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A Derivative Free Optimization method for reservoir characterization inverse problem

Hoël Langouët, Frédéric Delbos, Delphine Sinoquet and Sébastien Da Veiga

Reservoir characterization inverse problem aims at building reservoir models consistent with available production and seismic data for better forecasting of the production of a field . These observed data (pressures, oil/water/gas rates at the wells and 4D seismic data) are compared with simulated data to determine unknown petrophysical properties of the reservoir. The underlying optimization problem is usually formulated as the minimization of a least-squares objective function composed of two terms : the production data and the seismic data mismatch. In practice, this problem is often solved by nonlinear optimization methods, such as Sequential Quadratic Programming methods with derivatives approximated by finite differences. In applications involving 4D seismic data, the use of the classical Gauss-Newton algorithm is often infeasible because the computation of the Jacobian matrix is CPU time consuming and its storage is impossible for large datasets like seismic-related ones.

Consequently, this optimization problem requires dedicated techniques: derivatives are not available, the associated forward problems are CPU time consuming and some constraints may be introduced to handle a priori information. We propose a derivative free optimization method under constraints based on trust region approach coupled with local quadratic interpolating models of the cost function and of non linear constraints. Results obtained with this method on a synthetic reservoir application with the joint inversion of production data and 4D seismic data are presented. Its performance is compared with a classical SQP method (quasi-Newton approach based on classical BFGS approximation of the Hessian of the objective function with derivatives approximated by finite differences) in terms of number of simulations of the forward problem.

Introduction

The goal of reservoir characterization is the estimation of unknown reservoir parameters by integrating available data in order to take decisions for production scheme and to predict the production of the field in the future. Reservoir parameters can be classified in two classes: those related to the geological modeling (spatial distribution of porosity, permeability, faults), and those related to the fluid flow modeling (relative permeability curves, productivity index of the wells). These parameters cannot be directly determined by measurements (or only locally using well logs). This is the reason why this parameter estimation problem is formulated as an inverse problem with forward simulators that compute synthetic measurable data from the parameters : production data acquired at production/injection wells (e.g. bottom-hole pressure, gas-oil ratio, oil rate), time lapse seismic data (more precisely compressional and shear wave impedances for different seismic campaigns at different calendar times during the production of the field). The associated forward models consist of a fluid flow simulator and a petro-elastic model (PEM) based on rock physic Gassmann equations. For further details on this application see Roggero et al. (2008). Solving these forward problems is often CPU time consuming and does not provide the derivatives with respect to the parameters.

The optimization problem is formulated as the minimization of a least-squares objective function composed of two terms, one for the production data mismatch and one for the seismic data mismatch. Some weights are introduced to account for data uncertainties and modeling errors. In practice, these problems are often solved by nonlinear optimization methods, as SQP¹ method (Sinoquet and Delbos, 2008) with derivatives approximated by finite differences (FD).

In our application, using the classical Gauss-Newton algorithm is often infeasible because the computation of the Jacobian matrix is CPU time consuming and its storage is impossible for large datasets involving seismic data. Consequently, a natural alternative choice is a quasi-Newton approach based on classical BFGS approximation of the Hessian of the objective function with derivatives approximated by FD. Although these SQP methods are particularly efficient for the determination of active constraints, the number of function evaluations is usually too high for industrial problems with expensive simulators. Furthermore, the choice of the FD step, crucial for the convergence of this method, is generally cumbersome because it depends on the accuracy of the function computation which is difficult to estimate in practice. This is the reason why, we are interested in Derivative Free Optimization (DFO) methods.

There are mainly four classes of DFO methods in the literature. The first class is composed of direct search methods that explore the variable space by sampling points from a predefined class of geometric patterns or involve some random process (Nelder and Mead, 1965; Audet and Dennis, 2003; Kolda et al., 2003). These methods do not assume generally, smoothness of the objective function and therefore can be applied to a broad class of problems. But, on the other hand, a relatively large number of function evaluations are often required. These methods are theoretically simple and relatively easy to implement. The second class is the class of metaheuristic methods, for instance the evolution strategy (Hansen and Ostermeier, 1996), or the simulated annealing (Kirkpatrick et al., 1983): they explore the parameter space with a population of sampling points evolving towards the global optimum. This class of methods does not assume any regularity assumption on the objective function but requires a large number of function evaluations. The third class of methods combines gradient approximation techniques (e.g. finite difference (Sinoquet and Delbos, 2008) or simplex gradient (Kelley, 1999; Winslow et al., 1991)) with quasi-Newton methods. These methods are not always robust, especially in the presence of noise, which is often the case for derivative-free applications. The fourth class of methods is based on sequential minimizations of models of the objective function to limit the number of evaluations of the expensive function. These models can be local or global models:

- A global model constructed from a limited number of evaluations of f for parameters values

¹Sequential Quadratic Programming

chosen according to a relevant criterion (minimum prediction error, space filling, expected gain improvement.), can be, for instance, kriging models (Schonlau, 1997; Jones, 2001; Villemonteix, 2008) or Radial Basis Functions (RBF) (Gutmann, 2001; Regis and Shoemaker, 2007). But they are limited to small size problems (10-30 parameters).

