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Contaminant source localization via Bayesian global optimization

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Abstract. A Bayesian optimization approach to localize a contaminant source is proposed. The localization problem is illustrated with two 2D synthetic cases which display sharp transmissivity contrasts and specific connectivity patterns. These cases generate highly non-linear objective functions that present multiple local minima. A derivative-free global optimization algorithm relying on a Gaussian Process model and on the Expected Improvement criterion is used to efficiently localize the minimum of the objective function which identifies the contaminant source. In addition, the generated objective functions are made available as a benchmark to further allow the comparison of optimization algorithms on functions characterized by multiple minima and inspired by concrete field applications.

1 Introduction

The concept of polluter pays is not new (OECD, 1972) and holds for groundwater protection laws in many countries (USA, 1972; Swiss Confederation, 1983; European Union, 2000). The polluter can sometimes be identified by a specific chemical signature (Mansuy et al., 1997; Rachdawong and Christensen, 1997; Venkatramanan et al., 2016). However when signature is not unique, the ability to localize the contaminant source(s) using modeling technique can allow defining responsibilities or reducing decontamination costs. The topic is not recent and several approaches have been developed and proposed in the last three decades to identify contaminant source characteristics.

In their review of mathematical methods for groundwater pollution source identification, Atmadja and Bagtzoglou (2001a) classify existing approaches into four categories: *1) Optimization approaches*, in which forward simulations are run successively and the simulated concentrations are compared to measured concentrations (e.g., Gorelick et al., 1983; Wagner, 1992; Datta et al., 2011); *2) Probabilistic and geostatistical approaches*, in which the Advection Dispersion Equation (ADE) are solved backward in time based on the random walk particle methods (Bagtzoglou et al., 1992) or on stochastic differential equations (Wilson and Liu, 1994); *3) Analytical solution and regression approaches* (e.g., Ala and Domenico, 1992; Alapati and Kabala, 2000); *4) Direct approaches*, in which the ADE are solved backward in time based on deterministic direct approaches such as Tikhonov regularisation (Skaggs and Kabala, 1994; Atmadja and Bagtzoglou, 2001b), quasi-reversibility

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(Skaggs and Kabala, 1995), minimum relative entropy (Woodbury and Ulrych, 1996) or the backward bean equation (Atmadja and Bagtzoglou, 2001b).

A complementary classification is proposed by Amirabdollahian and Datta (2013) in their overview on contaminant source characteristics identification. Their classification is rather based on computational complexity and refines the *Optimization approaches* class mentioned above into three sub-classes: *1) Response Matrix*, in which unit responses are assembled linearly (e.g., Gorelick et al., 1983); *2) Embedded Optimization*, in which the objective function embeds directly mathematical equations of flow and transport (e.g., Mahar and Datta, 2001); *3) Linked Simulation-Optimization*, in which the optimization procedure calls numerical flow and transport simulators (e.g., Ayvaz, 2016). The proposed algorithm used hereafter belongs to this latter sub-class of algorithm.

In practice, geological media are heterogeneous. If one has a reasonable model of the underground heterogeneities, using an analytical solution will not allow integrating that information to identify contaminant source characteristics. To further simplify the classification proposed in the two reviews described above, we gather the different classes in two groups: backward or forward solver based approaches. Methods based on backward solvers consist in reversing the flow problem (Skaggs and Kabala, 1995; Milnes and Perrochet, 2007; Ababou et al., 2010). The ADE are solved backward in time. The transport physical processes are simulated 'backward' to localize the source and identify the release history. It regroups classes 2 and 4 as defined by Atmadja and Bagtzoglou (2001a). In that case, both flow-field and contaminated plume are assumed perfectly known. Methods using forward solvers are based on an inverse problem formulation (Aral et al., 2001; Yeh et al., 2007; Mirghani et al., 2012). The source location and release history are inferred from concentration samples. Parameter models are proposed and used as input in forward solver to simulate concentration breakthrough curves at the sample locations; when the mismatch between the simulated concentrations and the observed ones is within an acceptable level of error, the proposed model is accepted as a solution. This class of methods contains optimization methods as described by Atmadja and Bagtzoglou (2001a); Amirabdollahian and Datta (2013) but also posterior sampling methods which provide posterior probabilities of the solutions. In that class, less information about the contaminant plume is required and the method can be adapted to uncertain geology (Zhang et al., 2016).

Previous studies performed a characterization of the contaminant source in 1D (Woodbury and Ulrych, 1996), 2D (Singh and Datta, 2007) or 3D (Michalak and Kitanidis, 2004) modeling grids. The source is often identified along with other characteristics such as the release history(Aral and Guan, 1998), or the source geometry (Ayvaz, 2016). To the best of our knowledge, most existing studies consider the hydrogeological property field as homogeneous or multi-Gaussian like heterogeneous random field, which might not be the best representation of subsurface heterogeneity in flow and transport applications (Gómez-Hernández and Wen, 1998; Zinn and Harvey, 2003). One exception lies in the study conducted by Milnes and Perrochet (2007), reversing the flow, where the 2D synthetic aquifer represents channels and islands with a strong transmissivity contrast. So far, to the best of our knowledge, no geologically realistic medium has been used in an inverse problem formulation of contaminant source characteristics identification.

Optimization approaches to contaminant source characterization usually consist in minimizing an objective function that relies on a misfit between simulated measures and observations. The use of least square regression combined with linear

programming (Gorelick et al., 1983) assumes a linear system, which is not adapted for the contaminant source localization problem. Classical non-linear optimization techniques following a gradient based approach (Mahar and Datta, 2000; Datta et al., 2011) present the risk of being stuck in local minima. Employing a tabu search algorithm (Yeh et al., 2007) presents the same inconvenient as it explores neighbor solutions. Combining a gradient descent algorithm with a genetic algorithm (Aral et al., 2001; Ayvaz, 2016) decreases that risk, but the genetic algorithm might require a longer parameter exploration if the mutations are not guided by a smart rule. A Levenberg-Marquardt iterative algorithm (interpolates between the second order Gauss-Newton algorithm and the first order of a steepest descent algorithm Hansen and Vesselinov, 2016) might offer strategies to prevent being trapped in a local minimum. Simulated annealing (Amirabdollahian and Datta, 2014) allows for a broader exploration but at a very high cost. Bayesian optimization is a powerful approach that limits the risk of being trapped in local minima and explores smartly the parameter space by looking at figures of merit trading off exploitation of available results and space exploration such as the Expected Improvement (EI) criterion (Mockus, 1989; Jones et al., 1998a; Vazquez and Bect, 2010). To our knowledge, the latter method has not yet been tried on contaminant source characteristics identification problems.

