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A predictor-corrector algorithm to estimate the fractional flow in oil-water models

Gabriela B Savioli¹ and Elena M Fernández Berdaguer²

¹ Laboratorio de Ingeniería de Reservorios, IGPUBA and Departamento de Ingeniería Química, Facultad de Ingeniería, Universidad de Buenos Aires, Av. Las Heras 2214 Piso 3 C1127AAC Buenos Aires, Argentina
² Instituto de Cálculo, Facultad de Ciencias Exactas y Naturales, UBA-CONICET and Departamento de Matemática, Facultad de Ingeniería, Universidad de Buenos Aires, 1428 Buenos Aires, Argentina
E-mail: gsavioli@di.fcen.uba.ar, efernan@ic.fcen.uba.ar

Abstract. We introduce a predictor-corrector algorithm to estimate parameters in a nonlinear hyperbolic problem. It can be used to estimate the oil-fractional flow function from the Buckley-Leverett equation. The forward model is non-linear: the sought-for parameter is a function of the solution of the equation. Traditionally, the estimation of functions requires the selection of a fitting parametric model. The algorithm that we develop does not require a predetermined parameter model. Therefore, the estimation problem is carried out over a set of parameters which are functions. The algorithm is based on the linearization of the parameter-to-output mapping. This technique is new in the field of nonlinear estimation. It has the advantage of laying aside parametric models. The algorithm is iterative and is of predictor-corrector type. We present theoretical results on the inverse problem. We use synthetic data to test the new algorithm.

1. Introduction
The mathematical simulation of fluid flow through porous media is of vital importance to the management of underground resources, such as aquifers and petroleum reservoirs.

The motivation for the present work arises from a reservoir engineering problem: the estimation of the oil-water relative permeability curves. These curves are essential to perform predictions of oil recovery during a waterflooding process. In practice the estimation of such curves is carried out from measurements of saturations, flow rates or pressures taken during a laboratory displacement test.

The relative permeability curves, denoted by \( k_{ro} \) and \( k_{rw} \), appear as coefficients of the system of equations that rule the two phase flow through porous media. The general model consists of a coupled system of non-linear equations: an elliptic equation and a parabolic one, with boundary and initial conditions [12].

In models for mechanisms of water displacing oil, the equations have strong transport terms. In this case, capillarity forces can be disregarded and, therefore, the parabolic equation degenerates into a hyperbolic one [12]. We are left with the following hyperbolic-elliptic system...
on the unknowns $S$ (oil saturation) and $P$ (oil pressure):

$$\Phi \frac{\partial S(x,t)}{\partial t} + \frac{\partial f(S(x,t))}{\partial x} = 0, \quad x \in [0, L], \ t \in (0, T],$$  

$$\frac{\partial}{\partial x} \left( \lambda_T(S(x,t)) \frac{\partial P(x,t)}{\partial x} \right) = 0, \quad x \in (0, L), \ t \in [0, T]. \quad (2)$$

System (1)-(2) is completed with an initial condition for the hyperbolic equation and boundary conditions for the elliptic one. We recall that the oil saturation is not greater than one [1]. To solve the above system we first obtain the saturation $S$ from (1), then we use it to obtain $P$ from (2).

In the equations, $\Phi$ is the porosity of the media, $f$ the oil fractional flow and $\lambda_T$ the total mobility. The functions $f$ and $\lambda_T$ depend on $k_{ro}$ and $k_{rw}$, which are functions of the oil saturation $S$. It is possible to solve for $k_{ro}$ and $k_{rw}$ from $f$ and $\lambda_T$ [12].

The purpose of this paper is to deal with the inverse problem whose forward model is equation (1), known as the Buckley-Leverett equation, with initial condition

$$S(x,0) = g(x), \quad x \in [0, L]. \quad (3)$$

The forward model is non-linear because $f$ is a function of the solution of the system of equations.

