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On error sensitivity analysis in variationnal data assimilation

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Abstract: The problem of data assimilation for a nonlinear evolution model is considered with the aim to identify the initial condition. The equation for the error of the optimal solution through the errors of the input data is derived, based on the Hessian of the misfit functional. The solvability of the error equation is studied. The fundamental control functions are used for error analysis. The error sensitivity coefficients are obtained using the singular vectors of the specific response operators in the error equation. An application to the data assimilation problem in hydrology is given. Numerical results are presented.

Key-words: operator, optimal solution, Hessian, error equation, eigenvalues values, singular vectors, sensitivity coefficient

(Résumé : tsvp)

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Analyse de la sensibilité de l'erreur en assimilation variationnelle de données.

Résumé : Nous abordons dans cette étude, le problème d'assimilation de données sur un modèle d'évolution non linéaire, le but étant d'identifier la condition initiale. L'équation de l'erreur sur la condition initiale optimale est déduite au travers de l'erreur sur les données d'entrées (représentées ici par l'erreur modèle, l'erreur sur les observations et l'erreur sur la condition initiale). Cette équation d'erreur est basée uniquement sur le Hessien d'une nouvelle fonctionnelle coût prenant en compte ces erreurs. La définition de certains opérateurs attachés aux différentes erreurs permet d'effectuer une étude de l'erreur sur la condition initiale optimale. Les coefficients de sensibilité d'erreur sont obtenus à partir des valeurs propres et des vecteurs singuliers de ces opérateurs. Une application sur un modèle d'écoulement souterrain en zone non saturée est présentée ainsi que les résultats numériques.

Mots-clés : operateur, solution optimale, Hessien, équation d'erreur, valeurs propres, vecteurs singuliers, coefficient de sensilité

Contents

1 Introduction and statement of the problem

Consider the evolution problem

$$\begin{cases} \dfrac{\partial \varphi}{\partial t} = F(\varphi) + f, \quad t \in (0,T) \\ \varphi|_{t=0} = u, \end{cases} \tag{1.1}$$

where $\varphi = \varphi(t)$ is the unknown function belonging for any t to a Hilbert space X, $u \in X$, F is a nonlinear operator mapping X into X. Let $Y = L_2(0,T;X)$, $\|\cdot\|_Y = (\cdot,\cdot)_Y^{1/2}$, $f \in Y$.

Let us introduce the functional

$$S(u) = \frac{\alpha}{2}\|u - u_0\|_X^2 + \frac{1}{2}\|C\varphi - \varphi_{obs}\|_{Y_{obs}}^2, \tag{1.2}$$

where $\alpha = const \geq 0$, $u_0 \in X$, $\varphi_{obs} \in Y_{obs}$ are prescribed functions (observational data), Y_{obs} is a Hilbert space (observational space), $C : Y \to Y_{obs}$ a linear bounded operator.

Consider the following data assimilation problem with the aim to identify the initial condition: find u and φ such that

$$\begin{cases} \dfrac{\partial \varphi}{\partial t} = F(\varphi) + f, \quad t \in (0,T) \\ \varphi|_{t=0} = u \\ S(u) = \inf\limits_v S(v). \end{cases} \tag{1.3}$$

The necessary optimality condition reduces the problem (1.3) to the following system [15], [1]:

$$\begin{cases} \dfrac{\partial \varphi}{\partial t} = F(\varphi) + f, \quad t \in (0,T) \\ \varphi|_{t=0} = u, \end{cases} \tag{1.4}$$

$$\begin{cases} -\dfrac{\partial \varphi^*}{\partial t} - (F'(\varphi))^*\varphi^* = -C^*(C\varphi - \varphi_{obs}), \quad t \in (0,T) \\ \varphi^*|_{t=T} = 0, \end{cases} \tag{1.5}$$

$$\alpha(u - u_0) - \varphi^*|_{t=0} = 0 \tag{1.6}$$

with the unknowns φ, φ^*, and u, where $(F'(\varphi))^*$ is the adjoint to the Frechet derivative of F, and C^* is the adjoint to C defined by $(C\varphi, \psi)_{Y_{obs}} = (\varphi, C^*\psi)_Y$, $\varphi \in Y, \psi \in Y_{obs}$.

