Under-relaxed Quasi-Newton acceleration for an inverse fixed-point problem coming from Positron-Emission Tomography

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Abstract

Quasi-Newton acceleration is an interesting tool to improve the performance of numerical methods based on the fixed-point paradigm. In this work the quasi-Newton technique will be applied to an inverse problem that comes from Positron Emission Tomography, whose fixed-point counterpart has been introduced recently. It will be shown that the improvement caused by the quasi-Newton acceleration procedure is very impressive.

Key words: Positron Emission Tomography, Fixed-point methods, Quasi-Newton acceleration.

1 Introduction

Given a function $G : \mathbb{R}^n \to \mathbb{R}^n$ the fixed-point problem consists of finding $x \in \mathbb{R}^n$ such that $x = G(x)$. Associated to this problem one can define the nonlinear system of equations

$$F(x) = 0$$

(1)
where $F : \mathbb{R}^n \to \mathbb{R}^n$ is defined by $F(x) = x - G(x)$.

Quasi-Newton methods solve (1) with less computational effort (per iteration) than Newton’s method, without losing most of Newton’s good convergence properties. A quasi-Newton iteration can be seen as a generalization of the Newtonian iteration, in which one replaces the Jacobian matrix $F'(x)$ by some approximation, which may not involve calculations of derivatives. Here, we will discuss the use of quasi-Newton methods as accelerators of iterative procedures whose rate of convergence is merely linear. Since quasi-Newton methods usually converge superlinearly [28], we hope that this property will be inherited by the quasi-Newton acceleration of fixed-point iterations.

Fixed-point problems arise naturally in electronic structure calculation [21], complex models of transport [5], statistics [42], dynamic PET reconstruction [36, 37] and many other problems. PET reconstruction is the focus of our work. A major concern about the fixed-point iteration $x^{k+1} = G(x^k)$ is the fact that the iterates can converge with linear and extremely slow rate, motivating many acceleration studies [5, 14, 16, 20, 21, 24, 33, 38, 39, 41, 43, 44, 47].

Positron Emission Tomography (PET) is an imaging technique applied in nuclear medicine that produces images of physiological processes in 2D or 3D. This procedure has emerged as a research tool to study the brain and, despite its high cost, provides good diagnostic imaging in a minimally invasive manner, thus becoming a useful clinical tool. We are interested in the examination of cardiac myocardial perfusion, although the PET technique is also applied in a wide range of procedures, as detection and monitoring activity of malignant tumors and brain disorders, including early diagnosis of Alzheimer’s disease [32, 34, 36].

For low quality data, for example in tracers like $H_2^{15}O$ with low half-life (fast decay), new approaches based on the direct reconstruction of parameters from PET data instead of an intermediate image reconstruction step have evolved as promising tools [2, 3], at least for preclinical investigations.

In this paper we will present our experience with under-relaxed quasi-Newton acceleration techniques for reconstruction of the kinetic behavior of a radioactive tracer during cardiac perfusion with real PET data. We will show that significant improvement may be obtained in comparison with the original fixed-point algorithm.
2 Positron Emission Tomography (PET) Model

This section is based on the PhD Thesis of Reips [36], whose main objective was to reconstruct, directly, the kinetic behavior of radioactive water, \(\text{H}_2\text{^{15}O}\), based on real data obtained from PET scans during cardiac perfusion exams. In [36] the parameter identification problem associated with the inverse problem of image reconstruction was formulated. Its solution led to recover kinetic parameters associated to a suitable differential equations model.

In order to analyse PET data and estimate metabolic rates, compartmental models are generally used. These models are able to describe fairly well a large number of physiological processes within brain and heart. Many methods have been developed based on compartmental models. Cerebral oxygen processes were considered in [31], neuroreceptor ligand binding in [30], and quantification of blood flow in [1, 3, 4, 26, 25].

In compartmental models, each compartment defines one possible state (for example, physical location and chemical state) of the tracer. A single compartment uses to be a group of states [9]. Considering the PET image-sequence, fixed spatial compartments are areas defined by the concentration of a radioactive tracer (called activity) represented by a temporal function.

The images produced by PET scanners consist of many overlapping signals (measurements of radioactivity levels). Consequently, in order to isolate the desired component it is necessary to use a mathematical model, which includes all possible states (treated as a single compartment [45]) of the signal given by a PET-reconstruction sequence.

