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Hug model: parameter estimation via the ABC Shadow algorithm

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Abstract

Studying geological fluids mixing systems allows to understand interaction among water sources. The Hug model is an interaction point process model that can be used to estimate the number and the chemical composition of the water sources involved in a geological fluids mixing system from the chemical composition of samples REYPE (2022); REYPE et al. (2020, 2022). The source detection using the Hug model needs prior knowledge for the model parameters. The present work shows how the parameter estimation method known as the ABC Shadow algorithm STOICA et al. (2021, 2017) can be used in order to construct priors for the parameters of the Hug model. The long term perspective of this work is to integrate geological expertise within fully unsupervised models.

Introduction

The building of conceptual and quantitative models of fluid and mass transfer in the sub-surface and the Earth's crust rely on the analysis of hydrochemical data FAURE (1997); INGEBRITSEN, SANFORD, and NEUZIL (2006); YARDLEY and BODNAR (2014). Groundwater is the result of a mixing between water sources. Hence, the chemical composition of a sample of groundwater is link to the chemical composition of the water sources. The mass transfer occurring in the sub-surface is deduced by estimating the contribution of the water sources in samples.

However, the number and the composition of the water sources are not known. Thus, the water sources should be detected: their number and their chemical composition should be estimated. A toy example of mixing scenario between four sources (in blue) resulting in 200 samples (dots) is shown in Figure 1. This mixing system consider the composition in three hydrochemical parameters that can be concentration of ions or molecules, isotopic composition or ratios of hydrochemical parameters. The space made by the composition in the hydrochemical parameters is called data space.

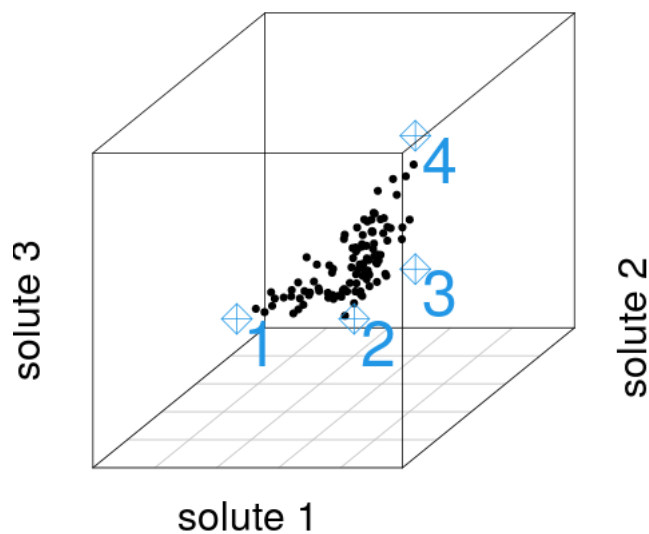


Figure 1: *Mixing scenario of four sources (in blue) in the three-dimensional space of hydrochemical parameters (solute1, solute2, solute3) called data space. The dots represent the position of the sample in the data space.*

In the literature, source detection is done mostly either graphically or in a supervised statistical analysis. Moreover, the detection often considers a subset of the hydrochemical parameters, that is to say the detection is performed by artificially combining results obtained on projections of the entire data space. Such a final result lacks of mathematical rigor and it can be biased. For instance, consider the situation when two sources have the same position in the projected data space but a different position in the whole data space. In this situation, the exact number of sources is never precisely detected.

The Hug model REYPE (2022); REYPE et al. (2020, 2022) is a point process especially built to detect the number of sources and their chemical composition in hydrochemical data. This point process considers the data as a cloud of points in a multidimensional space, with coordinates being the value of each hydrochemical parameter. The sources distribution in the data space is governed by a Gibbs point process. The density probability of this Gibbs point process is built by taking into account knowledge on the analyzed mixing system and assumptions used in the graphical detection methods. The conditions for using the Hug model are as follows. The datasets (*i.e.* the samples) are the result of a conservative mixing (*i.e.* no chemical reaction affects the considered hydrochemical parameters during the mixing process). The composition of the sources are supposed the same, or at least not significantly different for each data point.

The sources are estimated by the configuration that maximizes the joint probability density controlling the sources and the parameters distributions. This probability density is simulated by Markov chains Monte Carlo methods. The optimization procedure is implemented via a simulated annealing procedure, hence avoiding local maximum.

