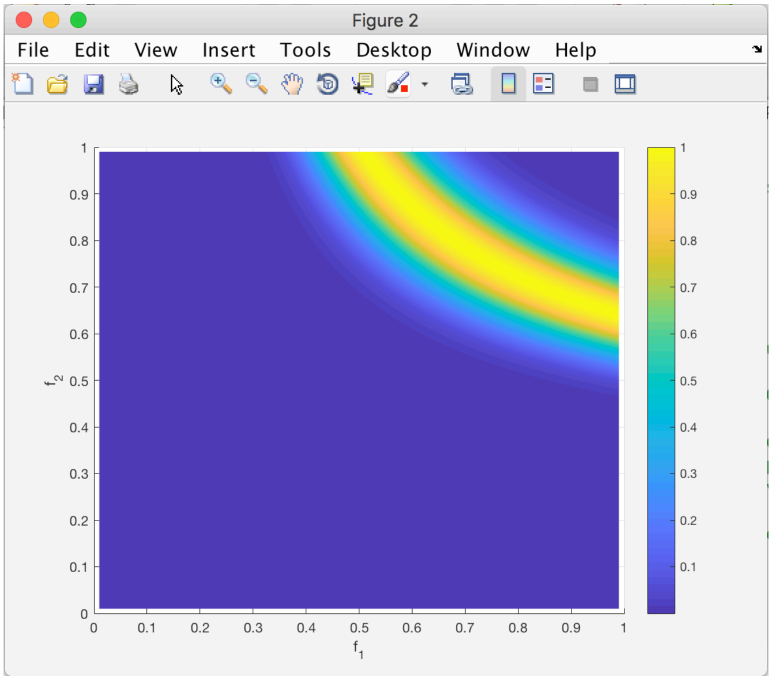
D. Inferring the shared fractions of two populations from BPC values using BPC2frac_GUI.m

BPC values have a functional relationship to the shared fraction of two detrital zircon populations (the fraction of age peaks of each population that is shared with the other population), which can be derived analytically (see paper text). Thus, a BPC value can non-uniquely constrain the shared fractions of both populations. This calculation is facilitated by the BPC2frac_GUI.m script. First, click the *"Infer shared fractions of parent populations from BPC"* button in the main menu. The following window should appear:



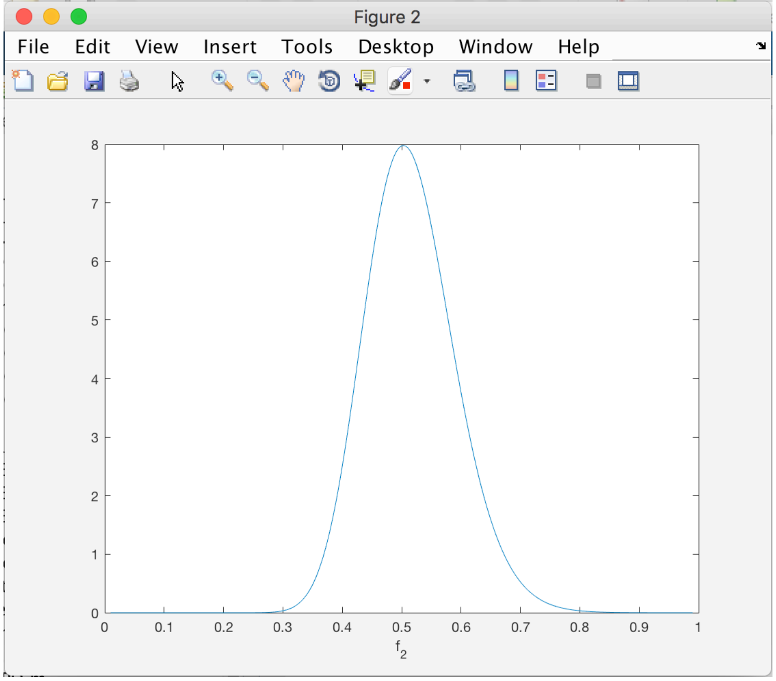
f1--this is the portion of the ages of population 1 that are contained within population 2, and may be known under special circumstances (see paper). If unknown, leave blank.

Fill out the text box fields, including BPC value and uncertainty, along with the sample sizes of the compared samples. The BPC age and uncertainty come from the results of part A. In specific circumstances, the shared proportion of one sample may be assumed. For instance, if two samples are taken from two positions on the same river network such that the water and sediment that flow past the first sample location subsequently flow past the second sample location, then all the age peaks in the first sample can be assumed to be shared with the second sample, resulting in an f1 value of 1 (see text for discussion). If f1 can be assumed, then enter it as well. If no f1 value is entered, then the output will appear like this:



Here, colors indicate the relative likelihood of coordinate pairs of (f1, f2) values. These values are obtained by solving Eqn. C.7 in Appendix C in the text numerically for the given BPC value and uncertainty. This result was generated for a BPC value of 0.75, uncertainty of 0.05, and sample sizes of 100 and 300.