The objective of this paper is threefold. Firstly, to assess the performance of an inverse problem formulation to identify contaminant source characteristics on a synthetic case that presents realistic hydrogeological property contrasts and connected structures, because 1) in spite of its advantages, inverse problem formulation to identify contaminant source characteristics has been employed only on multi-Gaussian type heterogeneities and 2) the type of heterogeneities strongly influences mass transport. Secondly, to verify the efficiency of an EI algorithm to identify contaminant source characteristics because such optimizers offer parameter space exploration possibilities that prevent being trapped in local minima at a much lower cost than with simulated annealing. Thirdly, to provide an open source benchmark that will allow testing and comparing optimization algorithms on application driven objective functions, as such objective functions are hardly available for the optimization community.

With this objective, we propose an original application of an EI algorithm to infer, in a deterministic inverse problem formulation, the contaminant source location in a 2D heterogeneous aquifer that presents realistic property contrasts and connectivity structures. To allow for a comparison between the optimizer exploration and an exhaustive search of the parameter space, the model grid is limited to 2D to keep reasonable computational cost for flow and transport simulations. The 2D synthetic model is generated with a multiple-point statistics (Guardiano and Srivastava, 1993) algorithm called *DeeSse* (Mariethoz et al., 2010), from a training image representing braided-river aquifer heterogeneous hydrogeological properties, that was generated by a pseudo-genetic algorithm (Pirot et al., 2015). The hydrogeological properties and flow boundary conditions are assumed perfectly known. The flow and transport equations are solved numerically by the *Groundwater* software (Cornaton, 2007). The optimization is performed using the DiceKriging and DiceOptim R packages (Roustant et al., 2012). In addition, we provide a benchmark for optimization algorithms, which relies on an objective function generator that can be customized by a choice between 2 geological scenarios, 2 possible locations for the contaminant sources and by the selection of observations among 25 wells. The performance of the EI algorithm is assessed by 100 replications from different initial designs.

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The paper is organized as follows. Section 2 describes the synthetic test case and the experimental setup. Section 3 explains the objective function generator. Section 4 details the steps of the EI algorithm. The results are presented in Section 5 and are discussed in Section 6. Conclusions are summed up in Section 7. The supplementary material provided online is listed in B.

2 Synthetic test cases

We consider two synthetic cases corresponding to 5 m thick × 600 m long × 300 m wide braided river aquifers. Each aquifer is represented by a unique, supposedly known 2D facies model (Figure 1) of 1 m by 1 m resolution to simplify the problem and to decrease the computing costs related to transport simulations. These 2D facies models (Figure 1), that present strong contrasts and possibly realistic spatial structures are obtained by MPS simulation, using the training image described in Figure

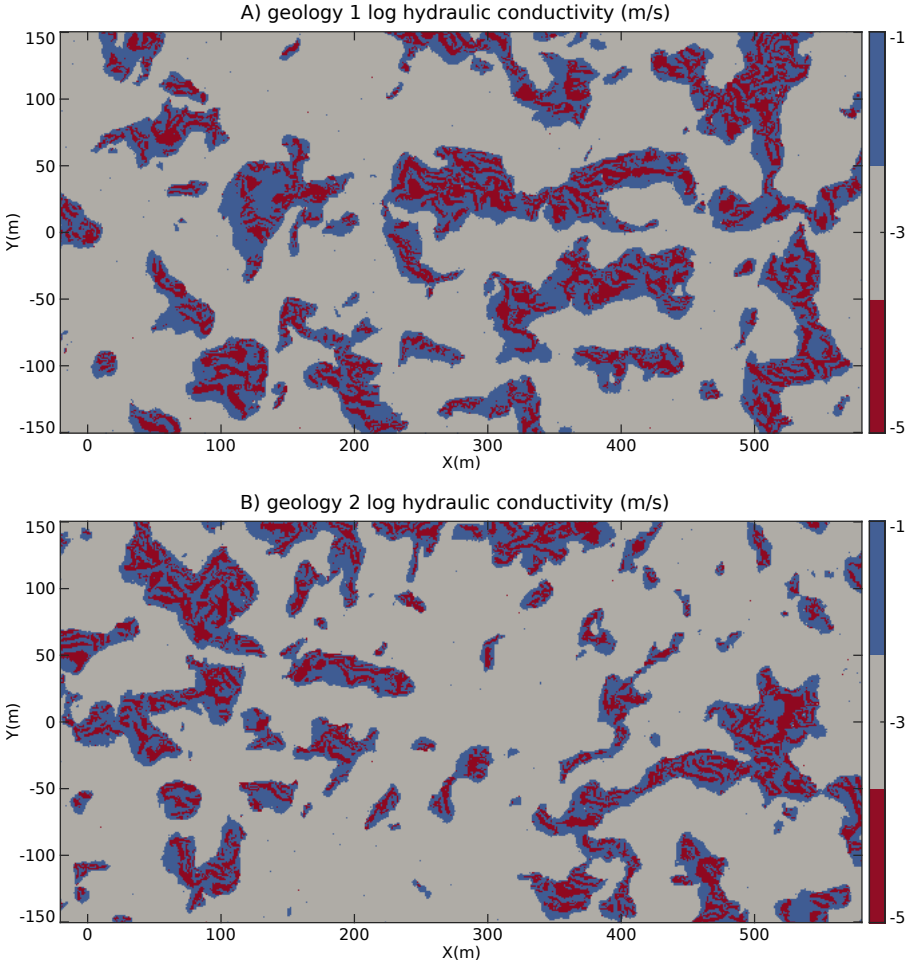

Figure 1. Experimental setup: 600m×300m 2D facies model of the aquifer; A) geology 1 and B) geology 2.

A1. The hydrogeological properties associated to the facies are given in Table 1 and are inspired from analogs described in the

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literature (Jussel et al., 1994; Bayer et al., 2011). Another possibility to obtain 2D horizontal models of braided river aquifers

facies	hydraulic conductivity $K(m/s)$	porosity	storage coefficient $S_s(m^{-1})$	molecular diffusion $D_m(m^2/s)$	longitudinal dispersivity $\alpha_L(m)$	transversal dispersivity $\alpha_{Th}(m)$
coarse sediments	10^{-1}	0.2	10^{-5}	10^{-9}	1	0.1
mixed sediments	10^{-3}	0.2	10^{-5}	10^{-9}	1	0.1
fine sediments	10^{-5}	0.2	10^{-5}	10^{-9}	1	0.1

Table 1. Hydrogeological parameters

from 3D models would have been to integrate vertically the hydraulic conductivity field, but as it smoothes out the hydraulic conductivity, the resulting 2D models present less contrasts and less realistic connected structures.