The Hug model need model parameters set by the user to detect the sources. This paper presents a method to estimate the model parameters from bidimensional sources in order to improve the detected sources: the ABC Shadow algorithm STOICA et al. (2021, 2017).

1 Materials and methods

1.1 Hug model

Considered data sets are made of measures of hydrochemical parameters for the collected samples. Each sample is a point in an abstract multidimensional space, called data space. Each sample coordinate represents the composition of a given hydrochemical parameters. The observed samples are the result of the mixing between the unknown sources.

The Hug model is a Gibbs point process that can be used to detect the number and the composition of the sources involved in a mixing system from the data. This point process takes into account the following assumptions:

- (a) the data points are rather close to the sources,
- (b) the data points are barycenters of the sources,
- (c) the number of sources is minimized,
- (d) the composition of the sources are significantly different from one source to another.

These assumptions are “translated” into a function U called energy function REYPE et al. (2022). Assume the model parameters vector θ known, the probability density of the Gibbs point process representing the Hug model writes as

$$p_{\mathbf{d}}(\mathbf{s}|\theta) = \frac{\exp(-U(\mathbf{s}|\theta))}{Z(\theta)}, \quad (1)$$

with $Z(\theta)$ the normalizing constant.

This probability density is simulated by using Metropolis-Hastings dynamics VAN LIESHOUT (2000); MØLLER and WAAGEPETERSEN (2003). The detection of the sources is made by estimating the configuration of sources that maximizes the previous probability density. This optimization problem is solved by using a simulated annealing algorithm that applies the previous Metropolis-Hastings dynamics REYPE (2022); REYPE et al. (2020, 2022). The Hug model is implemented by adapting the C++ library DRLib GEMMERLÉ, STOICA, and REYPE (2022). The purpose of this library is the modelling, the simulation and the inference of marked point processes.

1.2 Parameters estimation

The source detection depends on the values of the model parameters. Previous cited work used Approximate Bayesian Computation (ABC) strategy to chose appropriate values for the model parameters BLUM (2010). The principle of this technique is to compare realizations of simulated patterns of sources with configurations of known sources \mathbf{s}_{obs} . The parameters that produce statistics close to the observation are kept for building the posterior. This scheme is presented below:

ABC algorithm: set $\epsilon \in \mathbb{R}_+$.

- 1) generate ψ by $p(\psi)$
- 2) generate \mathbf{x} by $p(\mathbf{x}|\psi)$
- 3) while $d(t(\mathbf{s}_{obs}), t(\mathbf{x})) > \epsilon$
- 4) accept ψ as parameter of interest

The ABC method should choose a tolerance threshold ϵ , a distance d between the observed statistics of the pattern of known sources $t(\mathbf{s}_{obs})$ and the simulated statistics obtained from the model. An important problem to be considered is that for numerical efficiency, the proposed ϕ should be close to the parameter of interest θ . But this is exactly the problem to be solved: the prior to be used should be close to the unknown posterior.

In this paper, the ABC Shadow, STOICA et al. (2021, 2017) is used to estimate the model parameters from the posterior approximation. This choice is adopted since this algorithm does not exhibit the problems mentioned before. The ABC Shadow algorithm steps are:

ABC Shadow algorithm. Data: \mathbf{s}_{obs} the known sources, $\theta^{(0)} \in \Theta$ the parameter initial value, $\Delta \in \mathbb{R}_+$ the perturbation parameter and $N \in \mathbb{N}$ the number of iterations.

- 1) generate \mathbf{x} by $p(\mathbf{x}|\theta^{(0)})$
- 2) For $k = 1, \dots, N$
 - a) generate ψ uniformly on the ball $b(\theta_k, \Delta/2)$
 - b) set $\theta^{(k)} = \psi$ with probability

$$\alpha(\theta \rightarrow \psi) = \min \left\{ 1, \frac{p(\psi|\mathbf{s}_{obs}) Z(\psi) \exp(-U(\mathbf{x}|\theta)) \mathbb{1}_{b(\psi, \Delta/2)}(\theta)}{p(\theta|\mathbf{s}_{obs}) Z(\theta) \exp(-U(\mathbf{x}|\psi)) \mathbb{1}_{b(\theta, \Delta/2)}(\psi)} \right\}.$$