- A local model is generally based on linear or quadratic polynomial interpolation of evaluations of the objective function at sample sets (Conn et al., 2000, 2009a; Powell, 2006, 2007; Marazzi and Nocedal, 2002; Vanden Berghen, 2004). Some recent comparison (Langouët and Sinoquet, 2009) based on a benchmark proposed in Moré and Wild (2009), illustrates good performances of trust region model-based methods compared to three other approaches, even for noisy and piecewise-smooth problems. Even if the three others class of methods are still widely used in the engineering community, they require generally more simulations than the local trust region model-based methods.

In this paper, we propose an adapted method based on local surrogate models (Conn et al., 2000, 2009b; Powell, 2006) belonging to the fourth class of method: these methods are inspired by SQP methods with trust region globalization. The proposed Sequential Quadratic Approximation method (SQA) is an extension of NEWUOA, the efficient Derivative Free Optimization method of Powell (2006), for constrained optimization.

In the first part of this paper, we describe the main features of the SQA method. The second part presents results of this method applied to a challenging benchmark proposed by Jones (2008). The third part is dedicated to a 3D synthetic reservoir application with the joint inversion of production data and 4D seismic data.

SQA Method

The SQA method is a DFO method adapted to constrained optimization of nonlinear function

$$\begin{aligned} & \min_{x \in \mathbb{R}^n} f(x) \\ & \text{s.t.} \quad \begin{cases} C_{DB}(x) \leq 0, \\ C_{DF}(x) \leq 0, \end{cases} \end{aligned} \quad (1)$$

where the derivative free constraints C_{DF} (responses of simulator with unknown derivatives) and the constraints with given derivatives C_{DB} are separated ($C_{DB} : \mathbb{R}^n \rightarrow \mathbb{R}^{n_{DB}}$, $C_{DF} : \mathbb{R}^n \rightarrow \mathbb{R}^{n_{DF}}$).

The SQA algorithm is given in Algorithm 1. At an initial stage, a quadratic model \tilde{f} of the function f is constructed in a neighborhood of the current point. It interpolates m points² (usually $m = 2n + 1$ is chosen) in the admissible domain (at least matching linear constraints). For each derivative free constraint, a quadratic model \tilde{C}_{DF} is also constructed from the same interpolation points. Indeed, for any function f or C_{DF} and any poised set $Y = \{y^0, y^1, \dots, y^p\} \subset \mathbb{R}^n$, the minimum-norm interpolating polynomial Q and \tilde{C}_{DF} that interpolate f and C_{DF} on Y can be expressed as

$$\tilde{f}(x) = \sum_{i=0}^p f(y^i) l_i(x), \quad \tilde{C}_{DF}(x) = \sum_{i=0}^p C_{DF}(y^i) l_i(x), \quad (2)$$

where $\{l_i(x), i = 0, \dots, p\}$ is the set of minimum-norm Lagrange polynomials for Y (see Conn et al. (2009b)).

Then, at each iteration the problem is solve for the current precision on parameters ρ^3 : the current quadratic model \tilde{f} is minimized under constraints C_{DB} and models of derivative free constraints \tilde{C}_{DF}

²The incomplete quadratic models ($n + 2 \leq m \leq (n + 1)(n + 2)/2$) are completed by minimizing the Frobenius norm of the hessian matrix variations of the models (Powell, 2006)

³ ρ is the current resolution expected on x . It is updated during optimization process (see in Algorithm 1).

in a trust region of radius Δ around the optimal point by a SQP method:

$$\begin{aligned} & \min_{d \in \mathbb{R}^n} \tilde{f}(x_{opt} + d) \\ & \text{s.t.} \quad \begin{cases} C_{DB}(x_{opt} + d) \leq 0, \\ \tilde{C}_{DF}(x_{opt} + d) \leq 0, \\ \|d\| \leq \Delta. \end{cases} \end{aligned} \quad (3)$$

f and C_{DF} are evaluated at $x^* = x_{opt} + d_k$, solution of (2).

If the merit function

$$\varphi(x) = f(x) + \sum_{i=1}^{n_{DF}} \lambda_i C_{DF(i)}(x), \quad (4)$$

measuring the constraint violation and f , has decreased, x^* is validated as the new current optimal point x_{opt} , where λ is supposed to represent the unknown Lagrange multipliers in this algorithm. λ is set to a constant value that takes into account the normalization of the function f and the constraints C_{DF} .