In order to describe the interaction between compartments, one associates a constant capable to represent the velocity of absorption, i.e. the diffusion of the radioactive trace used by the PET scan. Thus, data concerning the rate at which the radioactive tracer is metabolized in the region of interest can be associated with rates of variation in time of the tracer concentrations in each compartment [9]. Moreover, the rate of passage of substances between the regions are represented by means of a constant linking these compartments.

In this way, it becomes possible to describe the kinetics behavior of a radioactive tracer in a physiological system employing a set of nonlinear differential equations. The variation of temporal concentration of the radioactive tracer is analyzed in a specific compartment and, thus, the quantities of interest can be determined.

The three-component reaction-diffusion model of [36] is a macroscopic model for cardiovascular perfusion that predicts the tracer activity (a tem-
poral function) if the reaction rates, velocities, and diffusion coefficients are known, based on compartmental models \[9, 45\]. The three components previously mentioned are denoted by arteries, veins and tissues (capillaries).

Let \( \Omega \subseteq \mathbb{R}^3 \) be a bounded domain representing the region of interest and let \( t \in \mathbb{R} \). We consider \( x \in \Omega \) as a macroscopic variable homogenizing microscopic flow patterns. Thus, for the activity \( u = u(x, t) \) we have

\[
u(x, t) = C_A(x, t) + C_V(x, t) + C_T(x, t)\]

and each concentration \( C \) is associated with local velocities \( V_A, V_V, V_T \) and local diffusion coefficients \( D_A, D_V, D_T \), respectively. Direct reconstructions of distributed parameters models from PET data can be found in \[3, 23\].

With the sinogram PET it is possible to formulate the dynamic inverse problem using a model encoded by an operator \( G \), that maps parameters \( p \) to a time evolution of activity \( u \):

\[
\varphi(Ku(x, t)) = f(x, t), \quad u = G(p), \tag{2}
\]

where \( f : \Omega \times \mathbb{R} \rightarrow \mathbb{R} \) is a sequence of measured PET data on a domain \( \Omega \), \( \varphi(z) \) denotes a Poisson random variable with expectation \( z \), and \( K : L^2(\Omega) \rightarrow L^2(\Omega) \) is the forward operator. As going into the details about \( K \) is beyond the scope of this work, we suggest the book of Wernick \[45\] for the interested reader.

Working with inverse problems have a disadvantage as the problem is usually ill-posed in the sense of Hadamard \[17\]. Thus, regularization methods are added and the solution of the above inverse problem is given by the following minimization problem

\[
(u, p) \in \arg \min_{(u, p)} \int_0^T \int_{\Omega} Ku(x, t) - f(x, t)\log(Ku(x, t))dx \ dt + \alpha R(p) \tag{3}
\]

where \( R \) is a regularization functional, which incorporates smoothness and a-priori information about typical values of the parameters. Several methods can be found in the literature applied to the regularization of ill-posed problems: Gauss-Newton \[6\], Levenberg-Marquardt methods \[18\], Landweber methods \[19, 35\] and Newton-type methods \[22\].

\[1\text{We denote by } L^2(X) \text{ the set of Lebesgue measurable functions such that } ||f||_{L^2(X)} < \infty, \text{ where } ||f||_{L^2(X)} = (\int |f|^2 \, d\mu)^{\frac{1}{2}}.\]
All the biological parameters represented in \( p \) are found by solving the minimization problem \([3]\). Moreover, using the differential equations model proposed in \([36]\) it is possible to predict the flow behavior of the radioactive tracer during the cardiac perfusion PET.

In order to solve \((3)\) for noise free-data, Reips \([36]\), as others in literature \([13, 15, 46]\), used the well-known Expectation Maximization (EM) Algorithm \([11]\). Thus, given an image \( u^k = G(p^k) \), one computes \( u^{k+\frac{1}{2}} \) by

\[
    u^{k+\frac{1}{2}} = \frac{u^k}{K^*1} K^* \left( \frac{f}{K u_k} \right),
\]

where \( 1 \) denotes the constant function equal one, \( K^* \) is the adjoint operator of \( K \) and \( u^{k+\frac{1}{2}}, u^k \) and \( f \) are spatially and temporally dependent of \( x \) and \( t \), respectively.