else set and $\theta^{(k)} = \theta^{(k-1)}$

- 3) set $\theta = \theta^{(N)}$

2 Results

2.1 Parameter estimation

The real data set, considered here, is presented in PINTI et al. (2020). In this data set the stable isotopic composition of chlorine $\delta^{37}\text{Cl}$, the stable isotopic composition of bromine $\delta^{81}\text{Br}$ and the stable isotopic composition of helium Rc/Ra ($^3\text{He}/^4\text{He}$ normalized to that of the Atmosphere and corrected for the air component) are measured on $m = 75$ samples from geothermal wells from Mexico and are supposed to be the result of a three-source mixing system (mantle, subduction and crust). Note that halogens and noble gases behave conservatively during fluid mixing and that the mixing trends in the two planes considered here are not affected by curvature. In PINTI et al. (2020), a source detection method is presented: on bi-dimensional data, the sources are the vertices of the smallest triangle, in terms of area, that contains the data. These bi-dimensional sources are used to estimate the model parameters of the Hug model by the ABC Shadow algorithm.

The empirical θ selected in REYPE et al. (2022) gives the visit map of Figure 2. The visit map estimates the probability that a point in the data space is in contact or visited by a source. The detected sources are given in Table 1. The distances between the detected sources and the known sources are the absolute values of the differences of their coordinates. They are given in Table 2.

	Rc/Ra		$\delta^{37}\text{Cl}$		$\delta^{81}\text{Br}$	
	mean	sd	mean	sd	mean	sd
1 (mantle)	0.69	0.06	0.7	0.07	0.59	0.13
2 (subduction)	0.6	0.08	0.29	0.07	0.3	0.14
3 (crust)	0.24	0.07	0.47	0.06	0.52	0.06

Table 1: Proposed sources computed from the empirical θ .

Sources	Rc/Ra	$\delta^{37}\text{Cl}$	$\delta^{81}\text{Br}$	Mean Distance by Source
1	0.01	0.00	0.13	0.05
2	0.01	0.02	0.17	0.07
3	0.03	0.02	0.01	0.02
Mean Distance by Dimension	0.02	0.01	0.10	0.04

Table 2: Distance between the proposed sources computed from the empirical θ and the sources estimated in PINTI et al. (2020).

