

AGEZ – Age Zircon model

DANIELE SILVESTRO^{1,2,3,4}

¹*Department of Biology, University of Fribourg, 1700 Fribourg, Switzerland;*

²*Swiss Institute of Bioinformatics, 1700 Fribourg, Switzerland;*

³*Department of Biological and Environmental Sciences, University of Gothenburg, 413 19
Gothenburg, Sweden;*

⁴*Gothenburg Global Biodiversity Center, 413 19 Gothenburg, Sweden;*

1 Methods

2 Main model parameters

3 Let us define a dataset of N dated zircons from S samples. We indicate with
4 $\mathbf{z} = \{z_1, \dots, z_N\}$ the (unknown) ages of the zircons and with $\mathbf{x} = \{x_1, \dots, x_S\}$ the ages of
5 the samples. The samples are ordered according on their depth and we assume their age
6 strictly follows that order such that $x_i > x_{i-1}$. We indicate the set of zircons found in a
7 sample s as \mathbf{z}^s .

8 The exact age of each zircon (z_i) is assumed to be unknown but linked to its
9 measured age, which is expressed as a mean μ_i and a standard deviation σ_i . The mean ages

μ and a standard deviations σ of all zircons represent the input data of the model, which
 aims to estimate the vector \mathbf{z} and the ages of all samples \mathbf{x} . Since the age of zircons can be
 measured based on different methods (e.g. $m \in \{1, \dots, M\}$, e.g. Zr-U-Pb, ZFT, Ar-Ar),
 the uncertainty around the true age of a zircon is assumed to be further affected by how it
 was measured. We compute the likelihood of the age of a zircon i based on a normal
 density (Fig. 1):

$$P(\mu_i | z_i, \sigma_i, \epsilon_m) \sim \mathcal{N}(z_i, \sigma_i + \epsilon_m) \quad (1)$$

where $\epsilon_m \in \mathbb{R}^+$ is the bias in the estimated error of the measurement method m . The
 parameters z_i and ϵ_m are considered as unknown and estimated from the data using a
 Bayesian algorithm.

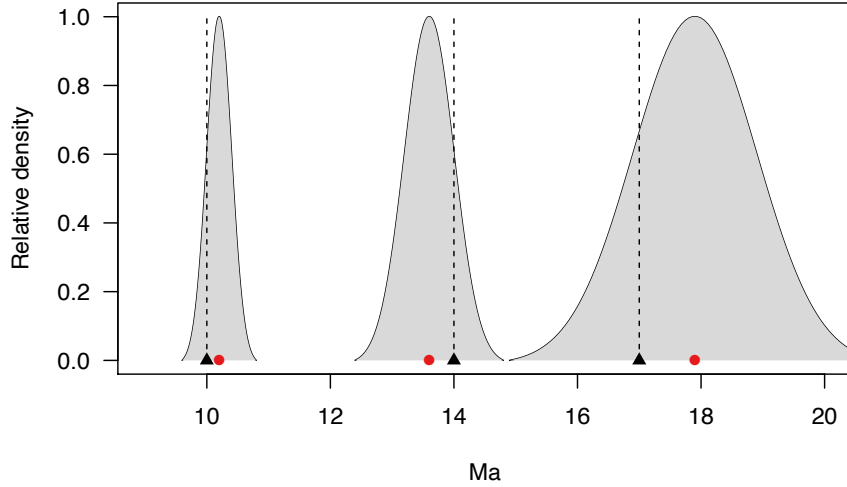


Figure 1: Example of three zircons with measured ages of 10, 14, and 17 Ma (μ ; indicated by the dashed vertical lines and black triangles) and standard deviations ($\sigma + \epsilon$; shown by the gray shaded areas). The sampled true ages of the zircons are indicated by the red circles.

The value of x_j , the age of the j^{th} sample, is determined by two latent variables (r_j
 and \mathbf{I}^j) and constrained by the sampled values of \mathbf{z} such that $x_i > x_{i-1}$ for $i \in \{2, \dots, S\}$.

Specifically, we define as

$$\zeta_j = \min(\mathbf{z}^s), \text{ for } s \in \{j, \dots, S\}, \quad (2)$$

the minimum age across all zircons included in sample j and in all older samples. Thus, ζ_j represents the upper (older) boundary for the age of sample j , which must be younger than all following samples (ordered by depth) and than its youngest zircon. Under this notation we define the age of a sample as:

$$x_j = \begin{cases} r_j(\zeta_j), & \text{if } j = 1 \\ x_{j-1} + r_j(\zeta_j - x_{j-1}), & \text{if } j > 1 \end{cases} \quad (3)$$