If f1 can be assumed, the output will appear like this:



Here, the plot shows the likelihoods of different values of f2 for the given value of f1. This example plot was generated using the same parameters as above, plus an f1 value of 1. In addition, the mean and standard deviation of this distribution are output to the MATLAB Command Window.

5. File architecture

File architecture of scripts for PME inference: Upon running, the script for inferring PMEs generates a new directory within the selected data folder, called 'chains/'. Within this directory, three .csv files per sample are generated, plus three additional .csv files for each possible pairing of samples in the data folder. For a given sample or sample pair, one of the two files contains a PME (a Markov chain), and is named with the sample name followed by 'chain.csv'. The first row of each 'chain.csv' file lists the knots for b-splining (see Section 2.1 of the text), and each following row corresponds to a different probability model that has been accepted into the PME. The columns store the values of the 100 model parameters of each of these probability models. The second of the two files per sample or sample pair contains a list of the log likelihood values of the PME inferred for that sample or sample pair. This second file is named with the sample name followed by 'logLk.csv'. The 'logLk.csv' file is a single column, where each row contains a log likelihood value that corresponds with the model in the same row of the 'chain.csv' file. The third file contains a list of log posterior probabilities for the models of the PME and ends with 'logPost.csv'.

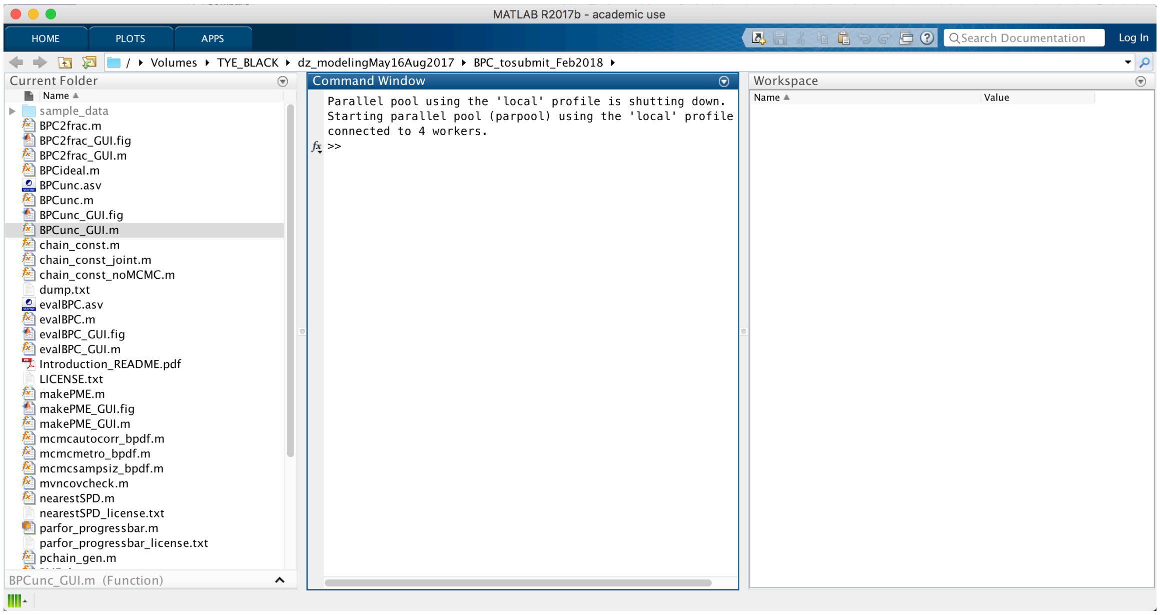
The files resulting from the comparison of two samples are named as above except the names of the two samples are concatenated such that the filenames read 'SampleName1_SampleName2chain.csv', where 'SampleName1' and 'SampleName2' are the filenames of the sample .csv files and 'chain.csv' could also be 'logLk.csv', 'logPost.csv', or 'log.txt'.

Log files. The scripts that infer PMEs and calculate BPC create log files. These logs can be found in the folder where the sample .csv files are located. The log records the settings for the run, and how long the run takes, and should be easily readable. Each line of the log file corresponds to a specific setting chosen on the BPConeclick interface, and successive runs will add onto the log document rather than replacing it.