Otherwise, another point is added in order to improve the quadratic models: a criterion based on the interpolating Lagrange polynomial is maximized, see Powell (2006). Finally, the trust region radius Δ is updated according to the comparison of the reduction of the merit function based on models \tilde{f} and \tilde{C}_{DF} and the effective reduction of the merit function based on f and C_{DF} :

$$R = \frac{\varphi(x_k) - \varphi(x_k + d_k)}{\tilde{\varphi}(x_k) - \tilde{\varphi}(x_k + d_k)}. \quad (5)$$

So, Δ is increased if the "modeled" merit function has the correct trends compared to the "real" merit function or decreased otherwise. The quadratic models \tilde{f} and \tilde{C}_{DF} are updated to interpolate the m closest points to the current optimal point (where f and C_{DF} were evaluated). The algorithm is stopped when the minimal trust region radius (accuracy on the solution requested by the user) is reached or when the maximum number of simulations given by the user has been performed.

MOPTA08 Benchmark

The MOPTA08 benchmark is a very complex and challenging minimization problem proposed by Jones (2008): it was built from a real automotive problem. The goal is to optimize vehicle performance subject to security constraints. The simulation (e.g. crash test) is very expensive in terms of computational time: 60 simulations can optimistically be computed per day. This function depends on 124 parameters under 68 derivative free constraints (blackbox constraints).

In order to share this application with the optimization community, Jones (2008) built kriging response surface of the objective function and of the constraints from simulations of the real problem. The main objective of this benchmark is to reduce the objective function value below a threshold of 228 (the initial function value is 251) in less than 1800 evaluations (15 times the number parameters which corresponds to one month of CPU time of the real simulator).

The result obtained by SQA method is presented in Figure 1, where the evolution of the objective function is depicted with respect to the number of simulations.

They are very promising: indeed, the threshold of 228 is reach in 800 simulations and all the constraints are satisfied. Jones has shown that lot of tested optimization methods failed to solve this problem: a classical SQP with finite differences, an evolution strategy method,... Only, one method based on RBF (radial basis functions) approximation of the objective function and of the constraints (Regis, 2009) gives similar performances than SQA method. With this application, we show the ability of SQA to

Algorithm 1 SQA Algorithm (Sequential Quadratic Approximation)

(1) Initialization : Select m initial interpolation points. x_{opt} is the initial point for which f is minimal among the m points. Determine the first quadratic model $\tilde{f} \approx f$ of the objective function f and the quadratic models \tilde{C}_{DF} of the derivative free constraints C_{DF} .

Δ is the trust region radius: $\rho = \Delta = \rho_{beg}$.

(2) Solve the problem for a precision on x : ρ

(a) (i) Minimize the model :

$$\min_d \tilde{f}(x_{opt} + d)$$

$$\text{s.t.} \begin{cases} \|d\| \leq \Delta, \\ C_{DB}(x_{opt} + d) \leq 0 \\ \tilde{C}_{DF}(x_{opt} + d) \leq 0 \end{cases}$$

(ii) If $\|d_k\| < \frac{1}{2}\rho$: \rightarrow (2)(b) (necessary to ensure the validity of the model before doing small steps).

(iii) Calculate $f(x_{opt} + d_k)$, $C_{DF}(x_{opt} + d_k)$,
 $\varphi(x_{opt} + d_k) = f(x_{opt} + d_k) + \sum_{i=1}^{n_{DF}} \lambda_i C_{DF(i)}(x_{opt} + d_k)$ and update the trust region radius Δ from the predictivity of the quadratic models $R = \frac{\varphi(x_{opt}) - \varphi(x_{opt} + d_k)}{\tilde{\varphi}_k(x_{opt}) - \tilde{\varphi}_k(x_{opt} + d_k)}$.
 Update interpolation points : $x_{opt} = x_{opt} + d_k$ if $\varphi(x_{opt} + d_k) < \varphi(x_{opt})$ and update the models \tilde{f} and \tilde{C}_{DF} in order to interpolate the function f and the derivative free constraints C_{DF} in $x_{opt} + d_k$.

(iv) If $R > 0.1 \rightarrow$ (2)(a)(i)
 Otherwise continue.

(b) Test the validity of the model \tilde{f} and \tilde{C}_{DF} . The model is considered valid if all the current interpolation points x_i , $i = 1, \dots, m$ are close to the optimal point x_{opt} , i.e. if the Euclidean distance $\|x_i - x_{opt}\| < 2\Delta$ for all x_i , $i = 1, \dots, m$.