where $r_j \in (0, 1)$ is an estimated sample-specific latent parameter determining how close x_j is to its lower boundary x_{j-1} (or to 0 if $j = 1$). Thus, when $r_j \approx 0$ the age of the sample is close to its younger boundary and when $r_j \approx 1$ the age of the sample is close to its older boundary. We also account for the fact that a zircon can be younger than the sample it was found in, for instance due to a dating error or a later recrystallization of the zircon. To account for this possibility, we additionally estimate a vector of identifiers $\mathbf{I} = \{I_1, \dots, I_N\}$ that define which zircons (identified by $I = 1$) are older than the sample and therefore used to determine its upper age boundary and which zircons (identified by $I = 0$) are younger than the age of the sample. Thus, the upper boundary of a sample age is:

$$\zeta_j = \min(\mathbf{z}^s \setminus \mathbf{I}_0^s), \text{ for } s \in \{j, \dots, N\}, \quad (4)$$

where $\mathbf{z}^s \setminus \mathbf{I}_0^s$ indicates the subset of zircons in sample s with indicator equal to 1.

We can now define the prior probability of z_i^j , i.e. the i^{th} zircon in sample j as a function of the age of the sample (x_j) and an estimated scale parameter s_j . Specifically we

38 model the prior distribution of zircons in a sample using a compound-Uniform-Cauchy
 39 distribution, defined as:

$$P(z_{i,j}|x_j, s_j) = \begin{cases} z_{i,j} \sim \mathcal{U}(0, 2x_j), & \text{if } z_{i,j} < x_j \\ z_{i,j} \sim \mathcal{C}(x_j, s_j), & \text{if } z_{i,j} \geq x_j \end{cases} \quad (5)$$

40 where s_j is the sample-specific scale parameter of the Cauchy distribution. Under this
 41 parameterization, the age of the zircons identified as younger than the sample will have a
 42 prior uniform probability ranging from 0 to the age of the sample and rescaled to integrate
 43 to 0.5. The other zircons will instead follow a half-Cauchy distribution with mode equal to
 44 the age of the sample (Fig. 2).