Suppose that $u_0 = \bar{u} + \xi_1$, $\varphi_{obs} = C\bar{\varphi} + \xi_2$, $f = \bar{f} + \xi_3$, where $\xi_1 \in X$, $\xi_2 \in Y_{obs}$, $\xi_3 \in Y$, and $\bar{\varphi}$ is the solution to the problem (1.1) with $u = \bar{u}$, $f = \bar{f}$:

$$\begin{cases} \dfrac{\partial \bar{\varphi}}{\partial t} &= F(\bar{\varphi}) + \bar{f}, \quad t \in (0,T) \\ \bar{\varphi}\big|_{t=0} &= \bar{u}. \end{cases} \tag{1.7}$$

The functions ξ_1, ξ_2, ξ_3 may be treated as the errors of the input data u_0, φ_{obs}, f.

Having supposed that the solution of the problem (1.4)–(1.6) exists, we will study the influence of the errors ξ_1, ξ_2, ξ_3 on the optimal solution u.

The first part of this paper is devoted to theoritical results: we derive the equation linking errors together, show its solvability, make some disgression for the case where the operator appering in the optimality system of error equation is time independant and self-adjoint through the Fourier analysis and also fundamental control functions under certain conditions. This is followed by The explicit expressions of singular vector and the value of the sensitivity coefficients.
In the second part of the paper will focus in the application in using model for underground flow.

2 Equation for the errors

The system (1.4)–(1.6) with the three unknowns φ, φ^*, u may be treated as an operator equation of the form

$$\mathcal{F}(U, U_d) = 0, \tag{2.1}$$

where $U = (\varphi, \varphi^*, u)$, $U_d = (u_0, \varphi_{obs}, f)$.

The following equality holds:

$$\mathcal{F}(\bar{U}, \bar{U}_d) = 0, \tag{2.2}$$

with $\bar{U} = (\bar{\varphi}, 0, \bar{u})$, $\bar{U}_d = (\bar{u}, C\bar{\varphi}, \bar{f})$. From (2.1)–(2.2), we get

$$\mathcal{F}(U, U_d) - \mathcal{F}(\bar{U}, \bar{U}_d) = 0. \tag{2.3}$$

Let $\delta U = U - \bar{U}$, $\delta U_d = U_d - \bar{U}_d$. Then (2.3) gives

$$\mathcal{F}(\bar{U} + \delta U, \bar{U}_d + \delta U_d) - \mathcal{F}(\bar{U}, \bar{U}_d) = 0. \tag{2.4}$$

From (2.4), with an accuracy of the second order in $\delta U, \delta U_d$, we obtain

$$\mathcal{F}'_U(\bar{U}, \bar{U}_d)\delta U + \mathcal{F}'_{U_d}(\bar{U}, \bar{U}_d)\delta U_d = 0, \tag{2.5}$$

where $\mathcal{F}'_U, \mathcal{F}'_{U_d}$ are the Gateâux derivatives with respect to U and U_d.

Let $\delta\varphi = \varphi - \bar{\varphi}$, $\delta u = u - \bar{u}$; then $\delta U = (\delta\varphi, \varphi^*, \delta u)$, $\delta U_d = (\xi_1, \xi_2, \xi_3)$. By calculating the derivatives $\mathcal{F}'_U, \mathcal{F}'_{U_d}$, it is easily seen that equation (2.5) is equivalent to the system:

$$\begin{cases} \dfrac{\partial \delta\varphi}{\partial t} - F'(\bar{\varphi})\delta\varphi &= \xi_3, \quad t \in (0,T), \\ \delta\varphi|_{t=0} &= \delta u, \end{cases} \tag{2.6}$$

$$\begin{cases} -\dfrac{\partial \varphi^*}{\partial t} - (F'(\bar{\varphi}))^*\varphi^* &= -C^*(C\delta\varphi - \xi_2), \\ \varphi^*|_{t=T} &= 0, \end{cases} \tag{2.7}$$

$$\alpha(\delta u - \xi_1) - \varphi^*|_{t=0} = 0, \tag{2.8}$$

where $\bar{\varphi}$ is the solution of the original problem (1.7).