As boundary conditions for the flow and transport model, we impose a differential head of 2m on the length of the model and no flow on the sides (Figure 2). We assume steady-state flow conditions to run transport simulations by solving the ADE with the finite elements code Groundwater (Cornaton, 2007).

The source of the contaminant is supposed to be unique, punctual and located within a search zone delimited by a 150 m $\times$ 150 m square-domain whose coordinates belong to $[20, 170] \times [-75, 75]$. Two reference locations (A and B) were chosen for the source of the contaminant. Source A is located at ($x_s^A = 89, y_s^A = -36$). Source B is located at ($x_s^B = 100, y_s^B = 10$). The initial contaminant mass distribution at time 0 follows a multi-Gaussian distribution centered on the source location and of standard deviation ($\sigma_x = 2.5$ m,$\sigma_y = 1.0$ m) for a total mass $m = 100$ Kg. The reference concentration curves $c_{obs}(i,t)$ are obtained for $i = 1, \cdots, 25$ groundwater monitoring wells (denoted by a circle or a triangle) in Figure 3 and for times $t = 1, \cdots, T$ days. Three concentration breakthrough curves recorded at the well number 2, 16, and 22 are given as examples at the bottom of the figure.

The unknown location of the contaminant source is denoted $\mathbf{x} = (x_s, y_s)$. We define $c_{sim}(\mathbf{x}, i, t)$ as the simulated concentration level obtained at (i,t) when the contaminant source is located at $\mathbf{x}$. The aim is to find $\mathbf{x}$ that minimizes the following misfit objective function:

$$f(\mathbf{x}) = \left(\sum_{i=1}^{25} \sum_{t=1}^{T} |c_{obs}(i,t) - c_{sim}(\mathbf{x}, i, t)|^p \right)^{\frac{1}{p}}, \quad (1)$$

which corresponds to an ℓ^p norm. At the location of the reference source, the function reaches its minimum: 0. In this synthetic study, we neglect measurement errors on c_{obs} or conceptual or numerical errors on c_{sim} that may result for example from an incomplete knowledge of the transmissivity field or boundary conditions, which would be important to consider in a real field application.

The search zone is restricted to a discrete domain Z, using a regular grid of 3 m resolution for the following reasons. First, in practical applications, the location of the source is often restricted to a given polygon thanks to historical information about possible industrial activities or accidents. Here, we apply the same principle but assume a simple geometry since it is a synthetic example. Second, this procedure and geometry allows us to provide an exhaustive computation of the objective function for the research community. Third, it is an interesting problem because most available optimization programs work

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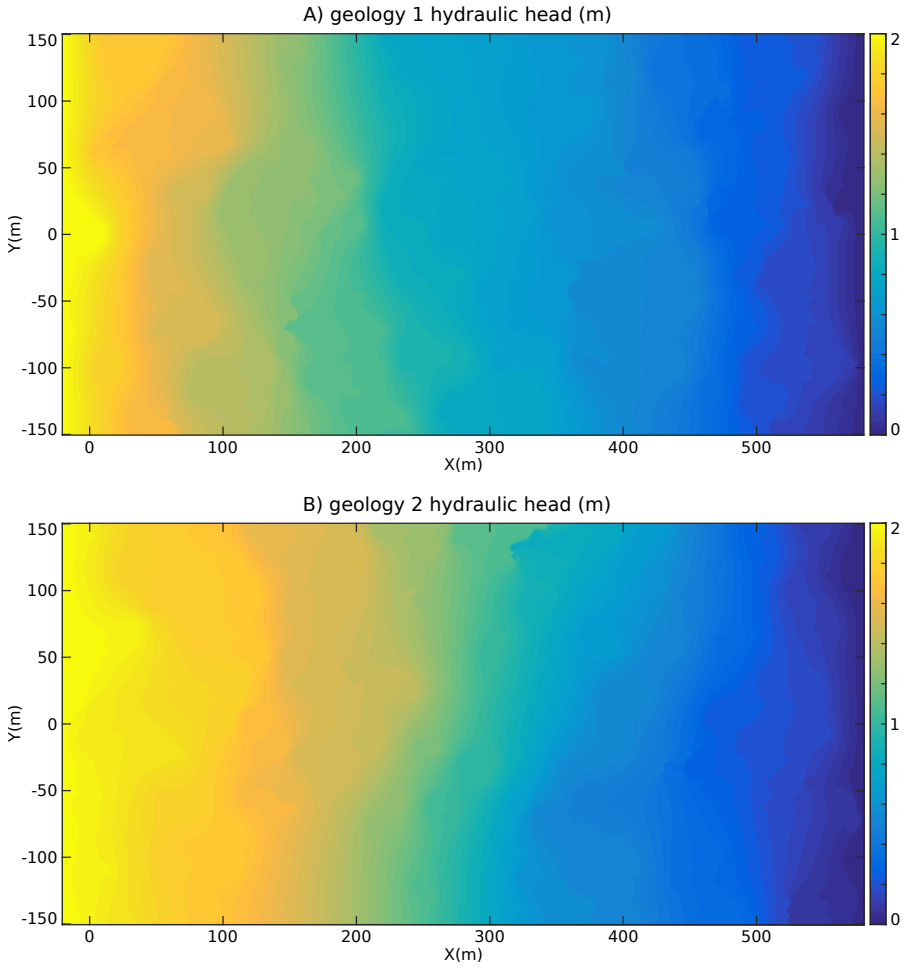

Figure 2. Steady state flow and boundary conditions for A) geology 1 and B) geology 2.

either on continuous domains or are dedicated to specific classes of optimization problems (Integer programming, mixed linear integer programming), and few seem to be available for non-linear optimization over finite sets beyond metaheuristics used in combinatorial optimization (Rios and Sahinidis, 2013). In the case of our contaminant localization problem, by the nature of the problem, we do have a continuous structure (objective function) where the domain is restricted to grid points. As an exhaustive evaluation of the objective function over Z is computationally expensive (depending on the mesh resolution), the aim of the optimization is to minimize the objective function f in the search zone within a limited number of iterations and for that purpose, we propose using an EI algorithm.