The parameter to be estimated is the oil-fractional flow function $f$. Observe in equation (1) that the support of function $f$ is the image of the solution $S(x,t)$. The curve $f$ must be inferred from measurements of saturation at different spatial points as a function of time taken during a displacement test of oil by water performed on a rock sample in the laboratory.

Traditionally, the estimation of functions requires the selection of a fitting model depending on few constant parameters and thus the optimum curve depends on that selection [3],[4],[10]. This approach has the drawback of imposing an a priori parametric model. The use of such models is currently the common practice among field engineers, different models yield different results and there is no objective criterion to choose among them. Another approach consists on discretizing the differential equations and using least squares on the discrete problem [9],[15].

The novelty of this work is to apply an alternative methodology based on the formulation of the inverse problem in functional spaces. We develop an algorithm that does not require a parametric model and thus provides a more objective fit. We prove the convergence of the algorithm. The estimation procedure is carried out linearizing the solution of the direct model with respect to the parameter in functional spaces. Up to now, this approach has been successfully applied to problems where the forward model is based on a linear partial differential equation [5],[7],[8],[14].

The estimation of the function $f$ is carried out iteratively. Since we do not know neither the shape nor the support of $f$, we need a predictor-corrector like algorithm. Briefly, at each iteration $k$, the new estimation is first predicted over the support of the previous one. Then, the correction step is performed in order to obtain the estimated function and its actual support at step $k + 1$.

The main contribution of this work is the formulation and application of the algorithm described above to estimate parameters in non-linear systems. The estimation is performed in functional spaces without the imposition of a priori parametric models. We present theoretical results on the inverse problem which are necessary to build the algorithm and prove its convergence under suitable hypothesis. The resulting method behaves very well in numerical tests. Because of its general theoretical formulation the method has the potential to be extended to solve more complex problems.
The paper is organized as follows: in section 2 we introduce the mathematical forward model; in section 3 we deal with the inverse problem, defining the set of admissible parameters and the parameter-to-output mapping. In section 4 we build the continuous estimation algorithm, we prove its convergence and we describe the discrete predictor-corrector algorithm. In section 5 the numerical tests are shown and finally, the conclusions are drawn in section 6.

2. The mathematical forward model

As we state in the introduction, our forward model is a simplified model for the displacement of oil by water in petroleum reservoirs. Under reasonable smoothness conditions on the function \( f \), problem (1),(3) can be written as

\[
\Phi \frac{\partial S(x,t)}{\partial t} + H(S(x,t))\frac{\partial S(x,t)}{\partial x} = 0, \quad x \in [0,L], \ t \in (0,T]; \quad S(x,0) = g(x), \quad x \in [0,L],
\]

where \( H(S) = f'(S) \).

Assuming the following: \( H \in C^{\infty}([0,1]); g \in C^1([0,L]); 0 \leq g(x) \leq S^+ < 1, \ x \in [0,L] \), the forward model is well-posed as the next proposition establishes (proposition 2.1.1 in the book by Serre [13]).

Proposition 1. We define \( T^* = +\infty \) if \( H \circ g \) is increasing, and \( T^* = - (\inf \left\{ d(H \circ g)/dx \right\})^{-1} \) otherwise. Then the initial value problem (4) possesses one and only one solution of class \( C^1 \) in the band \([0,L] \times [0,T^*]\) and does not possess any solutions in any greater band than \([0,L] \times [0,T^*]\).

From now on, we assume that the initial condition function \( g \) in (3) satisfies the assumption above.

We consider the case of smooth solutions of the inverse problem. In order to avoid shocks for an initial period of time we define the set of admissible parameters as,

\[
P = \{ H \in C^{\infty}([0,1]) : \ H \circ g \ is \ increasing \}.
\]

3. The inverse problem

Our objective is to estimate the oil fractional flow \( f \) given measurements of the saturation at a recording point \( x^{rec} \), \( S^{obs}(t) \), during a period of time \([0,T] \subset [0,T^*]\). To highlight the dependency of \( S \) on the parameter \( H \) we will denote \( S \) by \( S(H) \).