(i) If the model is not valid :

Improve the quality of the model \tilde{f} and \tilde{C}_{DF} :

$$\max_{d \in \mathcal{R}^n} |l_t(x_{opt} + d)|$$

$$\text{s.t.} \begin{cases} \|d\| \leq \bar{\Delta}, \\ C_{DB}(x_{opt} + d) \leq 0 \end{cases}$$

Calculate $f(x_{opt} + d_k)$ and $C_{DF}(x_{opt} + d_k)$, the worst point of the interpolation set is replaced by a new point closer to the current minimum.

Assuming that the accuracy of the updated models \tilde{f} and \tilde{C}_{DF} has been improved \rightarrow (2)(a)(i).

(ii) If the model is valid : If $\|d_k\| > \rho \rightarrow$ (2)(a)(i)
 Otherwise continue

(c) If $\rho > \rho_{end}$: reduction of ρ and $\Delta \rightarrow$ (2)(a) (zoom on x)
 Otherwise end of the algorithm.

deal with large size problem with a large number of constraints. In the next section, SQA is applied to a realistic reservoir application.

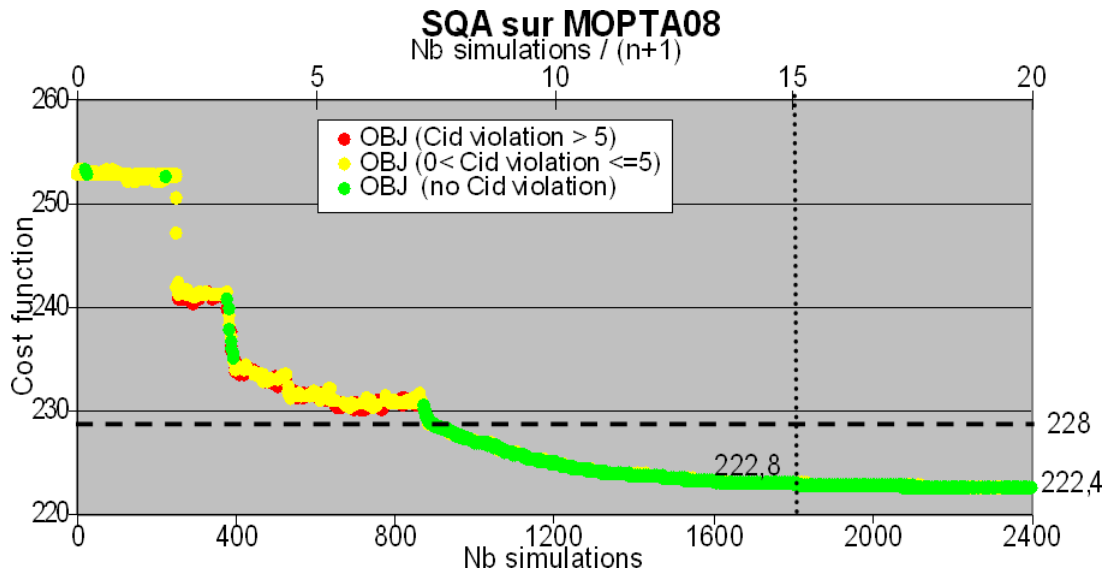


Figure 1: Objective function versus simulation number for optimization with SQA method for 249 interpolation points ($2n + 1$).

Reservoir application: inversion of monitor seismic datasets

The PUNQ test case is a 3D synthetic reservoir model derived from real field data. It was already used for comparative inversion studies in the European PUNQ project (Floris, 2001) and for validation of constrained modeling and optimization scheme development methods (Roggero, 2001). The top structure of the reservoir is presented in Figure 2.

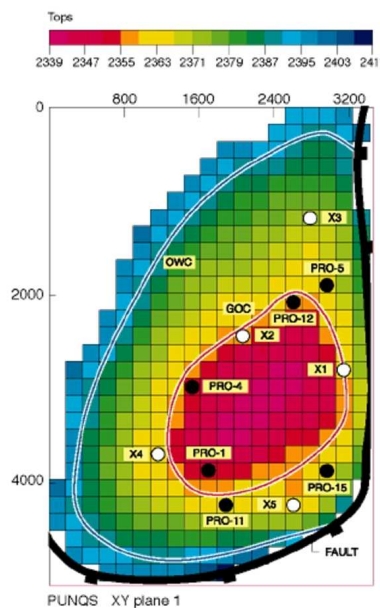


Figure 2: Top structure of the reservoir.

The reservoir is surrounded by an aquifer in the north and the west, and delimited by a fault in the south and the east. A small gas cap is initially present. The geological model is composed of five independent layers. The layers 1, 3, 4 and 5 are assumed to be of good quality, while the layer 2 is of poorer quality.