Note that this step is well defined since, as usual for EM, the operations are performed punctually, i.e., element by element. After solving the associated lagrangean functionals, we calculate all the biologicals parameters that composes the vector \( p \). The second half-step (backward splitting step) is defined by

\[
    p^{k+1} \in \arg \min_p \int_0^T \int_\Omega \omega_k(x,t)(G(p)(x,t) - u^{k+\frac{1}{2}}(x,t))^2 \, dx \, dt + \alpha R(p),
\]

where \( \omega_k = \frac{K^*1}{G(p^k)} \). The new image \( u^{k+1} \) is updated from the biological parameters found and the process is restarted.

Although the results in \([36]\) indicate that the model provides, with good accuracy, the activity of the radioactive tracer, the number of fixed point iterations that are necessary to obtain accurate results is very high, thus leading to unaffordable computational cost. Consequently, accelerating the Reaction-Diffusion Model from PET data is mandatory.

### 3 Quasi-Newton acceleration for PET calculations

For an arbitrary parameter \( p \in \mathbb{R}^n \) let us define \( p^+ = G(p) \) as the next iterate that comes from the application of the Forward-Backward Splitting (FBS) \([10]\) scheme to \((3)\). In this way, a fixed-point (FP) iteration is defined as an iteration of the FBS method.

As we mentioned before, solving a fixed-point problem corresponds to solve a nonlinear system of equations \( F(p) = 0 \), where \( F(p) = p - G(p) \).
However, the Jacobian of $F$ may not be available, or may be extremely difficult to compute.

In order to choose the most appropriate class of methods to improve the convergence rate of fixed-point iterates, the intrinsic characteristics of these problems must be taken into account. Usually [5, 16] practical fixed-point problems are high-dimensional, so it is interesting to use accelerators that do not require matrix inversion and that can be implemented using limited-memory techniques. In addition, line search procedures are not recommendable because the cost of function evaluations may be very high [16]. This means that we should accelerate employing well established quasi-Newton techniques that ensure local convergence without line searches.

We will show how to solve the associated nonlinear system $F(p) = 0$ using several quasi-Newton methods that belong to the secant type, because the approximate Jacobians satisfy the so called secant equation [28]. By definition, the FBS iteration corresponds to:

$$p^{k+1} = p^k - H_0 F(p^k)$$

with $H_0 = I$. Since this iteration converges locally at a linear rate, it is natural to conjecture that quasi-Newton methods based on

$$p^{k+1} = p^k - H_k F(p^k) \text{ or } p^{k+1} = p^k - B_k^{-1} F(p^k),$$

where $H_k$ satisfies the secant equation $H_{k+1}(F(p^{k+1}) - F(p^k)) = p^{k+1} - p^k$ (or alternatively, $B_{k+1}(p^{k+1} - p^k) = F(p^{k+1}) - F(p^k)$) with some minimal variation principle, probably converge superlinearly, thus accelerating the convergence of the FBS method.

In the following subsection we describe the quasi-Newton accelerators considered in this research.

### 3.1 Quasi-Newton methods employed in this study

We considered five different matrix updating schemes that satisfy the secant (or the inverse secant) equation, namely: Broyden’s First and Second Methods [7], Column Updating Method [27], Inverse Column Updating Method [29] and Thomas’ Method [40].

We may formulate the updating procedure of these methods by:

$$B_{k+1} = B_k + \frac{(y_k - B_k s_k) v_k^\top}{s_k^\top v_k},$$

where $s_k = x^{k+1} - x^k$, $y_k = F(x^{k+1}) - F(x^k)$ and $v_k \in \mathbb{R}^n$.  

6
The choice \( v_k = s_k \) defines Broyden’s First Method (BM1), \( v_k = e_k \) defines the Column Updating Method (COLUM), and \( v_k = \left( P_k + \frac{\|s_k\|^2}{2} I \right) s_k \) corresponds to Thomas’ method, where

\[
P_{k+1} = (1 + \|s_k\|) \left( \|s_k\| I + P_k - \frac{w_k w_k^\top}{w_k^\top s_k} \right), \quad P_0 = \rho^2 I.
\]

Applying the Sherman-Morrison formula to (6) we obtain

\[
B_{k+1}^{-1} = B_k^{-1} + \frac{(s_k - B_k^{-1} y_k) v_k^\top B_k^{-1}}{v_k B_k^{-1} y_k}
\]

or, equivalently,

\[
B_{k+1}^{-1} = (I + u_k v_k^\top) B_k^{-1} = \prod_{i=0}^k (I + u_i v_i^\top) B_0^{-1},
\]

where \( u_k = \frac{s_k - B_k^{-1} y_k}{v_k B_k^{-1} y_k} \). In order to save some memory storage, we used the updating trick described in [12], justified by the following lemma.