We precise the estimation problem: Find \( H \in C^{\infty}([0,1]) \) such that

\[
S(H)(x^{rec},t) = S^{obs}(t).
\]

The above correspondence between the parameter \( H \) and the observations \( S^{obs}(t) \) is the parameter-to-output mapping.

We analyze problem (6) assuming that there is no noise in the observations. The algorithm that we propose is based on the linearization of the parameter-to-output mapping \( S(H)(x^{rec}, \cdot) \) as a function of \( H \), about a particular function \( \bar{H} \):

\[
S(H) = S(\bar{H}) + S_H'(\bar{H})\delta H,
\]

where \( S'_H \) is the derivative of \( S \) with respect to \( H \) and \( \delta H = H - \bar{H} \).

Notice that we are differentiating with respect to the parameter \( H \), which is a function. Therefore \( S'_H \) is a functional derivative, the Fréchet derivative. We prove in [6] that the parameter-to-output mapping, \( S(H)(x^{rec},t) \), is Fréchet differentiable, as given by the following results.
3.1. Properties of the parameter-to-output mapping
We state the basic properties of the parameter-to-output mapping, which address practical questions related to the estimation problem (Chapter III of [2]). All the proofs can be found in [6].

**Identifiability.** Problem (6) is identifiable with respect to $P$.

**Continuity.** The parameter-to-output mapping satisfies:
\[
\left\| (S(H) - S(\tilde{H})) (x^{rec}, \cdot) \right\|_{C^1([0,T])} \leq K \left\| H - \tilde{H} \right\|_{C^1([0,1])},
\]
where $K$ is a constant which depends on the initial function $g$.

**Differentiability.** The mapping $S(H)(x^{rec}, \cdot)$ is Fréchet differentiable. Its differential at $H \in C^\infty([0,1])$ applied to $\delta H \in C^\infty([0,1])$ is given by
\[
(S'_H(H) \delta H)(x^{rec}, t) = w(x^{rec}, t) (\delta H \circ S)(x^{rec}, t),
\]
where $w(x, t)$ is the solution of
\[
w_t + H(S) w_x + H'(S) S_x w = -S_x, \quad w(x, 0) = 0,
\]
and $S$ is the solution of (4).

4. The estimation algorithm
The iterative algorithm, based on a linear equation that approximates (6), consists of:

(i) Give an approximation $\tilde{H}$ of $H$,

(ii) Calculate an increment $\delta H$ solving the linearized $S$ (see equation (7)), that is,
\[
(S'_H(\tilde{H}) \delta H)(x^{rec}, t) = S_{obs}(t) - S(\tilde{H})(x^{rec}, t).
\]

(iii) Update $H$ as $H_{new} = \tilde{H} + \delta H$.

The Fréchet derivative in (11) is computed using equation (9).

4.1. Convergence of the estimation algorithm
**Theorem 1.** If $H \in P$ there is a neighbourhood $N(H, \delta)$ of $H$ in $P$ such that if the initial guess $H^0$ belongs to $N(H, \delta)$ the algorithm is convergent.

**Proof.** Let $H$ be the solution of the estimation problem. We recall that the Fréchet derivative of $S$ with respect to $H$ can be identified with the function $w$ of equation (10). It is easy to see that, when $H \in P$, $S'_H(H): \delta H \to w(x^{rec}, t) (\delta H \circ S)(x^{rec}, t)$ has an inverse since $w(x^{rec}, t) \neq 0$ for every $t > 0$ [6].