There are additional log files created for each sample and each pair of samples while PMEs are being inferred, but these are unlikely to be easily readable by users. Log files are generated during each run of the script for PME inference and are stored in a 'chains/log/' directory within the data folder. The filenames of the log files match the filenames of the corresponding sample .csv files with "log.txt" appended.

6. General Notes, Common Problems, Clarifications

MATLAB may appear not to be busy even though the script is running: Once you start any of these scripts from the GUI (by clicking *"Generate PMEs"* or equivalent), the progress bar may appear under other MATLAB windows. In addition, a blinking cursor will appear in the MATLAB Command Window, and MATLAB will not display the word "Busy", as it usually does for a script run from the command line, even though the script is running. The screenshot below shows the MATLAB screen while the script is running. **This behavior will occur with all scripts included in our package when run from GUIs.**



```
Parallel pool using the 'local' profile is shutting down.
Starting parallel pool (parpool) using the 'local' profile
connected to 4 workers.
>>
```

The standalone applications can be slow to respond: As noted above, when the standalone applications are started or a button is clicked, the response of the application may be delayed. The standalone application will often be far more delayed than the MATLAB script. When this occurs, please wait for the application to respond rather than reissuing a command, which will cause operations to be run more than once.

Expected time for script running: The scripts that infer PMEs will take a significant amount of time to run. These scripts compare every possible pair of samples in an input dataset. Mathematically, the number of possible pairs in a given dataset is given by (N choose 2), where N is the number of samples in a given dataset. makePME.m and BPCunc.m both take minutes to tens of minutes for each sample plus an equivalent time for each possible sample pair. This time is distributed over as many cores as are available for processing, such that the total processing time (in hours) can be estimated as

$$T = (\sim 5\ minutes) * \frac{N + (N\ choose\ 2)}{\#\ cores}$$

These times were calculated on a 2014 Macbook Pro with 2.2 GHz, 4-core processor and 16 GB RAM. As noted above, changing the options on the scripts can have a significant effect on runtime. For instance, ignoring analytical uncertainties in grain ages should reduce processing time somewhat.

Progress is saved when running the scripts. The scripts that infer PMEs run a Monte Carlo-based analysis on each sample and each possible pair of samples in the input dataset, which takes significant time. These scripts immediately save the results of their analysis on each sample or pair of samples as soon as the analysis is complete. The scripts look for these files when run and do not run duplicate analyses for samples or sample pairs that have already been completed. Thus, if one of these scripts is interrupted in the middle of execution, it can be restarted without losing the analyses that have already been completed. Effectively, your progress is saved as the script runs. Previous analyses can be overwritten by checking the overwrite option on the BPConeclick interface.

BPC values and estimated uncertainties may differ slightly from run to run. Inferring PMEs is a Monte Carlo-based approach, meaning that they rely upon random sampling and are liable to be slightly different from one run to another. In general, the differences observed in calculated BPC values should be significantly less than the 1σ estimated uncertainty on that value, indicating that this variability is well within the limits of the resolution provided by the data. Estimated BPC uncertainties are likely to differ by ~10% (occasionally as high as 20%) of their value between runs. For typical BPC uncertainties for sample sizes n > 100, this results in possible variation of 0.01-0.02 from one run to another.

Exiting the scripts: The progress bars for the longer running scripts have cancel buttons that should halt execution if clicked. However, if operation does not stop, closing windows associated with the scripts/applications may not terminate these processes either. To quit the standalone applications prematurely, use your operating system's force quit/task manager option. To quit the MATLAB scripts prematurely, click on the command window to highlight it and then press Ctrl+C (Mac or Windows) to terminate the script.

Calculating PDF integrals from PME2CSV output: PME2CSV outputs a set of function values that correspond to a set of evenly spaced x values. These functions are PDFs and therefore must integrate to 1. The first content line of each PME2CSV output file lists the integrated area of each PDF included in the output file. These integrated areas are calculated using the Riemann

Summation method, meaning that each function value must be multiplied by the x-axis space between function values (Δx) in order to approximate the integral. Note that this method is less accurate when the number of output values is low. For instance, if only 1000 function values are queried from a PDF and there are some very steep and/or narrow age peaks, an integral estimated using the Riemann Sum method may produce a result that deviates from 1. As the number of queried function values increases, these deviating values should approach 1.

7. Tested hardware

This software has been successfully used on:

2014 Macbook Pro, 2.2 GHz, 4-core processor and 16 GB RAM,
MATLAB_R2017b, macOS 10.12.6

HP Windows 10 machine, 12-core processor and 64 GB RAM,
MATLAB_R2016b.