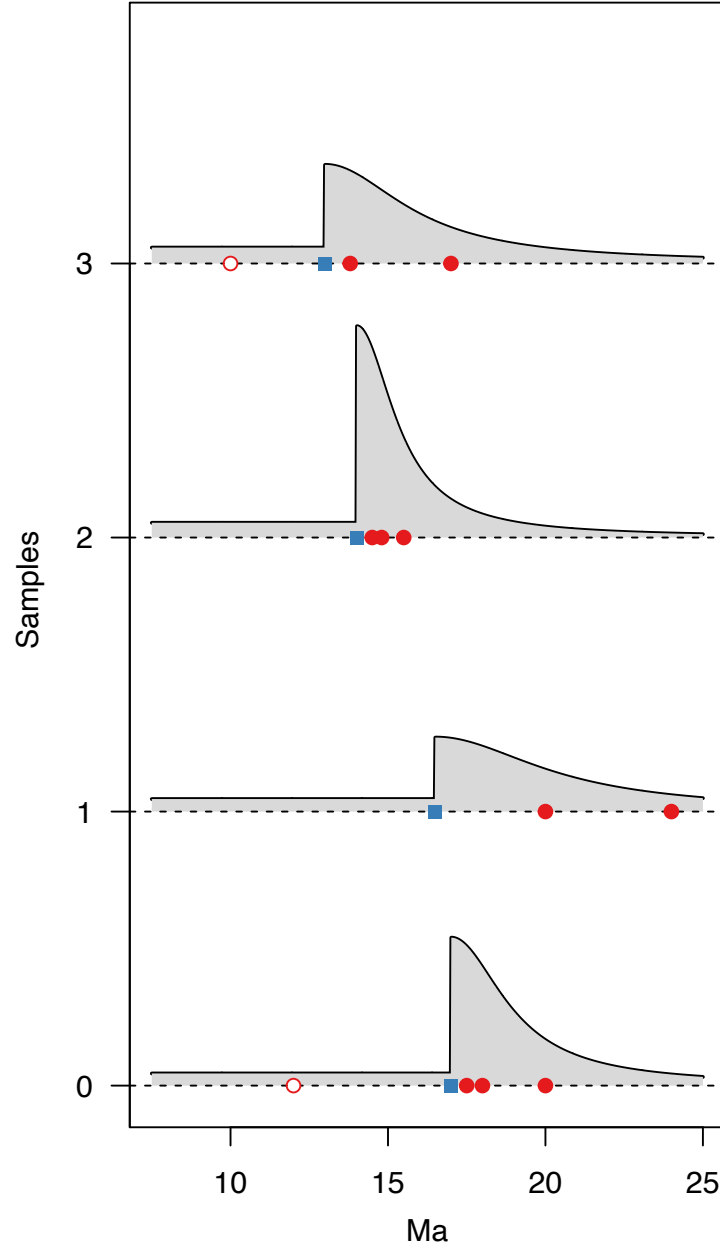


Figure 2: Probability distributions of zircon ages in four samples sorted from oldest (sample 0) to most recent (sample 3). Red filled circles indicate zircons identified as older than the age of the sample, shown as a blue square. Red empty circles indicate zircons identified as younger than the sample. The gray shaded areas display the relative probability distribution of the zircon ages multiplied by the probability of the respective indicator (here set to $P(I = 0) = 0.1$). We note that the maximum age of sample 1 (x_1) is not determined by its youngest zircon (of age 20 Ma), but by the age of the previous sample x_0 .

Priors and hyper-priors

We use a half-Cauchy prior for the vector of scale parameters of the compound Uniform-Cauchy distributions $\{s_1, \dots, s_S\} \sim \mathcal{C}^+(0, \beta)$, where the scale parameter β is assumed to be unknown and estimated through MCMC, with a gamma hyper-prior $\beta \sim \Gamma(10, 0.5)$. We set an exponential prior on the vector of parameters $\{\epsilon_1, \dots, \epsilon_M\} \sim \text{Exp}(0.1)$. We use a beta distribution as prior on the vector of parameters $\{r_1, \dots, r_S\} \sim \mathcal{B}(a, b)$ and consider the shape parameters a and b themselves as unknown parameters and assign them exponential hyper-priors, $a, b \sim \text{Exp}(0.1)$. Finally we use a Bernoulli distribution as prior on the indicators $\{I_1, \dots, I_N\}$ with parameter $p = 0.99$, thus assigning a 0.01 prior probability for a zircon to be younger than the sample it is assigned to. This informative prior assumes that only a small fraction of the zircons might have re-crystallized or is otherwise erroneously dated.

Parameter estimation

The model includes $2N + 2M + 2S + 3$ parameters (z and I , ϵ , s and r , a and b and β , respectively). All parameters are estimated through Metropolis-Hastings Markov chain Monte Carlo (MCMC). We use a sliding window proposal with reflection at the boundaries for r , normal kernel proposals for z , binomial proposals for I . We use multiplier proposals on all other parameters since they only span the positive range.

Adding a maximum age constraint

A maximum age constraint can be added to the age model by including an additional sample with a single age measures with no dating error. This artificial sample will therefore include a single measured age of fixed age μ^{S+1} and standard deviation $\sigma^{S+1} = 0$ to enforce a hard boundary. This artificial sample is assigned a fixed indicator

68 $I^{S+1} = 1$ and its true age is set equal to the measured one $x^{S+1} = \mu^{S+1}$. This approach
69 enforces a maximum age constraint to the estimated ages of all following samples.

$$x_j = \begin{cases} r_j(\zeta_j), & \text{if } j = 1 \\ x_{j-1} + r_j(\zeta_j - x_{j-1}), & \text{if } j > 1 \end{cases} \quad (6)$$

70 Results

71 The preliminary results obtained under this model are shown in Table 1.

Table 1: Estimated ages from preliminary MCMC analyses (5 replicates).

Sample name	Estimated ages (Ma)		
	mean	median	95% HPD interval
JG-R88-4	10.166	10.1492	9.1341 – 11.599
Z6	11.044	11.1778	9.6965 – 12.083
TVV-01	11.069	11.207	9.7002 – 12.104
JG-R88-2	11.0701	11.207	9.6982 – 12.104
Z5	11.078	11.2138	9.635 – 12.108
004	11.518	11.567	10.718 – 12.369
002	11.543	11.593	10.719 – 12.351
003	11.566	11.616	10.758 – 12.372
LV13	11.603	11.646	10.769 – 12.390
KS4	11.678	11.720	10.834 – 12.420
LV8	11.777	11.830	10.936 – 12.441
Z4	11.928	11.975	11.191 – 12.509
JG-R89-2	12.052	12.087	11.458 – 12.600
SEL-02	12.070	12.102	11.433 – 12.633
TVV-04	12.074	12.103	11.433 – 12.663
Z3	12.077	12.103	11.433 – 12.700
JG-R90-1	12.171	12.191	11.538 – 12.805
Z2	12.179	12.197	11.472 – 12.778
JG-R89-3	13.082	13.115	12.657 – 13.471
JG-R90-3	13.093	13.124	12.657 – 13.466
44011	13.095	13.125	12.657 – 13.466
JG-R89-1	13.096	13.127	12.657 – 13.469
UR-02	13.096	13.127	12.657 – 13.472
UR-01	13.229	13.241	12.700 – 13.761
Z1	15.097	14.769	12.207 – 17.879
44017	19.521	17.700	16.513 – 26.267