The algorithm can be regarded as a one step stationary iteration of the form
\[
H^{k+1} = G(H^k)
\]
where
\[
G(\tilde{H}) = \tilde{H} + (S'_H(\tilde{H}))^{-1} (S(H) - S(\tilde{H}))
\]
We will prove that $G$ is a contraction in a neighbourhood of $H$. To do so we use that $G$ has a continuous Fréchet derivative $G'$. The existence of the derivative of $G$ follows from the fact that
$S$ has a continuous second Fréchet derivative which is equal to $-w_z t$ [6]. Therefore the Fréchet derivative of $G$ can be computed as

$$G'(\tilde{H}) = \frac{(S(H) - S(\tilde{H}))(-w_z t)}{w^2}. \quad (14)$$

From (14), $G'(H) = 0$. Then, given a constant $\alpha < 1$, there is a ball $B(H, \delta)$ with center $H$ and radius $\delta$ such that $\|G'(\tilde{H})\| < \alpha$ for every $\tilde{H} \in B(H, \delta)$. Therefore

$$\|G(H) - G(\tilde{H})\| < \alpha \|H - \tilde{H}\|, \text{ for every } \tilde{H} \in B(H, \delta). \quad (15)$$

4.2. Numerical Implementation. The predictor-corrector algorithm

The estimation of the function $H$ is carried out iteratively. Notice that we do not know neither the shape of $H$ nor the support of $H$. To estimate the function $H$ including the support, we use a predictor-corrector like algorithm. We denote the support of $H$ by $\text{supp}(H)$.

The discretization is carried out by expanding $H$ at each iteration in a basis of first order splines. Since we do not know the domain of $H$, we choose a partition of the domain that depends on the previous iteration. Therefore the nodes of the basis change at each iteration.

**Predictor-corrector Algorithm**

(i) Initial Step

Given the observations $S^\text{obs}_j$ at points $t_j \in [0, T], \ j = 1, \ldots, M$; and an initial guess $H^0$, we solve the initial value problem (4) with $H = H^0$ thus obtaining $S^0(x, t)$. Next we select the nodes for the first order spline expansion as $z^0_j = S^0(x_{rec}, t(j))$, where $l(j) = M - j + 1$. We expand the already known $H^0$ in the chosen basis $\psi^0_j$:

$$H^0(z) = \sum_{j=1}^{M} \gamma^0_j \psi^0_j(z), \quad z \in [S^0(x_{rec}, t_M), \ S^0(x_{rec}, t_1)].$$

(ii) Procedure at Step $k$

We assume that we have $H^k$ expressed in its spline basis $\psi^k_j$ and also $S^k(x_{rec}, t_j)$.

- **Predictor Step to obtain $H^{k+1}$:**
  First we compute $w_k$ solving (10) with $H = H^k$ and $S = S^k$. Then $\delta H^k$ is computed as [11]

$$\delta H^k(S(x_{rec}, t_j)) = \frac{S^\text{obs}_j - S^k(x_{rec}, t_j)}{w_k(x_{rec}, t_j)} = \delta \gamma^k_j. \quad (16)$$

Therefore $H^{k+1}$ expressed in the basis $\psi^k_j$ is

$$(H^{k+1}/\text{supp}(H^k))(z) = \sum_{j=1}^{M} (\gamma^k_j + \delta \gamma^k_j) \psi^k_j(z), \quad z \in [S^k(x_{rec}, t_M), \ S^k(x_{rec}, t_1)].$$

- **Corrector Step to obtain $H^{k+1}$:**
  With $H^{k+1}$ expressed in the basis $\psi^k_j$ we solve the initial value problem (4) obtaining $S^{k+1}(x, t)$. In order to obtain the new basis $\psi^{k+1}_j(z)\!$ we define the new nodes as $z^{k+1}_j = S^{k+1}(x_{rec}, t(j))$. Therefore we express $H^{k+1}$ in the new basis $\psi^{k+1}_j$ as

$$(H^{k+1}/\text{supp}(H^{k+1}))(z) = \sum_{j=1}^{M} \gamma^{k+1}_j \psi^{k+1}_j(z), \quad z \in [S^{k+1}(x_{rec}, t_M), \ S^{k+1}(x_{rec}, t_1)].$$
Figure 1: Convergence of $H^k$

(iii) Compute the residual $\|S_{\text{obs}}^j(\cdot) - S^{k+1}(x_{\text{rec}}, \cdot)\|$.