The initial model consists of a $19 \times 28 \times 5$ grid, with a constant step of 180 m in the horizontal X and Y directions. In order to illustrate the potential of the algorithm on large seismic data sets, we decided to build a larger model. Therefore, our reference model consists of a $76 \times 56 \times 5$ grid, with a constant step of 45 m in the X direction and 90 m in the Y direction. Each geological unit is modeled by one layer, with a Gaussian distribution of the porosities and a spherical variogram. The geostatistical simulation parameters are listed in Table 1. The permeability on each layer is defined by a $(\log K - \phi)$ relationship, i.e. $\log(K_x) = A\phi + B$ with constant ratios K_y/K_x and K_z/K_x . The corresponding reference parameters are given in Table 1.

Table 1: Corresponding reference of geostatistical simulation parameters.

	ϕ mean	ϕ variance	A	B	K_y/K_x	K_z/K_x
Layer 1	0.1722	0.0078	8.585	0.701	1	0.364
Layer 2	0.0802	0.0004	14.383	0.258	1	0.339
Layer 3	0.1677	0.0050	8.683	0.781	1	0.314
Layer 4	0.1615	0.0006	4.209	1.789	1	0.211
Layer 5	0.1892	0.0049	8.98	0.793	1	0.296

Then, the geostatistical simulations are upscaled to come back to the original $19 \times 28 \times 5$ grid in order to work with a faster fluid flow simulation in the reservoir. The synthetic production data are produced by a numerical simulation using the ATHOS model over a eight-year period. The production results selected as synthetic measurements are the gas oil ratio (GOR), the bottomhole pressure (BHP) and the water cut value (WCUT) at the six producing wells (PRO-1, 4, 5, 11, 12 and 15). We give on the left of Figure 3 the reference production data for all wells.

Then, pressure and saturations maps simulated by the ATHOS model at times 0 days, 181 days (half a year) and 2192 days (six years) are extracted and downscaled to the $76 \times 56 \times 5$ grid. A petro-elastic model (PEM) involving Gassmann and Hertz equations is defined with given bulk and dry modulus, bulk densities and Hertz exponents. The combination of downscaled pressure and saturations maps with this petroelastic model allows to compute synthetic P and S impedance maps at times 0, 181 and 2192 days. These maps serve as a synthetic 4D seismic data set. An example of the reference impedance map on layer 5 at time 0 and Delta impedance maps at times 181 and 2192 is depicted on the right of Figure 3.

For history matching, the parameters of the simulation model are constrained by both production and seismic data. An optimal matching is sought by minimization of an objective function defined as follows:

$$f(x) = \frac{1}{2} \sum_{i=1}^6 \sum_{j=1}^{n_p} (d_{P_i}^{sim}(x, t_j) - d_{P_i}^{obs}(t_j))^2 + \frac{1}{2} \sum_{k=1}^{n_{grid}} (d_S^{sim}(x, k) - d_S^{obs}(k))^2, \quad (6)$$

where $i = 1, \dots, 6$ is the well index, $t_j, j = 1, \dots, n_p$ are the measurement times of production data and $k = 1, \dots, n_{grid}$ denotes the cell indices. The geometric data, the geological structure, the fluid properties and the geomechanical parameters of the PEM are presumed known. The inversion parameters are the porosity means (one for each layer), the A and B coefficients for the permeabilities (two coefficients

per layer) and the permeability ratios (two ratios per layer). These parameters are submitted to bound constraints.