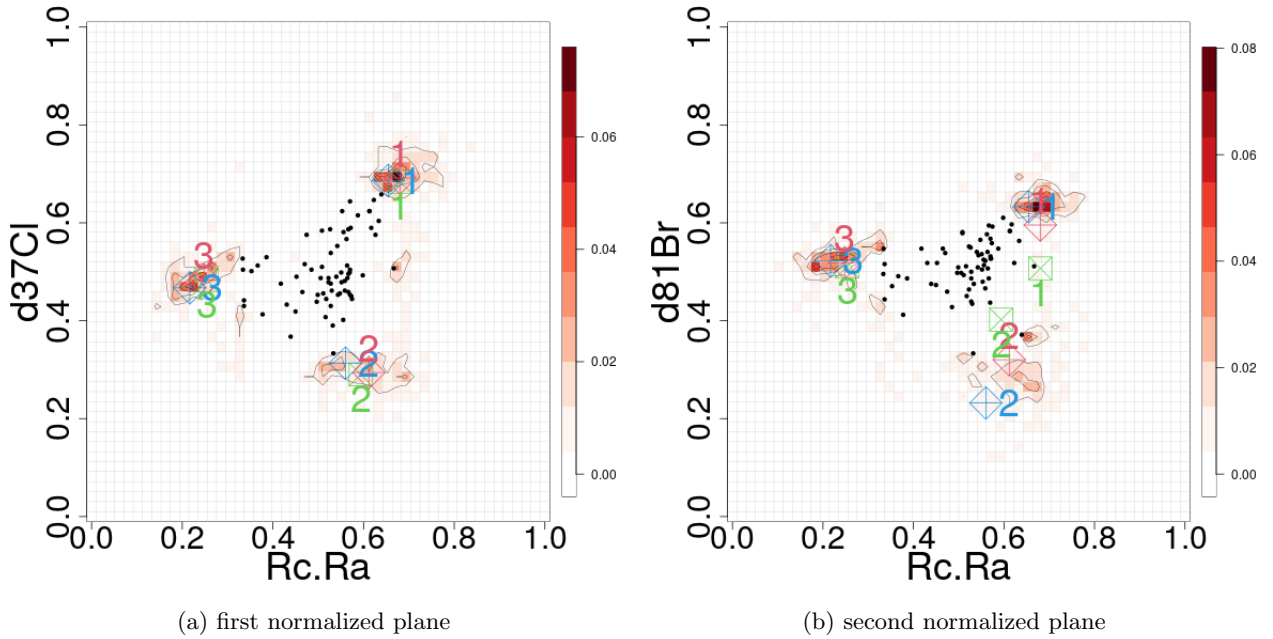


Figure 2: Visit map computed applied to the real data set PINTI *et al.* (2020) using the empirical prior for θ . The blue symbols represent the sources reconstructed by PINTI *et al.* (2020). The detection results obtained with the Hug model are represented by the green symbols and the red symbols. The first ones represent the clusters centers (means) obtained after the aggregation of the outputs of the optimization algorithm, while the second ones indicate the median points of each cluster.

For the ABC Shadow algorithm, the ranges of value that θ can takes are given in Table 3. The summary statistics of the posterior approximation of θ are given in Table 4 while the histograms of θ are presented in Figure 3.

	Initial value	min value	max value
θ_1	1.0	0.0	10000.0
θ_2	1.0	0.0	10000.0
θ_3	1.0	-10000.0	10000.0
θ_4	1.0	0.0	10000.0

Table 3: Initialization of the parameter for the ABC Shadow algorithm.

	Q25	Q50	Q75	mean	mode	sd
θ_1	13.98	22.77	35.08	26.1	14.83	15.9
θ_2	1500.25	2893.75	3857.65	2570.99	3906.32	1282.21
θ_3	865.92	1942.69	2624.99	1720.65	2686.69	932.69
θ_4	0.13	0.26	0.49	0.36	0.11	0.33

Table 4: Summary statistics of the posterior estimation of θ .