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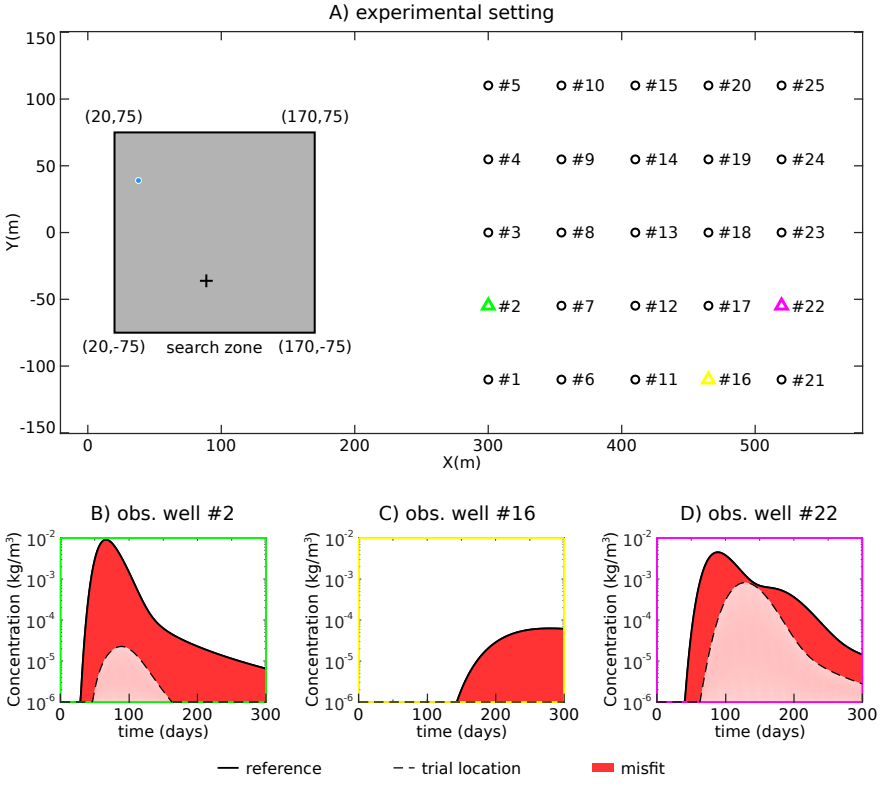

Figure 3. Misfit objective function settings; A) Location of the search zone (grey area) and of the 25 groundwater monitoring wells within the hydrogeological model boundaries; the cross marks the reference location of the contaminant while the blue dot denotes the trial location of the contaminant; B), C) and D) misfit components resulting from the comparison of the concentration breakthrough curves simulated at the trial location with the recorded ones for the reference location at wells 2, 16, and 22 respectively

3 Benchmark generator

By considering misfit functions parameterized by our different geologies, contaminant source locations or norms, a set of pre-computed objective functions was generated. It is used in this paper for testing a global optimization technique (EI algorithm). More precisely, misfit values varying over time at each of the 25 wells were calculated for 2 geological geometries, 2 reference locations (A and B) for the contaminant source and 2 types of norms used in the misfit objective function ($p = 1$ and $p = 2$) at a full factorial design of candidate points in the search zone Z. By allowing the possibility to consider any combination of observation wells among the 25, it leads to $2^3 \times (2^{25} - 1)$ possible test functions (i.e. more than 268×10^6 test cases). As these functions are known through their respective 51^2 values at the discretized source space Z, they can be re-interpolated (e.g. using splines) for continuous optimization purposes. Here we rather consider the discrete problem of selecting the optimal location among 51^2 candidates and for that goal, we will apply a straightforward discretized version of an EI algorithm as

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presented in the next section. The data and some R functions to generate benchmarks for any input parameters are provided on GitHub at https://github.com/gpirot/BGICLP. A brief description of the repository is given in the appendix of this paper.

4 Optimization methodology

The optimization algorithm used hereafter to minimize $f(\mathbf{x})$ over the domain belongs to a class of Bayesian optimization algorithms (Mockus, 1989; Shahriari et al., 2016). The Bayesian aspect refers to placing a random process prior Y on the unknown function f (possibly computationally expensive) and updating its probability distribution thanks to available evaluation results, and the optimization part relies on using conditional distributions of Y to iteratively choose points with the identification of f's global optimum/optimizer(s) in view. The crux is to fit adequate probabilistic models and also to design adapted *acquisition functions* (a.k.a *infill sampling criteria* in surrogate-based optimization) in order to drive algorithms to an efficient optimization.

A very popular class of probabilistic models used in such context rely on Gaussian Processes (GP), that are fully specified by a mean function $m(\mathbf{x})$ and a covariance function $k(\mathbf{x},\mathbf{x}')$. In this work, we use ordinary kriging with a Matérn ($\nu = 3/2$) covariance function (See Roustant et al. (2012) for details) and the kernel parameters are estimated by maximum likelihood using the DiceKriging R package. While it is also possible to appeal to a transformation of the response in GP-based optimization (See, e.g., Jones et al., 1998a), on the considered data it did not lead to substantial differences in optimization performance despite the non-negativity of the misfit.

Denoting training inputs and outputs as $\mathbf{X}_n = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$ and $\mathbf{f}_n = \{f(\mathbf{x}_1), f(\mathbf{x}_2), \ldots, f(\mathbf{x}_n)\}$, assuming a GP prior with a constant unkown mean (endowed with an improper uniform prior) leads to a Gaussian conditional distribution with the following marginal predictive mean and variance:

$$m(\mathbf{x}) = \hat{\mu} + \mathbf{k}(\mathbf{x})^T K^{-1}(\mathbf{f}_n - \hat{\mu}\mathbf{1}) \tag{2}$$

$$s^2(\mathbf{x}) = k(\mathbf{x},\mathbf{x}) - \mathbf{k}(\mathbf{x})^T K^{-1}\mathbf{k}(\mathbf{x}) + \frac{(1 - \mathbf{k}(\mathbf{x})^T K^{-1}\mathbf{1})^2}{\mathbf{1}^T K^{-1}\mathbf{1}}, \tag{3}$$

where K is the $n \times n$ prior covariance matrix (assumed invertible here) of responses at training inputs, with $K_{i,j} = k(\mathbf{x}_i, \mathbf{x}_j)$, $\mathbf{k}(\mathbf{x}) = (k(\mathbf{x},\mathbf{x}_1), ..., k(\mathbf{x},\mathbf{x}_n))^T$ is an $n \times 1$ covariance vector and $\hat{\mu} = \frac{\mathbf{1}^T K^{-1}\mathbf{f}_n}{\mathbf{1}^T K^{-1}\mathbf{1}}$ is the best linear unbiased estimate of μ.