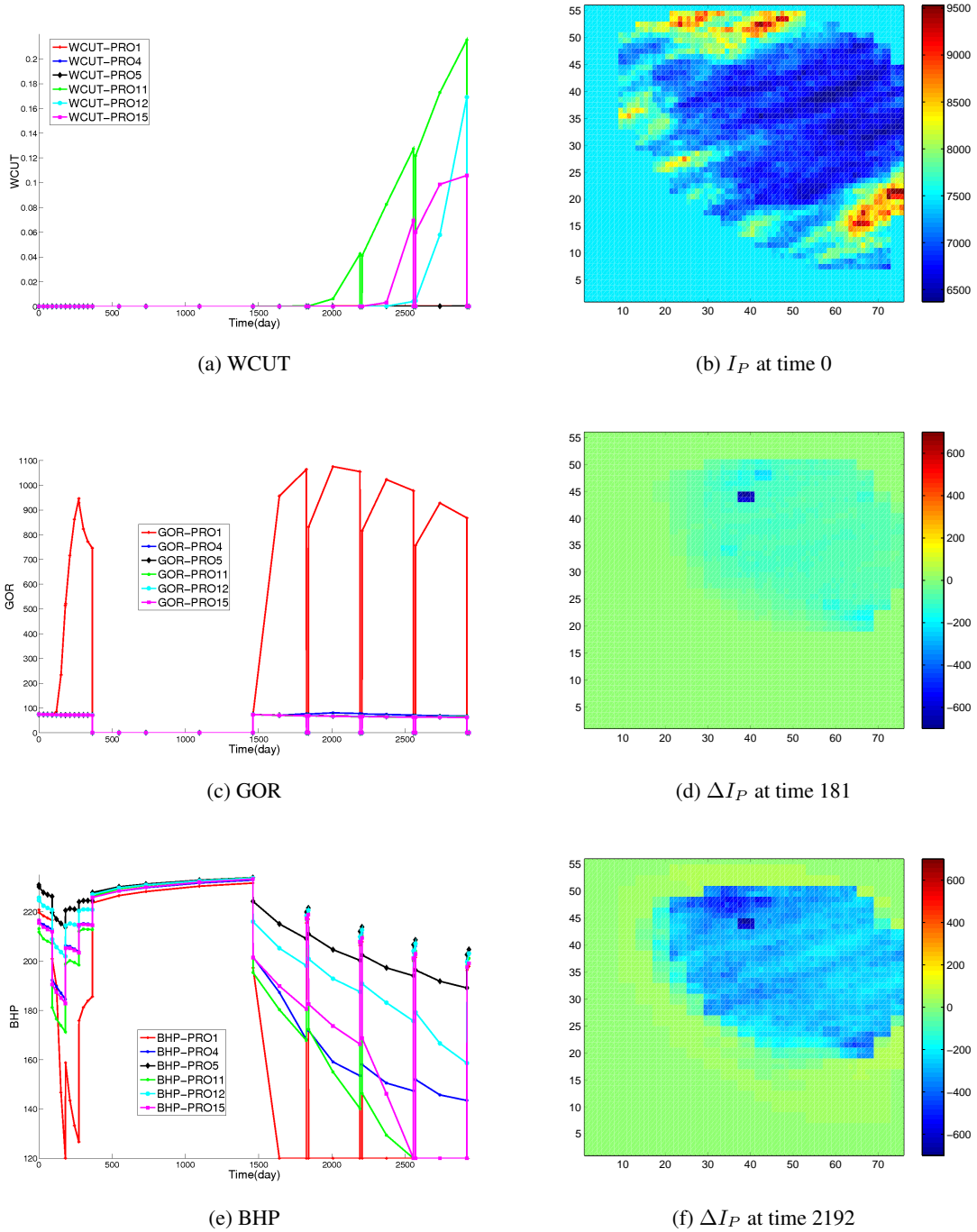


Figure 3: PUNQ field: Reference production data (left), seismic data (P impedance map) for layer 5 (right).

The SQPAL BFGS method (Sinoquet and Delbos, 2008), the SQA method for different number of interpolation points ($2n + 1$, $n + 6$ and $n + 2$) and the SQPAL Gauss Newton (GN) method are applied to the minimization problem of the objective function (6) with respect to these 25 inversion parameters un-

der bound constraints. Both BFGS and Gauss-Newton approaches belong to the class of Quasi-Newton methods which solve sequentially a minimization problem based on a quadratic objective function with the same gradient as the original objective function and an approximation of its Hessian matrix:

$$\min_d \frac{1}{2} d^T \tilde{H} d + g^T d. \quad (7)$$

The BFGS formula provides an update of the approximation of the Hessian matrix at each iteration depending on the gradients of the objective function and of the parameter values

$$\tilde{H}_{k+1} = \tilde{H}_k + \frac{\gamma_k \gamma_k^T}{\gamma_k^T \delta_k} - \frac{H_k \delta_k \delta_k^T H_k^T}{\delta_k^T H_k^T \delta_k}, \quad (8)$$

with $\delta_k = x_{k+1} - x_k$ and $\gamma_k = \nabla_x f(x_{k+1}, \lambda_{k+1}) - \nabla_x f(x_k, \lambda_k)$. For Gauss-Newton method, the approximation of the Hessian matrix is computed from the Jacobian matrix J , first derivatives of the calculated data ($J_{ij} = \frac{\partial d_i}{\partial x_j}$):