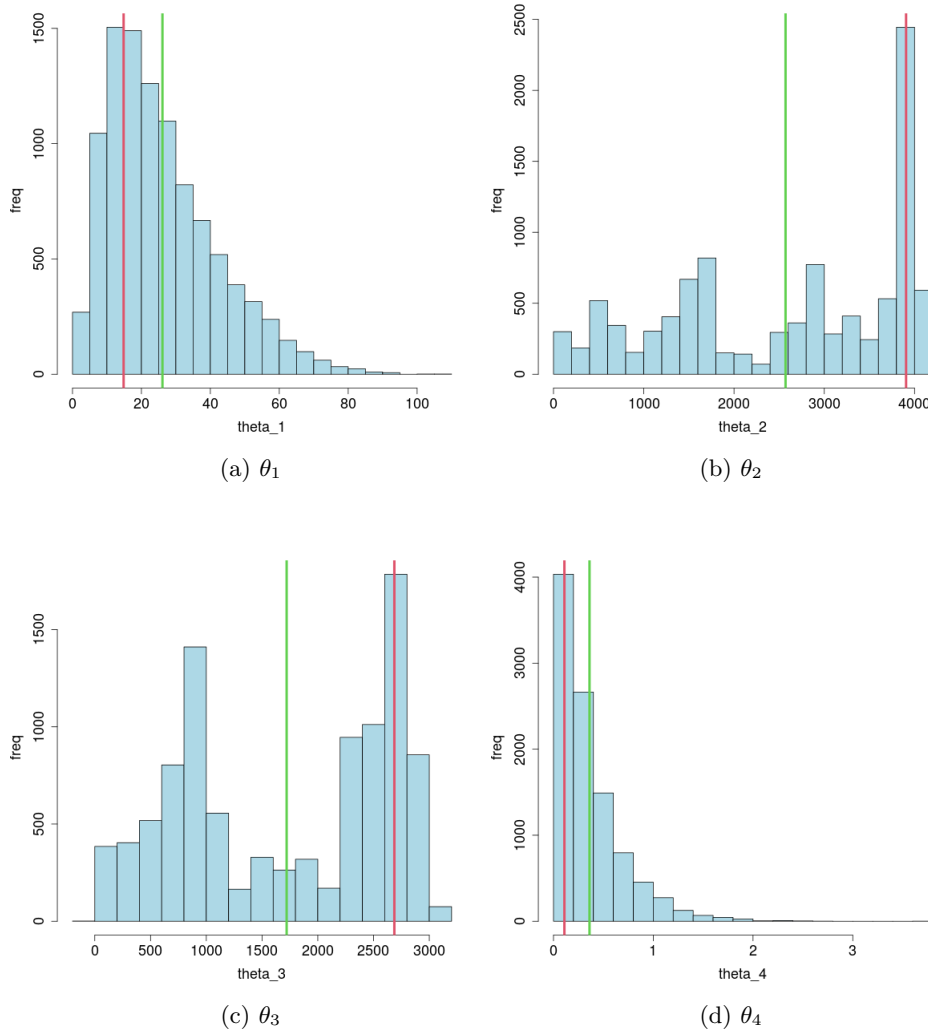


Figure 3: *Histogram of the posterior approximation of θ . The mean value are colored in green and the modal value in red.*

The posterior mean values of θ are used to make a new detection of the sources by the Hug model in Figure 4. Graphically, the areas containing the sources are smaller than with the empirical θ . The proposed sources computed from the estimation of θ are given in Table 5. As expected, the standard deviations of the sources are smaller with the estimated θ . Moreover, the distance between the proposed sources and the sources presented in PINTI et al. (2020) are also smaller. Based on this analysis, the detection method performs more accurately whenever the estimated θ are used.

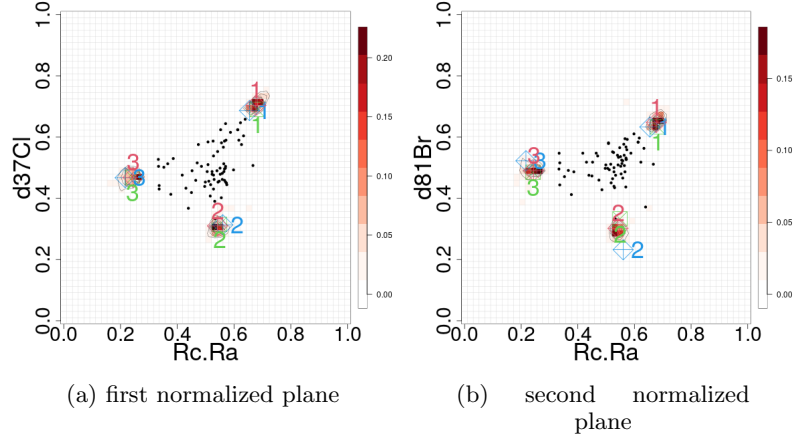


Figure 4: Visit map computed from the estimated θ for the real dataset PINTI et al. (2020). The blue symbols represent the sources reconstructed by PINTI et al. (2020), the green symbols are the centers of the clusters and the red symbols are the median points.

	"Rc/Ra"		"delta37Cl"		"delta81Br"	
	mean	sd	mean	sd	mean	sd
1 (mantle)	0.68	0.04	0.69	0.08	0.63	0.08
2 (subduction)	0.55	0.03	0.31	0.03	0.33	0.1
3 (crust)	0.24	0.04	0.47	0.03	0.48	0.04

Table 5: Proposed sources computed from the estimated θ .

Sources	Rc/Ra	$\delta^{37}\text{Cl}$	$\delta^{81}\text{Br}$	Mean Distance by Source
1	0.03	0.0	0.0	0.01
2	0.01	0.0	0.1	0.04
3	0.02	0.0	0.04	0.02
Mean Distance by Dimension	0.02	0.0	0.05	0.02

Table 6: Distance between the proposed sources computed from the empirical θ and the sources estimated in PINTI et al. (2020).

Conclusions and perspectives

This paper presented the ABC Shadow algorithm in order to determine appropriate parameters for the Hug model. This approach requires expert geologists knowledge. This knowledge is used either for an initial set up of the parameters in order to obtain a first source detection, or for manual detection of these sources. The pre-detected sources are used to estimate the model parameters that are finally plugged in the Hug model detection method in order to get final results. A visual inspection of the visit maps obtained from the detection with new parameters indicates a general improvement of the obtained results. As a perspective, we mention here the continuation of this study while taking into account data uncertainties. This work is in progress.

Acknowledgments

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