The optimization algorithm typically starts with constructing a space-filling design $\mathbf{X}_{n_0} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_{n_0}\}$ (See, e.g., (Dupuy et al., 2015)) and evaluating $f(\mathbf{X}_{n_0})$ to initialize the knowledge of the algorithm (e.g., 9 blue dots in the left panel of Figure 4A). Here the initial $\mathbf{X}_{n_0}$ is generated based on latin hypercube sampling (McKay et al., 1979). Then, the algorithm begins its iterations. In each iteration, the ensemble of n available evaluations $\mathbf{f}_n = \{f(\mathbf{x}_1), f(\mathbf{x}_2), \ldots, f(\mathbf{x}_n)\}$ is used to train the GP model and make predictions at yet unexplored decision space locations. The predictive distributions is then used to compute the so called Expected Improvement criterion (Mockus, 1989) which indicates at each point in the decision space by how much the objective function value may be decreased relative to $f_{\min} = \min \mathbf{f}_n$, in expectation:

$$\mathrm{EI}_n(\mathbf{x}) = \mathbb{E}_n\left[\max(0, f_{\min} - Y(\mathbf{x}))\right]. \tag{4}$$

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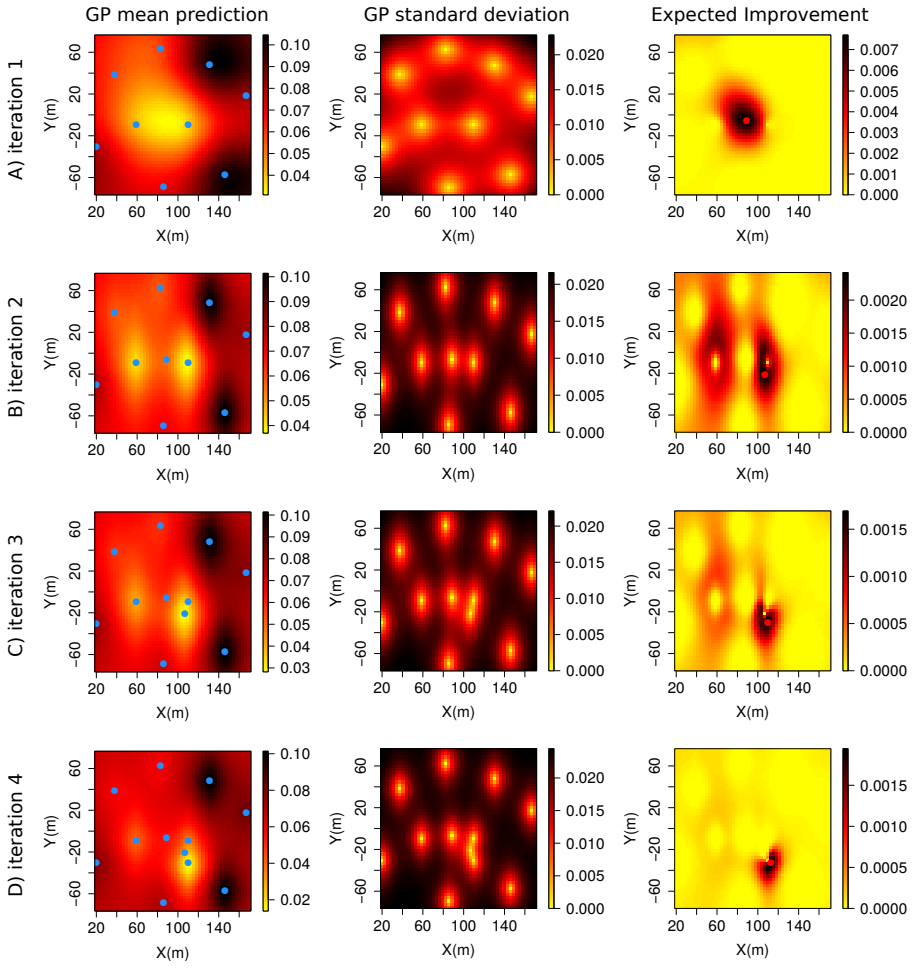

Figure 4. Illustration of the first four EI algorithm iterations for scenario 1; the sub-figures in the left column illustrate the prediction mean of f over the two-dimensional decision space at each iteration; the blue dots indicate the decision space locations where f was previously evaluated; the sub-figures in the center column illustrate the prediction variance of f over the two-dimensional decision space at each iteration; the sub-figures in the right column illustrate the expected improvement map over the two-dimensional decision space at each iteration; the red dot denotes the decision space location with the maximum EI value.

The EI criterion offers a good balance between exploitation of regions with low predictive mean values and exploration of regions with high predictive means, which provides an efficient optimization search scheme (e.g., red dot in the right panel of Figure 4A). It turns out that EI could be calculated analytically (Mockus, 1989; Jones et al., 1998b). In our discrete settings with moderate number of search points, the EI can be computed at all unevaluated locations of f (e.g. right panels of Figure 4). The decision space location with the largest EI value is considered as the next point $\mathbf{x}_{n+1}$ (e.g. red dot on right panels of Figure 4) to evaluate f. The optimization is run using the DiceKriging and DiceOptim R packages Roustant et al. (2012).

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Here the number of iterations is fixed in advance, so that it stops when the maximum number of iterations allowed is reached. Covariance parameters are updated after each iteration by Maximum Likelihood Estimation.

5 Results

Using information from the 25 observation wells, the optimization algorithm is applied over 4 configurations that depend on the retained geology and on the contaminant source location as described in Table 2, with the ℓ^2 norm taken for the objective function $f(x)$. Starting from a specific initial design, the exploration of the objective function by the EI algorithm (aiming at

case	type of geology	source coordinate
1	geology 1	$(89, -36)$
2	geology 1	$(100, 10)$
3	geology 2	$(89, -36)$
4	geology 2	$(100, 10)$

Table 2. Description of the 4 configurations.

the contaminant source localization), are displayed in Figure 5 for each scenario. These objective functions display multiple local minima, narrow valleys and sometimes very flat bottoms. These characteristics are making the search for the global minimum rather challenging especially for gradient based techniques. The locations explored by the EI algorithm are plotted over the 3m $\times$ 3m discretization of the objective function f. The white and blue dots represent respectively the initial and then explored locations where the objective function was evaluated by the algorithm. In most cases, the minimum of the discretized objective function is reached in less than 50 evaluations. The geology seems to be the dominating factor for the global patterns of the objective function. Note that for scenarios 2 & 4, the contaminant source is located at $(100, 10)$, which is not on the discretized grid of the objective function; the closest point on the discretized grid is $(101, 9)$. For scenarios 4, it implies that the contaminant reference source located at $(100, 10)$ and the minimum of the objective function located at $(80, 18)$ are 25m apart.