$$\tilde{H} = J^T J. \quad (9)$$

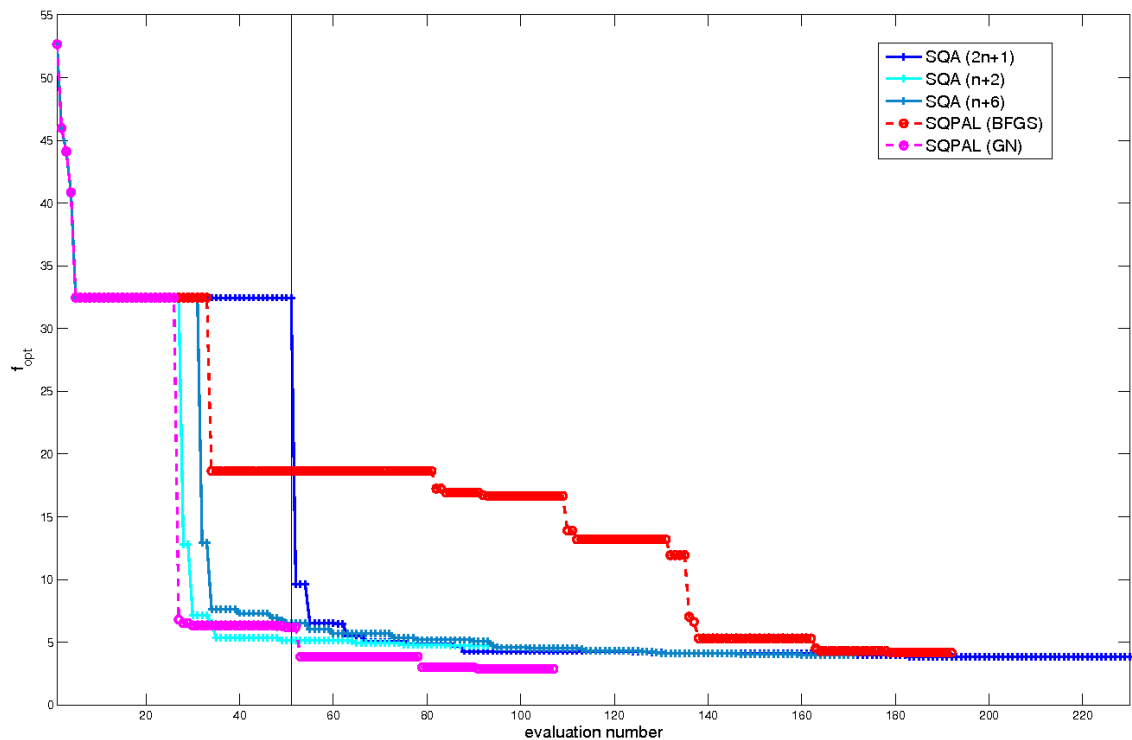


Figure 4: Objective function versus simulation numbers for five optimization runs, respectively with SQA for different numbers of interpolation points (solid lines, blue crosses), with BFGS method with line search globalization (dashed line, red circles), and with GN method (dashed line, pink circles).

In both cases, the first derivatives of the objective function (BFGS) or of the calculated data (Gauss-Newton) are computed by finite differences which requires at each iteration $n + 1$ simulations of the forward operator. Moreover, Gauss-Newton approach needs the storage of the Jacobian matrix of size $n \times n_{data}$ ($n_{data} = n_p + n_{grid}$ is the total number of observed data). The storage of such a matrix

becomes cumbersome for joint inversion of production data and seismic data because of the huge number of measurements. In our application case, this storage is still possible for 128500 measurements but it will be untractable for more complex problems with larger number of measurements. The SQA method requires as the BFGS method only the storage of the gradient and of the Hessian matrix of size depending only on the number of parameters.

The results obtained by the five methods are presented in Figure 4, where the evolution of the objective function is depicted with respect to the number of fluid flow and petroelastic simulations. In all cases, we can observe that the objective function decreases: the five different methods seem to converge to a local minimum. As expected, we can also notice that SQA (version $2n + 1$ interpolation points) requires more evaluations during the initialization phase than SQPAL ($m = 2n + 1$ compared to FD computations which require $n + 1$) and others SQA (version $n + 6$ and $n + 2$). However, SQA achieves in all cases a greater reduction of the objective function much faster than SQPAL BFGS. This is the key advantage of SQA versus SQPAL BFGS: it allows to reduce the number of evaluations of the simulator, which are very CPU time consuming. We can also observe that SQPAL GN achieves a fastest reduction of the objective function than other methods through the use of information of the jacobian matrix. SQA (version $n + 2$) is the only method with performances closed to SQPAL GN.

The production data at well 12 obtained by the initial model and the SQA matched model are compared to the reference data on the left of Figure 5. SQA provides a model which is much closer to the reference production data than the initial model. The reference, initial, and optimal impedance map of layer 5 at time 0 obtained with the SQA method is given on the right of Figure 5. We can observe that SQA succeeds to give a good match also for seismic data.

SQA method is then able to solve this large size reservoir history matching problem (in terms of number of measurements) without requiring to store the large size Jacobian matrix. It is quite encouraging for future real applications involving complex datasets and computationnaly expensive simulators.