**Lemma 3.1** Let \( d_k = -B_k^{-1} F(x_k) \), \( z_k = B_k^{-1} y_k \), \( \bar{z}_i = B_i^{-1} y_k \), \( \gamma_i = \frac{s_i^\top \bar{z}_i}{s_i^\top z_i} \), and \( \tau_k = \frac{s_k^\top d_k}{s_k^\top z_k} \). Consider \( x^{k+1} = x_k + \alpha_k d_k \) and assume that \( s_i^\top z_i \neq 0 \), \( i = 0, 1, \ldots, k - 1 \). Then,

(i) \( d_{k+1} = d_k - s_k + \tau_k (s_k - z_k) \) and

(ii) \( z_{i+1} = z_i + \frac{\gamma_i}{\tau_i} (d_{i+1} - (1 - \alpha_i) d_i) \).

**Proof.** See Lemma 2.2 of [12].

On the other hand, among the methods inspired by the inverse secant equation, we used Broyden’s Second Method (BM2) and the Inverse Column-Updating Method (ICOLUM). For these methods, we have

\[
B_{k+1}^{-1} = B_k^{-1} + \frac{(s_k - B_k^{-1} y_k) v_k^\top}{v_k^\top B_k^{-1} y_k},
\]

where \( v_k = y_k \) for BM2 and \( v_k = e_k \) for ICOLUM.

Note that we can write (9) as

\[
B_{k+1}^{-1} = B_k^{-1} + w_k v_k^\top = B_0^{-1} + \sum_{i=0}^k w_i v_i^\top
\]
where
\[ w_k = \frac{s_k - B_k^{-1}y_k}{v_k y_k}. \]

4 Computational Experience

The codes that produced the experiments presented here were written in Fortran 77 with double precision. We used gfortran-4.6 on an Intel CORE I3-2310M@2.10 GHz with 100 Gb of HD and 4Gb of Ram.

The variables considered in this model are
\[ p = (k_1, k_2, k_3, V_{xA}, V_{yA}, V_{xT}, V_{yT}, V_{xV}, V_{yV}, D_A, D_T, D_V)^\top, \]
where \( k_1, k_2, \) and \( k_3 \) represent the fluid exchange between arteries, tissues (capillaries), and veins. \( V_A, V_T, \) and \( V_V \) are the velocity parameters, and \( D_A, D_T, \) and \( D_V \) are the diffusion parameters in arteries, tissues and veins, respectively. The Parameters \( D_A, D_T, D_V, \) and \( k_i, i = 1, 2, 3 \) are nonnegative [36].

As stopping criteria we considered the following sensibility measure:
\[ \frac{\|p_{i+1}^k - p_i^k\|_F}{\|p_{i+1}^k\|_F} < 10^{-4}, \]
where \( p_i^k \) represents a component of vector \( p \) defined in (11) at iteration \( k \).

We also limited the number of iterations by \( \max\{100, n^2\} \), where \( n \) is the dimension of vector \( p \), and the computer time (for quasi-Newton methods) by 600 seconds.

Now, we define the test problems and present the results.

4.1 Numerical Problems and Results

For all the examples analyzed, let us consider an operator \( K \) (size 16512 × 4225) associated with the real PET scanner, as shown in Figure 1.

We will consider a 65 × 65 image in a domain \( \Omega \). For the initial concentration of the radioactive tracer in arteries, \( C_A \), we used
\[ C_A(x, y, 0) = \tau(1 - x^2)(50 - y)y, \]
characterizing the image exposed in Figure 2.

For the initial concentration in tissues and veins we used
\[ C_T(x, y, 0) = 0 \text{ and } C_V(x, y, 0) = 0. \]
Figure 1: Real PET image for an observation operator $K$.

Figure 2: Initial concentration of radioactive tracer in artery.

For defining the time step we used $\tau = 3 \times 10^{-5}$. Data are generated from forward simulations of the PDE system with subsequent generation of Poisson noise.
Example 1  For this example, the initial values of the biological parameters are defined in Table 1 where $\alpha$ is the a priori regularization and $\xi$ the gradient regularization parameter. The column $(\cdot)^*$ is related with the typical value used in a priori regularization [36].