The problem (2.6)–(2.8) is a linear data assimilation problem; it is equivalent to the following minimization problem: find u and φ such that

$$\begin{cases} \dfrac{\partial \varphi}{\partial t} - F'(\bar{\varphi})\varphi &= \xi_3, \quad t \in (0,T) \\ \varphi|_{t=0} &= u \\ S_1(u) &= \inf_v S_1(v), \end{cases} \tag{2.9}$$

where

$$S_1(u) = \frac{\alpha}{2}\|u - \xi_1\|_X^2 + \frac{1}{2}\|C\varphi - \xi_2\|_{Y_{obs}}^2. \tag{2.10}$$

Consider the Hessian H of the functional (2.10); it is defined by the successive solutions of the following problems:

$$\begin{cases} \dfrac{\partial \psi}{\partial t} - F'(\bar{\varphi})\psi &= 0, \; t \in (0,T), \\ \psi|_{t=0} &= v, \end{cases} \tag{2.11}$$

$$\begin{cases} -\dfrac{\partial \psi^*}{\partial t} - (F'(\bar{\varphi}))^*\psi^* &= -C^*C\psi, \quad t \in (0,T) \\ \psi^*|_{t=T} &= 0, \end{cases} \tag{2.12}$$

$$Hv = \alpha v - \psi^*|_{t=0}. \tag{2.13}$$

Let us introduce the operator R_2 acting on the functions $g \in Y_{obs}$ according to the formula

$$R_2 g = \theta^*|_{t=0}, \tag{2.14}$$

where θ^* is the solution to the adjoint problem

$$\begin{cases} -\dfrac{\partial \theta^*}{\partial t} - (F'(\bar{\varphi}))^*\theta^* = C^*g, \quad t \in (0,T) \\ \theta^*|_{t=T} = 0. \end{cases} \tag{2.15}$$

We introduce also the operator $R_3 : Y \to X$ defined successively by the formulas:

$$\begin{cases} \dfrac{\partial \theta_1}{\partial t} - F'(\bar{\varphi})\theta_1 = h, \ h \in Y, \\ \theta_1|_{t=0} = 0, \end{cases} \tag{2.16}$$

$$\begin{cases} -\dfrac{\partial \theta_1^*}{\partial t} - (F'(\bar{\varphi}))^*\theta_1^* = -C^*C\theta_1, \quad t \in (0,T) \\ \theta_1^*|_{t=T} = 0, \end{cases} \tag{2.17}$$

$$R_3 h = \theta_1^*|_{t=0}. \tag{2.18}$$

From (2.11)–(2.18) we conclude that the system (2.6)–(2.8) is equivalent to the one equation for δu:

$$H\delta u = R_1\xi_1 + R_2\xi_2 + R_3\xi_3, \tag{2.19}$$

where $R_1 = \alpha E$, and E is the identity operator in X.

3 Solvability of the error equation

To study the solvability of the error equation (2.19), we suppose that the original model satisfies the following conditions:

(i) the solution to the problem

$$\begin{cases} \dfrac{\partial \psi}{\partial t} - F'(\bar{\varphi})\psi = f, \quad t \in (0,T) \\ \psi|_{t=0} = v, \end{cases} \tag{3.1}$$

meets the inequality

$$\|\psi\|_Y \le c_1(\|f\|_Y + \|v\|_X), \quad c_1 = const > 0; \tag{3.2}$$

(ii) the solution of the adjoint problem

$$\begin{cases} -\dfrac{\partial \psi^*}{\partial t} - (F'(\bar{\varphi}))^*\psi^* = p, \quad t \in (0,T) \\ \psi^*|_{t=T} = 0, \end{cases} \tag{3.3}$$

satisfies

$$\|\psi^*\|_Y + \|\psi^*|_{t=0}\|_X \le c_1^*\|p\|_Y, \quad c_1^* = const > 0; \tag{3.4}$$