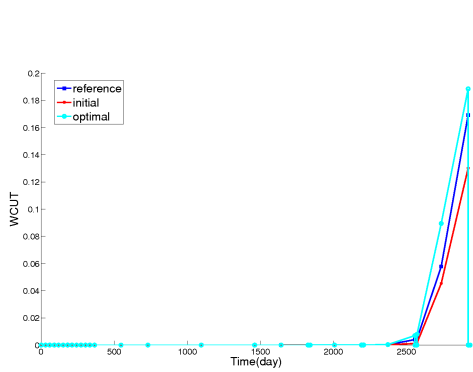
Conclusions

In this paper, we proposed a Derivative Free Optimization method based on Sequential Quadratic Approximations (SQA) of the objective function to solve the joint inversion of production and 4D seismic data. As shown on a realistic application, this method allows to limit the number of evaluations of the computationnaly expensive forward problem compared to classical optimization method coupled with gradient approximated by finite differences as BFGS Quasi-Newton method. We compared also SQA method with Gauss-Newton method : in that case, we obtained comparable results when using a small number of interpolation points to build the quadratic model of the objective function (a quadratic polynomial model built from $n + 2$ points). These results are very encouraging for applications with a large number of measurements: for such cases, Gauss-Newton method is not applicable due to storage requirement (the Jacobian matrix is too huge to be stored).

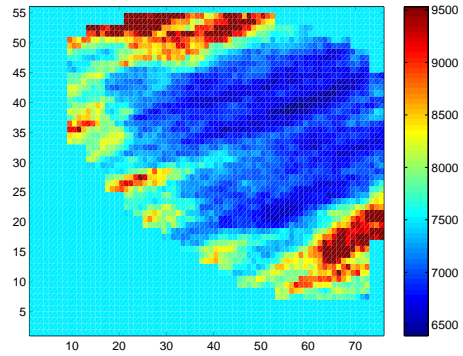
An other interesting feature of SQA method shown in the paper is its ability to deal efficiently with nonlinear constraints (with or without given derivatives). SQA succeeded to solve a challenging optimization benchmark with 68 black-box constraints (with unknown derivatives) and 124 parameters. A study of a reservoir engineering application with nonlinear constraints is in progress and preliminary results are presented in Metla et al. (2010). The aim of this work is to compute parameter uncertainty estimations and confidence intervals of a forecast response based on solutions of history matching problems.

In order to take into account the nature of the objective function in history matching problem, namely its least-square characteristic, we are currently working on adapting SQA method to construct several models to form the objective function (basically, one model for each data misfit or for each type of data misfit), following the idea proposed by Zhang et al. (2009). The objective is to obtain more ac-

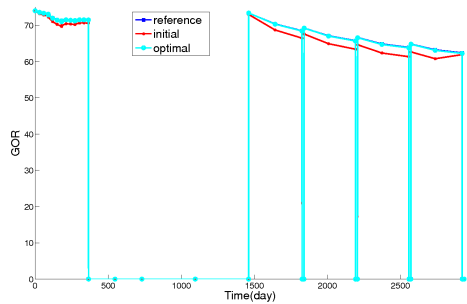
curate models taking into account the characteristics of the objective function, and then obtain a faster convergence.



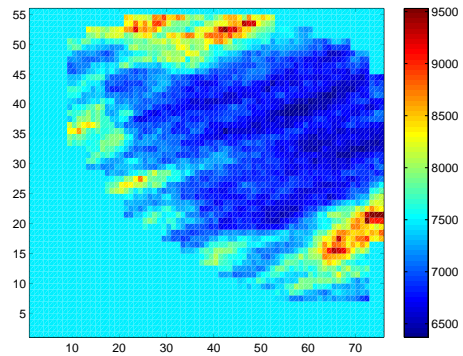
(a) WCUT for well 12



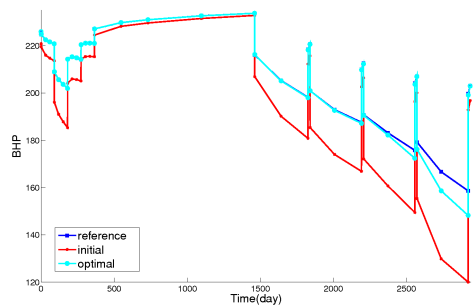
(b) Initial



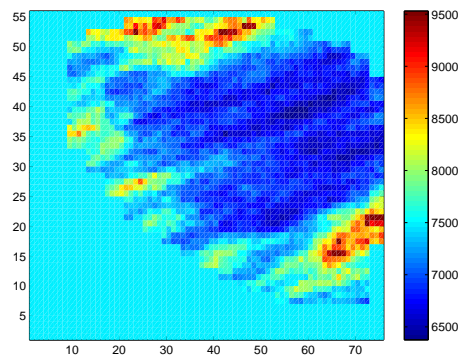
(c) GOR for well 12



(d) Reference



(e) BHP for well 12



(f) Optimal

Figure 5: Comparison between reference production data (blue) and simulated production data for initial point (red) and optimal point obtained with SQA (cyan) (left). P Impedance maps at time 0 obtained with SQA (right).

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