Table 1: Input data for Example 1

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Initial Value</th>
<th>$(\cdot)^*$</th>
<th>a priori Regul. ($\alpha$)</th>
<th>Grad. Regul. ($\xi$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_1$ (1/cm)</td>
<td>0.90 (0)</td>
<td>0.89</td>
<td>0.01287520644013148965</td>
<td>0.0008</td>
</tr>
<tr>
<td>$k_2$ (1/cm)</td>
<td>0.75</td>
<td>0.70</td>
<td>0.01286792647011880155</td>
<td>0.0001</td>
</tr>
<tr>
<td>$k_3$ (1/cm)</td>
<td>0.90</td>
<td>0.85</td>
<td>0.01287621626481284896</td>
<td>0.0001</td>
</tr>
<tr>
<td>$V_{zA}$ (cm/s)</td>
<td>1e-4</td>
<td>0.10</td>
<td>0.001024495</td>
<td>0.0001</td>
</tr>
<tr>
<td>$V_{yA}$ (cm/s)</td>
<td>700.0</td>
<td>15.0</td>
<td>1.100</td>
<td>0.0001</td>
</tr>
<tr>
<td>$V_{zT}$ (cm/s)</td>
<td>-50.0</td>
<td>-5.0</td>
<td>1.122098745999</td>
<td>0.0001</td>
</tr>
<tr>
<td>$V_{yT}$ (cm/s)</td>
<td>1e-4</td>
<td>0.10</td>
<td>0.001024495</td>
<td>0.0001</td>
</tr>
<tr>
<td>$V_{xV}$ (cm/s)</td>
<td>1e-4</td>
<td>0.10</td>
<td>0.001024495</td>
<td>0.0001</td>
</tr>
<tr>
<td>$V_{yV}$ (cm/s)</td>
<td>700.0</td>
<td>15.0</td>
<td>1.10000000001</td>
<td>0.0001</td>
</tr>
<tr>
<td>$D_A$ (cm²/s)</td>
<td>3e-7</td>
<td>1e-3</td>
<td>0.0003344</td>
<td>0.000444</td>
</tr>
<tr>
<td>$D_T$ (cm²/s)</td>
<td>3e-6</td>
<td>1e-2</td>
<td>0.000344</td>
<td>0.000444</td>
</tr>
<tr>
<td>$D_V$ (cm²/s)</td>
<td>3e-7</td>
<td>1e-3</td>
<td>0.0003344</td>
<td>0.000444</td>
</tr>
</tbody>
</table>

We also evaluated the radioactive flux behavior when $k_1$ is zero for some interval. In Table 1 the symbol (0) indicates that $k_1$ is not constant throughout the region of interest. When $k_1 = 0$ there is no material exchange between arteries and tissues, which means that the concentration of radioactive tracer in this region is null.

Applying quasi-Newton acceleration we reduced significantly the number of iterations. Table 2 reports the performance of fixed-point method (FBS) and quasi-Newton acceleration for Example 1. In this table, we use the following notations:

NI: number of iterations.

TIME: CPU time (in seconds), measured with the function etime.

RES: value of $||F(\bar{x})||$, where $\bar{x}$ is the solution computed by the algorithm.

10
SENS: sensibility measure used as stopping condition.

Table 2: Performance of methods for Example 1

<table>
<thead>
<tr>
<th>Method</th>
<th>NI</th>
<th>TIME</th>
<th>RES</th>
<th>SENS</th>
</tr>
</thead>
<tbody>
<tr>
<td>FBS</td>
<td>317</td>
<td>4138.5</td>
<td>6.6958</td>
<td>9.99e-5</td>
</tr>
<tr>
<td>BM1</td>
<td>2</td>
<td>53.699</td>
<td>7.97e-3</td>
<td>5.51e-5</td>
</tr>
<tr>
<td>BM2</td>
<td>2</td>
<td>58.959</td>
<td>7.97e-3</td>
<td>5.52e-5</td>
</tr>
<tr>
<td>COLUM</td>
<td>2</td>
<td>59.827</td>
<td>9.29e-3</td>
<td>5.54e-5</td>
</tr>
<tr>
<td>ICOLUM</td>
<td>2</td>
<td>60.703</td>
<td>1.46e-2</td>
<td>5.58e-5</td>
</tr>
<tr>
<td>THM</td>
<td>2</td>
<td>59.827</td>
<td>7.97e-3</td>
<td>5.51e-5</td>
</tr>
</tbody>
</table>

Figure 3: Images generated by methods FBS (left) and BM2 (right).