(iv) If residual $< \text{TOL}$, then $H^{k+1}$ is the solution. STOP

(v) If not, $k = k + 1$, GO TO (ii).

5. Numerical tests

We illustrate the performance of the algorithm with two examples. The purpose of the first example is to analyze the behavior of the predictor-corrector algorithm. The purpose of the second example is to show the ability of the algorithm to recover the 'true' shape of a typical fractional flow function.

5.1. First example

In this case, $L = 1$, $T = 0.1$, the exact function is $H(z) = e^z$; the initial condition is $g(x) = x^3$; the observations $S_{\text{obs}}^j$ are the evaluation of the exact solution at $x = 0.44$ and times $t_j = j \times 0.001$, $j = 1, \ldots, 100$; and the accuracy required for convergence is TOL $= 10^{-7}$.

Figure 1 illustrates the behavior of the predictor-corrector procedure. We plot the predictor and corrector steps for iterations one to three. That is, the figure depicts $H^k$ spanned in the 'old' basis $\psi_k^j$ (dotted line) and in the new one $\psi_{k+1}^j$ (solid line). Notice how the domains are modified in each iteration.

The functions $H^k$ are in the space spanned by the first order splines $\psi_k^j$ which have a discontinuous derivative at the nodes. That is, the discontinuities of $(H^k)'$ affect $u^k$ (solution of (10)) and those of $w^k$ reflect on $\delta H^k$ (16). That explains the discontinuities observed in the plot.

Figure 2 shows the convergence of the predictor-corrector procedure. Convergence was achieved in 20 iterations. We plot the 'true' parameter $H$, some iterations of the algorithm and the final estimate $H^{20}$. An almost exact match to the 'true' function is obtained.

5.2. Second example

In this case the fractional flow curve $f(S)$ has a typical shape because we apply the well known potential model for oil and water relative permeabilities $k_{ro}$ and $k_{rw}[4][10]$. Selecting
\[ k_{ro}(S) = S^2, \quad k_{rw}(S) = 0.2 (1 - S)^2, \quad f(S) \] results \[ f(S) = \frac{S^2}{0.2 (1 - S)^2 + S^2} \] (17)

In Figure 4 we plot the exact solution \( H \), the initial guess \( H^0 \), the first iteration \( H^1 \) and the optimum estimated \( H^0 \).

For the numerical tests \( L = 1, T = 1 \), the observations \( S_{\text{obs}}(t_j) \) are the evaluation of the exact solution at \( x = 0.98 \) and times \( t_j = j \times 0.05, j = 1, \ldots, 20 \). The accuracy required for
convergence is $\text{TOL} = 10^{-7}$. Convergence was achieved in 9 iterations. We observe that the optimum estimated $H^9$ is an excellent approximation of the 'true' function $H$. The fractional flow is obtained numerically, integrating the estimated function $H(S)$.

6. Conclusions

We have developed a discrete predictor-corrector algorithm to estimate a parameter that appears as a coefficient of a nonlinear hyperbolic equation. The sought-for parameter is the oil fractional flow function in oil-water systems. The problem is non-linear, the parameter is a function of the solution of the forward model. The iterative algorithm is based on the linearization of the parameter-to-output mapping. This technique is new in the field of non-linear estimation. It has the advantage of laying aside parametric models. The algorithm estimates the function as well as its domain. We proved its convergence. We presented two numerical experiments that validate the method. The algorithm was tested with data based on the potential model for the relative permeabilities. It was successful recovering that model. The highlight is that we did not prescribe any particular model of the function parameter. That makes us believe that the algorithm has the ability to recover the true shape of the sought-for function.

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