Remark 3.1. The conditions (i), (ii) are satisfied if, for example, the operator $-F'(\bar\varphi)$ is positive definite: $-(F'(\bar\varphi)w, w)_Y \ge \gamma\|w\|_Y^2$, $\gamma = const > 0$, $\forall w \in Y$. Indeed, from (3.1) we get

$$\Big(\frac{\partial\psi}{\partial t}, \psi\Big)_X - (F'(\bar\varphi)\psi, \psi)_X = (f, \psi)_X,$$

whence,

$$\frac{1}{2}\int_0^T \frac{d}{dt}(\psi, \psi)_X dt - \int_0^T (F'(\bar\varphi)\psi, \psi)_X dt = \int_0^T (f, \psi)_X dt,$$

and by virtue of positive definiteness of $-F'(\bar\varphi)$,

$$\frac{1}{2}\|\psi|_{t=T}\|_X^2 + \gamma\|\psi\|_Y^2 \le (f, \psi)_Y + \frac{1}{2}\|\psi|_{t=0}\|_X^2 \le \|f\|_Y\|\psi\|_Y + \frac{1}{2}\|v\|_X^2,$$

or

$$\gamma\|\psi\|_Y^2 \le \frac{1}{2\gamma}\|f\|_Y^2 + \frac{\gamma}{2}\|\psi\|_Y^2 + \frac{1}{2}\|v\|_X^2.$$

The last inequality gives (3.2) with $c_1 = max(\gamma^{-1}, \gamma^{-1/2})$. Similarly, the inequality (3.4) is obtained.

In the finite-dimensional case, when $X = \mathbf{R}^n, n \in \mathbf{N}$, the inequalities (3.2), (3.4) are valid without positive definiteness requirement if the $n \times n$-matrix $F'(\bar\varphi)$ is regular enough (for instance, having the elements continuous in t).

Under the hypotheses (i), (ii) the following statement is valid.

Lemma 3.1. *The operator H acts in X with domain of definition $D(H) = X$, it is bounded, self-adjoint, and positive semi-definite. If $\alpha > 0$, the operator H is positive definite.*

Proof. Let $v \in X$, and ψ be the solution to (2.11). By (3.2), $\|\psi\|_Y \le c_1\|v\|_X$. For the solution ψ^* of (2.12) the inequality (3.4) holds:

$$\|\psi^*\|_Y + \|\psi^*|_{t=0}\|_X \le c_1^*\|C^*C\psi\|_Y.$$

Hence, from (2.13),

$$\|Hv\|_X = \|\alpha v - \psi^*|_{t=0}\|_X \le \alpha\|v\|_X + \|\psi^*|_{t=0}\|_X \le$$

$$\leq \alpha\|v\|_X + c_1^*\|C^*C\psi\|_Y \leq \alpha\|v\|_X + c_1^*c_1\|C^*C\|\|v\|_X,$$

and, therefore, H is bounded. Further, we have for $v, w \in X$:

$$(Hv, w)_X = (\alpha v - \psi^*|_{t=0}, w)_X = \alpha(v, w)_X - (\psi^*|_{t=0}, w)_X =$$

$$= \alpha(v, w)_X + (C^*C\psi, \psi_1)_Y = \alpha(v, w)_X + (C\psi, C\psi_1)_{Y_{obs}},$$

where ψ_1 is the solution to (2.11) with $v = w$. Hence, H is self-adjoint, and

$$(Hv, v)_X = \alpha(v, v)_X + (C\psi, C\psi)_{Y_{obs}} \geq 0,$$

that is, H is positive semi-definite. Moreover, H is positive definite if $\alpha > 0$.

Corollary 3.1. The following estimate is valid:

$$(Hv, v)_X \geq \mu_{\min}(v, v)_X, \quad \forall v \in X, \tag{3.5}$$

where $\mu_{\min}$ is the lower spectrum bound of the operator H, and $\mu_{\min} \geq \alpha$.

Let us prove the following solvability theorem.