The images displayed in Figure 3 refer to the parameter $V_{x,T}$ calculated through the methods FBS and BM2. Observe that, although the images are visually very similar, the numerical values obtained are different. From the theoretical point of view, the quasi-Newton methods improved the solution, since the image found is closest to a fixed-point of the problem. However, from a practical point of view, the ideal solution should resemble to the image obtained via Forward-Backward Splitting method. For this reason we decided to limit the step size at each quasi-Newton iteration by a steplength $\alpha_k$, thus

$$p^{k+1} = p^k + \alpha_k s^k$$

where $s^k$ is the quasi-Newton direction. We used $\alpha_k = 0.1$ and $\alpha_k = 0.01$, the value $\alpha_k = 1$ represents the pure quasi-Newton step, whereas $\alpha_k < 1$
corresponds to “under-relaxed” quasi-Newton iterations. After this step correction, we could approach very well the images, as exemplified for parameter $V_2\tau$ in Figure 4.

![Figure 4: Images generated by methods FBS (left) and BM2 with $\alpha_k = 0.01$ (right).](image)

The performance of quasi-Newton methods for the step sizes $\alpha_k = 0.1$ and $\alpha_k = 0.01$ are displayed in Table 3. The result for the FBS method was omitted as it is independent of the step size $\alpha_k$.

<table>
<thead>
<tr>
<th></th>
<th>$\alpha_k = 0.1$</th>
<th></th>
<th>$\alpha_k = 0.01$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>NI</td>
<td>TIME</td>
<td>RES</td>
</tr>
</tbody>
</table>

Figure 5 exposes the convergence graph of the methods tested for Example 1. Note that, even restricting the step size, the number of iterations reduction was approximately 98% and, most importantly, maintaining the quality of the solution.

In the Figures 6-15 we present the images that represent the reconstruction of the biological parameters for Example 1 using Broyden’s second
method. The reconstruction of parameters $k_2$ and $k_3$ was omitted since these parameters were constant, with $k_2 \approx 0.7278$ and $k_3 \approx 0.8733$.

Figure 5: Convergence behavior of methods for Example 1.

Figure 6: Reconstruction of $k_1$.

Figure 7: Reconstruction of $V_{x,A}$. 
Figure 8: Reconstruction of $V_{yA}$.

Figure 9: Reconstruction of $V_{xT}$.

Figure 10: Reconstruction of $V_{yT}$.

Figure 11: Reconstruction of $V_{xV}$.

Figure 12: Reconstruction of $V_{yV}$.

Figure 13: Reconstruction of $D_{xA}$. 
Example 2 In this last example we will analyze the radioactive tracer behavior considering a slightly different case. The initial values corresponding to the parameters $k_1$ and $k_2$ have zeros in the central region, which visually corresponds to the gaps shown on Figure 16. With this definition, we consider the presence of something that hinders the flow, such as a tumor, for example. The new initial values used in this experiment and the performance of the algorithms for this instance are displayed in Table 4 and Table 5, respectively.

These results showed a significant reduction in the number of iterations and computer time. This reduction was approximately 98% for $\alpha_k = 0.01$, the step size by means of which we obtained the best results. Moreover, can see in Figure 17 that the quality of the solution was preserved.
Table 4: Initial data for Example 2