The performance of the optimization algorithm is assessed on 100 replications. Each replication is characterized by a specific and uniformly drawn 9-point initial design. Each run is allowed a total budget of 100 evaluations of the objective function. The performance depends on the number of iterations required to locate the minimum of the objective function $\min_{\mathbf{x}} f(\mathbf{x})$. It can be assessed directly by looking at the optimality gap, i.e., the distance between the location of the best estimated minimum $f_{\min}$ of the objective function and the location of its true minimum $\min_{\mathbf{x}} f(\mathbf{x})$ as a function of the number of evaluations of f (Figure 6A to D). Another possibility is to look at the normalized best found minimum misfit between the true minimum $\min_{\mathbf{x}} f(\mathbf{x})$ and the best estimated minimum of the objective function $f_{\min}$ as a function of number of evaluations of f (Figure 6E to H). Both indicators behave similarly. Finally, the performance of the localization algorithms can be assessed by analyzing the distribution of the distance of the explored location that is closest to the true contaminant source over the 100 replications for a given number of iterations (Figure 7). Independently from the considered scenario, the bin counts for lowest values significantly increase when the number of iterations increase, and the bin counts for distances over 20 m rapidly come down to 0.

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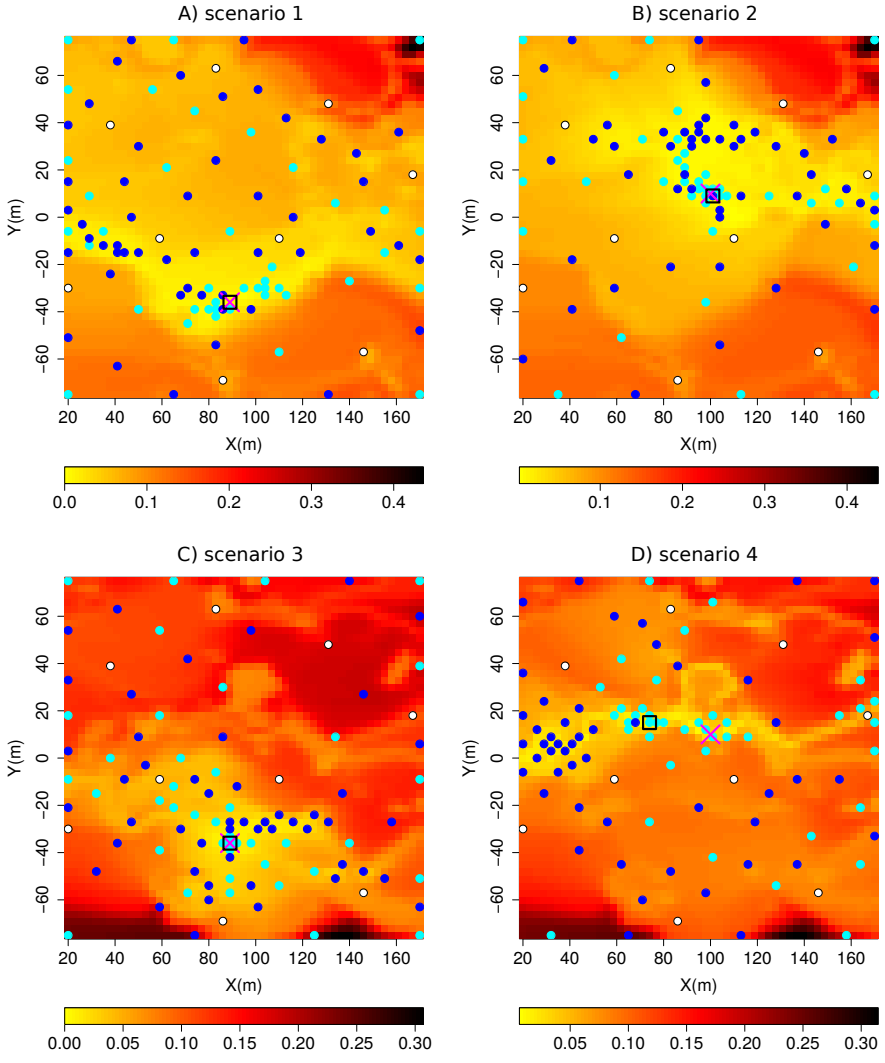

Figure 5. Solution exploration results for the 4 scenarios over the cost functions; A & B for geology 1; C & D for geology 2; A & C for initial contaminant location at $(89, -36)$; B & D for contaminant initial location at $(100, 10)$.

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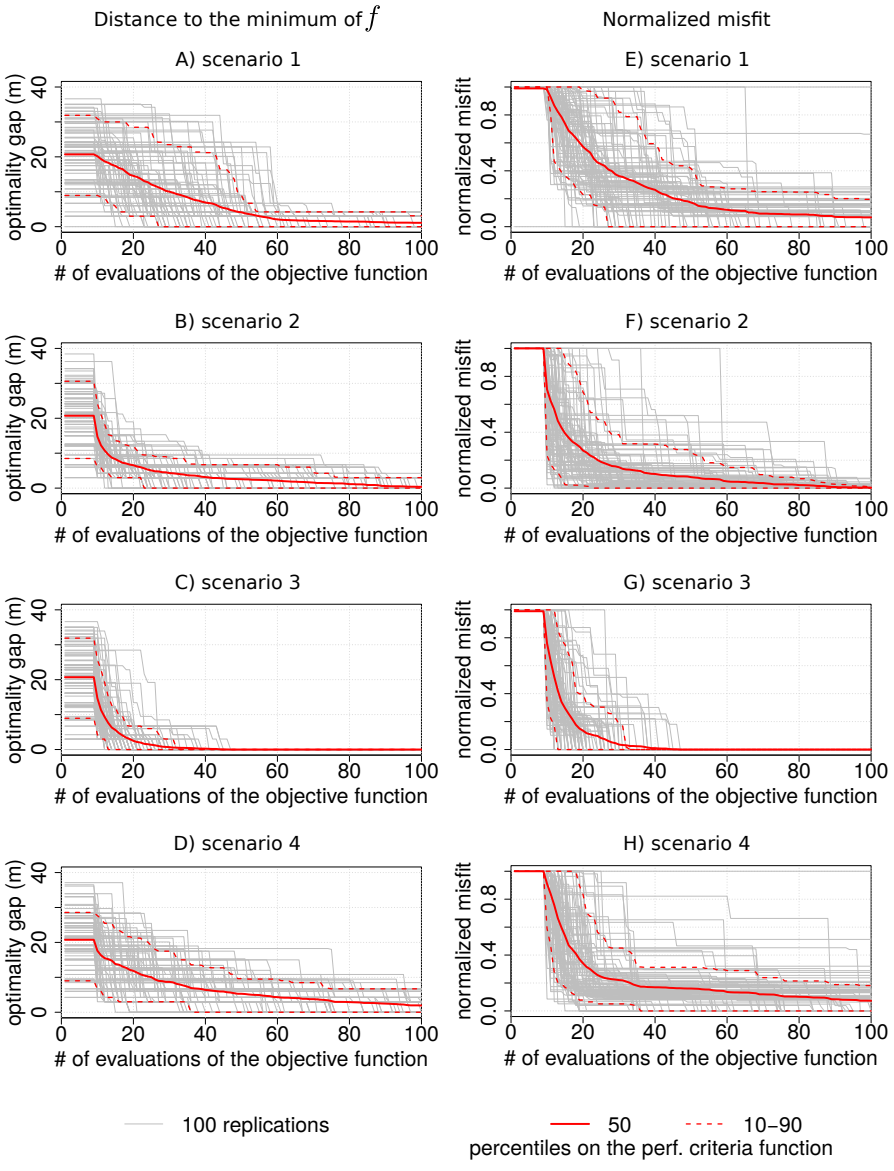