Theorem 3.1. *Under the hypotheses* (i), (ii)*, for* $\alpha > 0$*, the error equation* (2.19) *has a unique solution* $\delta u \in X$*, and*

$$\|\delta u\|_X \leq \frac{\alpha}{\mu_{\min}}\|\xi_1\|_X + \frac{c_1^*}{\mu_{\min}}\|C^*\|\|\xi_2\|_{Y_{obs}} + \frac{c_1 c_1^*}{\mu_{\min}}\|C^*C\|\|\xi_3\|_Y. \tag{3.6}$$

Proof. If $\alpha > 0$, from Corollary 3.1, there exist a unique solution δu of the error equation (2.19), and

$$\|\delta u\|_X \leq \frac{1}{\mu_{\min}}\|R_1\xi_1 + R_2\xi_2 + R_3\xi_3\|_X. \tag{3.7}$$

For the solution θ^* of (2.15) for $g = \xi_2$ we get from (3.4):

$$\|R_2\xi_2\|_X = \|\theta^*|_{t=0}\|_X \leq c_1^*\|C^*\xi_2\|_Y \leq c_1^*\|C^*\|\|\xi_2\|_{Y_{obs}}. \tag{3.8}$$

Similarly, the solution θ_1^* of (2.17) satisfies the inequality (3.4), and

$$\|R_3\xi_3\|_X = \|\theta_1^*|_{t=0}\|_X \leq c_1^*\|C^*C\theta_1\|_Y,$$

where θ_1 is the solution to (2.16) for $h = \xi_3$. Due to (3.2), $\|\theta_1\|_Y \le c_1\|\xi_3\|_Y$, then

$$\|R_3\xi_3\|_X \le c_1^* c_1 \|C^*C\| \|\xi_3\|_Y. \tag{3.9}$$

From (3.7)–(3.9) we obtain (3.6). This ends the proof.

Remark 3.2. For $\alpha = 0$, the theorem holds true also if $\mu_{\min} > 0$. It is true, for instance, in the case that $Y_{obs} = Y$, $C = E$, $X = \mathbf{R}^n$, $n \in \mathbf{N}$.

As follows from equation (2.19) and Theorem 3.1, the error δu of the optimal solution depends on the errors ξ_1, ξ_2, ξ_3 linearly and continuously. The influence of the errors ξ_1, ξ_2, ξ_3 on the value of δu is determined by the operators $H^{-1}R_1, H^{-1}R_2, H^{-1}R_3$, respectively. The values of the norms of these operators may be considered as an influence criteria: the less is the norm of the operator $H^{-1}R_i$, the less impact on δu is given by the corresponding error ξ_i. This criteria may be used also for choosing the regularization parameter α ([28], [19]).

In some cases, the method of eigenfunctions (Fourier method) may be used for the error analysis.

4 The Fourier method for error analysis

Consider the case that $Y_{obs} = Y$, $C = E$ (the identity operator). Let $F'(\bar{\varphi}) = (F'(\bar{\varphi}))^* = -A$ be a t-independent self-adjoint operator such that A generates an orthonormal basis in X consisting of eigenfunctions w_k: $Aw_k = \lambda_k w_k$, $(w_k, w_j)_X = \delta_{kj}$, where λ_k are the corresponding eigenvalues of A, and δ_{kj} the Kronecker delta. The Fourier expansion

$$u = \sum_j u_j w_j, \quad u_j = (u, w_j)_X$$

holds for any function $u \in X$.

Consider the eigenvalue problem

$$Hv = \mu v \tag{4.1}$$

for the operator H defined by (2.11)–(2.13). It is easily seen that (4.1) is equivalent to the system:

$$\begin{cases} \dfrac{\partial \psi}{\partial t} - F'(\bar{\varphi})\psi &= 0, \ t \in (0,T), \\ \psi|_{t=0} &= v, \end{cases} \tag{4.2}$$

$$\begin{cases} -\dfrac{\partial \psi^*}{\partial t} - (F'(\bar{\varphi}))^*\psi^* &= -\psi, \ \ t \in (0,T) \\ \psi^*|_{t=T} &= 0, \end{cases} \tag{4.3}$$

$$\alpha v - \psi^*|_{t=0} = \mu v. \tag{4.4}$$

We will seek the solution of (4.2)–(4.4) in the form $v = w_k$, $\psi = \psi_{(k)}(t)w_k$, $\psi^* = \psi^*_{(k)}(t)w_k$. Then from (4.2)–(4.4) we come to the system