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Initial Value</th>
<th>(·)*</th>
<th>a priori Regul. (α)</th>
<th>Grad. Regul. (ξ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_1$ (1/cm)</td>
<td>0.90 (0)</td>
<td>0.89</td>
<td>0.017148965</td>
<td>0.0008</td>
</tr>
<tr>
<td>$k_2$ (1/cm)</td>
<td>0.75 (0)</td>
<td>0.70</td>
<td>0.016801553</td>
<td>0.0001</td>
</tr>
<tr>
<td>$k_3$ (1/cm)</td>
<td>0.01</td>
<td>0.85</td>
<td>0.051822197678965</td>
<td>0.0001</td>
</tr>
<tr>
<td>$V_{x,A}$ (cm/s)</td>
<td>1e-4</td>
<td>0.10</td>
<td>0.001024495</td>
<td>0.0001</td>
</tr>
<tr>
<td>$V_{y,A}$ (cm/s)</td>
<td>700.0</td>
<td>15.0</td>
<td>1.1</td>
<td>0.0001</td>
</tr>
<tr>
<td>$V_{x,T}$ (cm/s)</td>
<td>-50.0</td>
<td>-5.0</td>
<td>1.22098745999</td>
<td>0.0001</td>
</tr>
<tr>
<td>$V_{y,T}$ (cm/s)</td>
<td>1e-4</td>
<td>0.10</td>
<td>0.001024495</td>
<td>0.0001</td>
</tr>
<tr>
<td>$V_{x,V}$ (cm/s)</td>
<td>1e-4</td>
<td>0.10</td>
<td>0.001024495</td>
<td>0.0001</td>
</tr>
<tr>
<td>$V_{y,V}$ (cm/s)</td>
<td>700.0</td>
<td>15.0</td>
<td>1.1000000001</td>
<td>0.0001</td>
</tr>
<tr>
<td>$D_A$ (cm²/s)</td>
<td>3e-7</td>
<td>1e-3</td>
<td>0.0003344</td>
<td>0.000444</td>
</tr>
<tr>
<td>$D_T$ (cm²/s)</td>
<td>3e-6</td>
<td>1e-2</td>
<td>0.000344</td>
<td>0.000444</td>
</tr>
<tr>
<td>$D_V$ (cm²/s)</td>
<td>3e-7</td>
<td>1e-3</td>
<td>0.0003344</td>
<td>0.000444</td>
</tr>
</tbody>
</table>

Table 5: Performance of methods for Example 2

<table>
<thead>
<tr>
<th></th>
<th>$\alpha_k = 0.1$</th>
<th></th>
<th>$\alpha_k = 0.01$</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>NI</td>
<td>TIME</td>
<td>RES</td>
<td>SENS</td>
</tr>
</tbody>
</table>

Figure 17: Convergence behavior of methods for Example 2.
Next, in Figures 18 and 19, we compare the images related to the reconstruction of the parameters $k_1$ and $V_x T$, two of the parameters that presented more difficulties to approximate the values obtained by FBS method.

Figure 18: Reconstruction of $k_1$ by FBS (left) and BM2 (right).

Figure 19: Reconstruction of $V_x T$ by FBS (left) and BM2 (right).

Figures 20 to 28 involve the recovery of the remaining biological parameters for Example 2 using BM2 method. The case of parameter $k_3$ was omitted since this parameter was constant, with $k_3 \approx 0.0109$. 
Figure 20: Reconstruction of $k_2$.

Figure 21: Reconstruction of $V_{xA}$.

Figure 22: Reconstruction of $V_{yA}$.

Figure 23: Reconstruction of $V_{yT}$.

Figure 24: Reconstruction of $V_{xT}$.

Figure 25: Reconstruction of $V_{yV}$.
In Figures 29-36, we display the concentration of radioactive material in tissues $C_T$ and veins $C_V$, and the image $u$, for different stages of time.
Figure 29: Reconstruction of $C_T - t_3$.

Figure 30: Reconstruction of $C_T - t_{12}$.

Figure 31: Reconstruction of $C_V - t_3$.

Figure 32: Reconstruction of $C_V - t_{12}$.
Figure 33: Reconstruction of $u - t_3$.

Figure 34: Reconstruction of $u - t_6$.

Figure 35: Reconstruction of $u - t_9$.

Figure 36: Reconstruction of $u - t_{12}$.

5 Conclusions

We showed that under-relaxed versions of quasi-Newton methods are very efficient to accelerate the behavior of Fixed-Point methods associated to a tomographic reconstruction problem. The fact that we need under-relaxation ($\alpha_k \approx 0.01$) is very interesting and reflects a characteristic of many inverse problems [1]. As so happens to occur with very ill-conditioned linear and nonlinear systems of equations, the “exact solution” is not the one that we wish in practice and all the vast theory of regularization is related with this fact. Under-relaxation is one of the techniques that have been associated with regularization in order to obtain physically meaningful solutions of inverse problems. It is somewhat surprising that such device works extremely
well when coupled to quasi-Newton acceleration.

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References


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