Figure 6. Performances of the EI optimization algorithm as a function of number of evaluations of the objective function for 100 different initial design; A), B), C) & D) distance of the best solution to the location of the objective function minimum; E), F), G) & H) normalized misfit; A) & E) scenario 1; B) & F) scenario 2 ; C) & G) scenario 3 ; D) & H) scenario 4.

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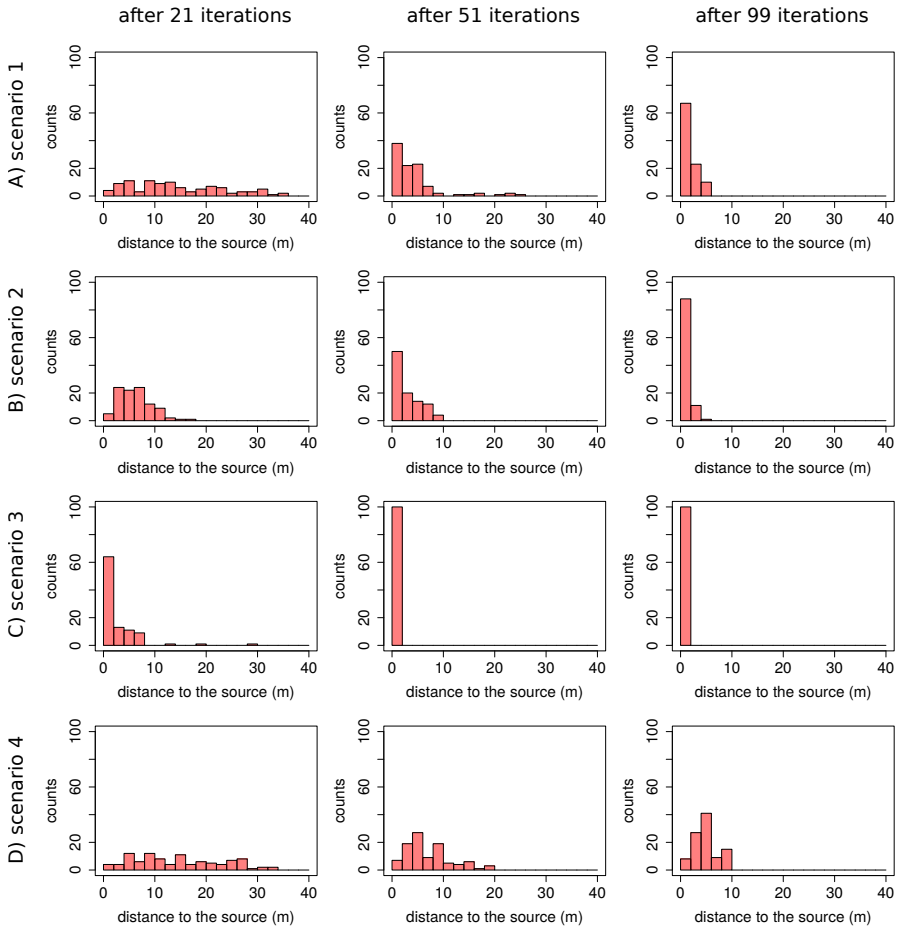

Figure 7. Distance to the contaminant source distribution for 100 replications for the best solution given by the EI algorithm ; row A) to D) for scenarios 1 to 4.

6 Discussion

Successively kriging the misfit of simulated versus observed concentrations and computing the expected improvement criterion, the proposed optimization algorithm localizes efficiently the source of a contaminant in a 2D geological environment representing realistic patterns and property contrasts. It requires only about 50 evaluations of the objective function instead of more than 2600 for an exhaustive evaluation on the discretized search zone ($\sim 1.9\%$). One can note that the total number of candidate points would increase exponentially in the number of dimensions of the parameter space, discarding exhaustive search already from moderate dimensions when assuming a high resolution.

The comparison of the different scenarios reveals that the geology controls the main features of the objective functions, which reinforce the importance of realistic geological structures in contaminant source localization problems. Of course, the shape and location of lower values of the objective functions are controlled by the true location of the contaminant source.

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The results presented here are based on an objective function f computed with $p = 2$, which corresponds to an ℓ^2 norm. As the choice of the norm strongly influences the flat or deep aspect of valleys (low value zones) of the objective function, we additionally tested the EI algorithm on the 4 scenarios for ℓ^1 norm objective functions. We found that squared ℓ^2 norm lead to flatter wide valleys of low values for the objective functions, which might not favor the efficiency of the EI optimizer. However, the results and performances of the EI algorithm are very similar for the different tested norms.

By making source code of the function generator available for public use, we provide a benchmark of objective functions, driven by real hydrogeological applications, for testing and comparing optimization techniques. This benchmark will fill a gap for the community of applied mathematicians and statisticians who develop optimization algorithm and who want to test their tools on possibly realistic objective functions. In addition, hydrogeologists benefit of the code provided in the GitHub repository so that they can implement the proposed optimization algorithm in their applications. For the given test case and its given structure, it does not seem relevant to apply off-the-shelf combinatorial algorithms. However it would be certainly of interest to compare to genetic/evolutionary algorithms compatible with such settings. Also, to enable comparisons with a broader class of derivative-free and also derivative-based algorithms, a pragmatic approach here would be to re-interpolate the data (with a careful inspection of the optima of the interpolator, i.e. a check that it is not perturbing the problem by too many potential artifacts) and conduct a benchmark involving Bayesian optimization (with EI and potentially also other infill sampling criteria) against a selection of state-of-the-art algorithms.