$$\begin{cases} \dfrac{\partial \psi_{(k)}(t)}{\partial t}w_k + \lambda_k \psi_{(k)}(t)w_k &= 0,\ t\in(0,T), \\ \psi_{(k)}|_{t=0}w_k &= w_k, \end{cases} \tag{4.5}$$

$$\begin{cases} -\dfrac{\partial \psi^*_{(k)}(t)}{\partial t}w_k + \lambda_k \psi^*_{(k)}(t)w_k &= -\psi_{(k)}(t)w_k,\ \ t\in(0,T) \\ \psi^*_{(k)}|_{t=T}w_k &= 0, \end{cases} \tag{4.6}$$

$$\alpha w_k - \psi^*_{(k)}|_{t=0}w_k = \mu w_k. \tag{4.7}$$

From (4.5), (4.6) we get

$$\psi_{(k)}(t) = e^{-\lambda_k t},\ \ \psi^*_{(k)}(t) = \frac{1}{2\lambda_k}e^{\lambda_k t}(e^{-2\lambda_k T} - e^{-2\lambda_k t}). \tag{4.8}$$

Substituting $\psi^*_{(k)}|_{t=0} = (e^{-2\lambda_k T} - 1)/(2\lambda_k)$ into (4.7), we obtain $\mu = \alpha + (1 - e^{-2\lambda_k T})/(2\lambda_k)$. Thus, we have proved the following statement.

Lemma 4.1. *The eigenfunctions of the operator $H : X \to X$ form an orthogonal basis in X consisting of the eigenfunctions w_k of the operator A. The eigenvalues of H are defined by the formula*

$$\mu_k = \alpha + \frac{1}{2\lambda_k}(1 - e^{-2\lambda_k T}), \tag{4.9}$$

where λ_k are the corresponding eigenvalues of the operator A.

In this case, we may perform the Fourier analysis of the error equation (2.19). Let us represent the errors ξ_1, ξ_2, ξ_3 as the series

$$\xi_1 = \sum_k \xi_{1,k}w_k,\ \ \xi_2 = \sum_k \xi_{2,k}(t)w_k,\ \ \xi_3 = \sum_k \xi_{3,k}(t)w_k, \tag{4.10}$$

where $\xi_{i,k} = (\xi_i, w_k)_X$, $i = 1,2,3$.

The error δu of the optimal solution will be found also as the series:

$$\delta u = \sum_k (\delta u)_k w_k,\ \ (\delta u)_k = (\delta u, w_k)_X. \tag{4.11}$$

Substituting the expansions (4.10), (4.11) into (2.19), we get for the Fourier coefficients:

$$\mu_k(\delta u)_k = \alpha\xi_{1,k} + (R_2\xi_2, w_k)_X + (R_3\xi_3, w_k)_X. \tag{4.12}$$

By definition of R_2 and R_3,

$$(R_2\xi_2, w_k)_X = \sum_j (R_2\xi_{2,j}(t)w_j, w_k)_X = \sum_j (\theta^*|_{t=0}, w_k)_X,$$

$$(R_3\xi_3, w_k)_X = \sum_j (R_3\xi_{3,j}(t)w_j, w_k)_X = \sum_j (\theta_1^*|_{t=0}, w_k)_X,$$

where θ^* is the solution to (2.15) with $g = \xi_{2,j}(t)w_j$, and θ_1^* is the solution to (2.16)–(2.17) with $h = \xi_{3,j}(t)w_j$:

$$\theta^* = \int_t^T e^{-\lambda_k(s-t)}\xi_{2,j}(s)ds w_j,$$

$$\theta_1^* = -\int_t^T e^{-\lambda_k(\tau-t)} \int_0^\tau e^{-\lambda_k(\tau-s)}\xi_{3,j}(s)dsd\tau w_j.$$

Hence,

$$(R_2\xi_2, w_k)_X = \int_0^T e^{-\lambda_k s}\xi_{2,k}(s)ds, \quad (R_3\xi_3, w_k)_X =$$

$$= -\int_0^T e^{-\lambda_k\tau} \int_0^\tau e^{-\lambda_k(\tau-s)}\xi_{3,k}(s)dsd\tau = \frac{1}{2\lambda_k}\int_0^T e^{\lambda_k s}(e^{-2\lambda_k T} - e^{-2\lambda_k s})\xi_{3,k}(s)ds. \tag{4.13}$$

From Lemma 4.1 and (4.12)–(4.13) we come to the relation between the Fourier coefficients:

$$(\delta u)_k = \frac{\alpha}{\mu_k}\xi_{1,k} + \frac{1}{\mu_k}\int_0^T e^{-\lambda_k s}\xi_{2,k}(s)ds + \frac{1}{\mu_k}\frac{1}{2\lambda_k}\int_0^T e^{\lambda_k s}(e^{-2\lambda_k T} - e^{-2\lambda_k s})\xi_{3,k}(s)ds, \tag{4.14}$$

where $\mu_k = \alpha + (1 - e^{-2\lambda_k T})/(2\lambda_k)$.

The equation (4.14) relates the Fourier coefficients of the error δu of the optimal solution to the Fourier coefficients of the errors ξ_1, ξ_2, ξ_3. The impact of the error ξ_1

is defined by the multiplier α/μ_k, the impact of the observation error ξ_2 is defined by $\int\limits_0^T e^{-\lambda_k s}\xi_{2,k}(s)ds/\mu_k$, and the effect of the model error ξ_3 is determined by the third summand in (4.14).

5 Fundamental control functions

Consider the case that $Y_{obs} = Y$, $C = E$. We assume that the hypotheses (i), (ii) are satisfied and the operator H defined by (2.11)–(2.13) is positive and has a complete orthonormal system in X of eigenfunctions v_k corresponding to the eigenvalues μ_k:

$$Hv_k = \mu_k v_k, \tag{5.1}$$

where $(v_k, v_l)_X = \delta_{kl}, \ k, l = 1, 2, \ldots$

Remark 5.1. In the finite-dimensional case, when $X = \mathbf{R}^n, n \in \mathbf{N}$, the last condition on H is always satisfied (even if $\alpha = 0$). Concerning the infinite-dimensional case, see [26].

It is easily seen that the eigenvalue problem (5.1) is equivalent to the system:

$$\begin{cases} \dfrac{\partial \varphi_k}{\partial t} - F'(\bar\varphi)\varphi_k &= 0, \ t \in (0, T), \\ \varphi_k|_{t=0} &= v_k, \end{cases} \tag{5.2}$$

$$\begin{cases} -\dfrac{\partial \varphi_k^*}{\partial t} - (F'(\bar\varphi))^*\varphi_k^* &= -\varphi_k, \ \ t \in (0, T) \\ \varphi_k^*|_{t=T} &= 0, \end{cases} \tag{5.3}$$

$$\alpha v_k - \varphi_k^*|_{t=0} = \mu_k v_k. \tag{5.4}$$

We say that the system of functions $\{\varphi_k, \varphi_k^*, v_k\}$ is the system of *fundamental control functions* by the analogy with the Poincaré-Steklov operator theory [10]. For self-adjoint positive definite operator $-F'(\bar\varphi)$ these functions were considered in [26].

Let W be the Hilbert space of real-valued functions with the inner product and the norm:

$$(\varphi, \psi)_W = \Big(\frac{\partial \varphi}{\partial t} - F'(\bar\varphi)\varphi, \frac{\partial \psi}{\partial t} - F'(\bar\varphi)\psi\Big)_Y + (\varphi|_{t=0}, \psi|_{t=0})_X,$$

$$\|\varphi\|_W = (\varphi, \varphi)_W^{1/2}.$$

We introduce the subspace $W_0 = \{\varphi \in W : \frac{\partial \varphi}{\partial t} - F'(\bar{\varphi})\varphi = 0\}$. It is easy to show that W_0 is closed in W. We consider also the subspace

$$W_1 = \Big\{\varphi \in W : -\frac{\partial \varphi}{\partial t} - (F'(\bar{\varphi}))^*\varphi \in W, \ \ \varphi|_{t=T} = 0\Big\},$$

putting

$$(\varphi, \psi)_{W_1} = \Big(-\frac{\partial \varphi}{\partial t} - (F'(\bar{\varphi}))^*\varphi, -\frac{\partial \psi}{\partial t} - (F'(\bar{\varphi}))^*\psi\Big)_W.$$

The following statement holds.