Strong assumptions have been made to localize the contaminant source in the presented application. The hydrogeolological properties and the flow boundary conditions are supposed to be perfectly known and the hydrogeological model is spatially limited to two dimensions. Because of their expensive computing costs, three-dimensional applications will not allow for an exhaustive search of the solution; this is why they may require optimization algorithms such as the one proposed in this paper in a near future. Further research should also take into account the uncertainty related to hydrogeological properties characterization and flow and transport boundary conditions. Some steps have already been made in that direction (Koch and Nowak, 2016) but were limited to multi-Gaussian conductivity fields. In addition, a regular grid discretization might compromise the location of the contaminant source in the presence of strong flow path: in a real application, the contaminant source encounters a very low probability to be located on a grid node. This problem could be avoided by using adaptive meshing, which would require more computing resources.

7 Conclusions

The use of 2D hydraulic conductivity fields that present sharp contrasts and specific connectivity patterns produces complex objective functions with multiple local minima. The proposed benchmark tool resulting from these complex functions offers challenging testing for developers of optimization algorithms. The EI algorithm used in this 2D study localized efficiently the contaminant source that is located on a grid node. More generally, the proposed algorithm is an interesting approach for combinatorial optimization algorithm.To improve the limitation imposed by a source centered on the nodes of a fixed mesh, which is independent of the optimization algorithm, future research could be conducted on optimization embedding adaptive

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meshing in flow and transport simulations; another possibility would be to relax the constraint on mass distribution of the initial plume as a way to deal with its related uncertainty. The good performance of the algorithm on this 2D case is encouraging to continue toward 3D applications and toward integration of geological uncertainty in contaminant source localization problems.

Code and data availability. The data and some R functions to generate benchmarks for any input parameters are provided on GitHub at https://github.com/gpirot/BGICLP. A brief description of the repository is given in the appendix of this paper.

Appendix A: Training Image

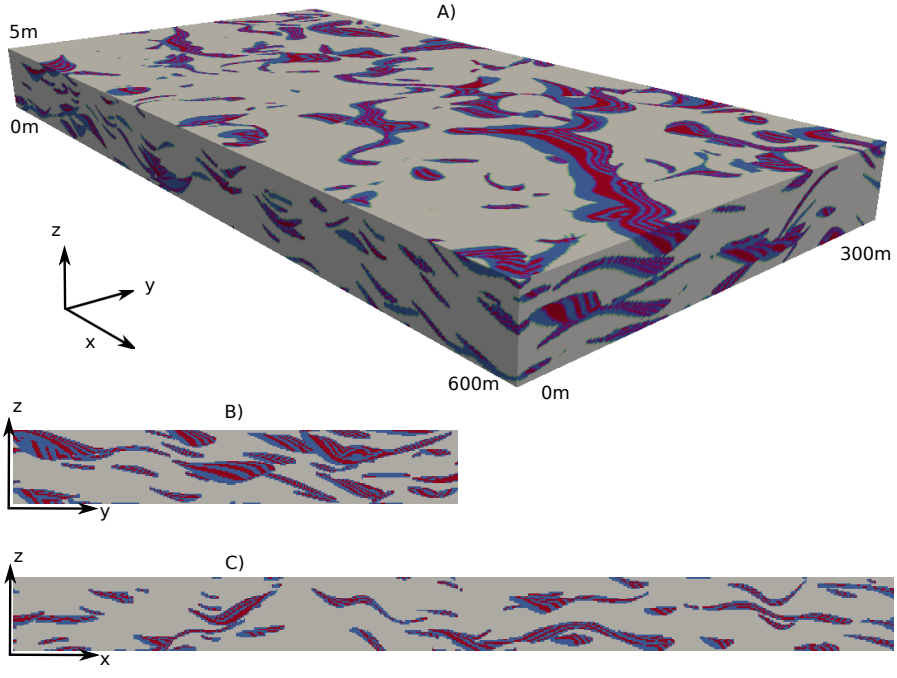

Figure A1. 600m ×300m ×5m training image with vertical scale exaggerated by 10; A) 3D representation; B) vertical section transversal to the main flow direction; C) vertical section longitudinal to the main flow direction. This three-dimensional model was generated by a pseudo-genetic algorithm proposed by Pirot et al. (2015). It is obtained by imitation of successive erosion and deposition events. Successive conditional simulations of topographies (Pirot et al., 2014) stacked together produce successive layers that are filled by heterogeneous geological facies according to a rule mimicking flow and sedimentation processes.

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Appendix B: Supplementary material

The electronic supplementary material provided on the GitHub repository at https://github.com/gpirot/BGICLP with this paper contains 3 folders and 2 R-scripts.

The 'data' folder contains 1) the evaluation of sub-functions

$$f^p(\mathbf{x}, i) = \sum_t |c_{obs}(i,t) - c_{sim}(\mathbf{x}, i, t)|^p$$

over Z at $i = 1, \cdots, 25$ observation wells for each of the 8 possible configurations (2 geologies, 2 sources, 2 norms) in the 'grid_25_wells_*.txt' files, 2) the $\mathbf{x}$ coordinates of the search zone Z and 3).

The 'figures' folder contains illustrations of $f(\mathbf{x})$ over Z for each of the 4 configurations when considering the 25 wells with the ℓ^2 norm.

The 'src' folder contains 3 R scripts. The 'image.scale.R' script, created by Pretty R at inside-R.org is used for graphic illustration purposes. The 'generate_lhs_on_grid.R' script allows generating initial point designs by latin hypercube sampling. The 'functionGenerator.R' script takes as arguments a selection of observation wells $\mathcal{W}$, a type of geology, the source coordinates and the type of norm used. It produces the evaluation of the function

$$f^p(\mathbf{x}, \mathcal{W}) = \sum_{i \in \mathcal{W}} f^p(\mathbf{x}, i)$$

over Z. When all wells are considered, $f^p(\mathbf{x}, \mathcal{W})$ resumes to $f(\mathbf{x})$ in Eq. 1.

The 'plotGeneratedFunction.R' script illustrates the use of the function generator and saves the plot in the 'figures' folder. The 'runEGO.R' script gives an example of how to use the proposed optimization algorithm.

Competing interests. The authors declare that they have no conflict of interest.

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