Lemma 5.1. *The functions* $\{\varphi_k\}, \{\varphi_k^*\}, \{v_k\}$ *defined by formulas* (5.2)–(5.4) *form complete orthonormal systems in* W_0, W_1, X, *respectively.*

Proof. Since $(v_k, v_l)_X = \delta_{kl}$, we have

$$(\varphi_k, \varphi_l)_W = \Big(\frac{\partial \varphi_k}{\partial t} - F'(\bar{\varphi})\varphi_k, \frac{\partial \varphi_l}{\partial t} - F'(\bar{\varphi})\varphi_l\Big)_Y + (\varphi_k|_{t=0}, \varphi_l|_{t=0})_X =$$

$$= (\varphi_k|_{t=0}, \varphi_l|_{t=0})_X = (v_k, v_l)_X = \delta_{kl},$$

$$(\varphi_k^*, \varphi_k^*)_{W_1} = \Big(-\frac{\partial \varphi_k^*}{\partial t} - (F'(\bar{\varphi}))^*\varphi_k^*, -\frac{\partial \varphi_l^*}{\partial t} - (F'(\bar{\varphi}))^*\varphi_l^*\Big)_W = (\varphi_k, \varphi_l)_W = \delta_{kl}.$$

Let $\varphi \in W_0$ and $(\varphi, \varphi_k)_W = 0$ for all $k = 1, 2, \ldots$ Then

$$(\varphi, \varphi_k)_W = \Big(\frac{\partial \varphi}{\partial t} - F'(\bar{\varphi})\varphi, \frac{\partial \varphi_k}{\partial t} - F'(\bar{\varphi})\varphi_k\Big)_Y + (\varphi|_{t=0}, \varphi_k|_{t=0})_X = (\varphi|_{t=0}, v_k)_X = 0, \ \ k = 1, 2, \ldots$$

Because of the completeness of $\{v_k\}$ in X we find that $\varphi|_{t=0} = 0$. Then, $\varphi = 0$, which leads to the completeness of $\{\varphi_k\}$ in W_0. Analogously, we show that $\{\varphi_k^*\}$ is complete in W_1.

Using the fundamental control functions, we can obtain the solution of the error equation (2.19) in the explicit form. The equation (2.19) is equivalent to the system (2.6)–(2.8) and may be written as the following system:

$$\left\{ \begin{array}{rcl} \frac{\partial \psi}{\partial t} - F'(\bar{\varphi})\psi &=& 0, \ t \in (0, T), \\ \psi|_{t=0} &=& \delta u, \end{array} \right. \tag{5.5}$$

$$\left\{ \begin{array}{rcl} -\frac{\partial \psi^*}{\partial t} - (F'(\bar{\varphi}))^*\psi^* &=& -\psi, \ \ t \in (0, T) \\ \psi^*|_{t=T} &=& 0, \end{array} \right. \tag{5.6}$$

$$\alpha\delta u - \psi^*|_{t=0} = P, \tag{5.7}$$

where $P = R_1\xi_1 + R_2\xi_2 + R_3\xi_3$ is the right-hand side of (2.19).

The following theorem holds.

Theorem 5.1. *The solution* $\psi, \psi^*, \delta u$ *of the system* (5.5)–(5.7) *may be represented in the form:*

$$\psi = \sum_k a_k\varphi_k, \quad \psi^* = \sum_k a_k\varphi_k^*, \quad \delta u = \sum_k a_k v_k, \tag{5.8}$$

where $\varphi_k, \varphi_k^*, v_k$ *are the fundamental control functions defined by* (5.2)–(5.4), $a_k = (P, v_k)_X/\mu_k$, *the series for* $\psi, \psi^*, \delta u$ *converging in* W_0, W_1, X, *respectively.*

Proof. The system (5.5)–(5.7) is equivalent to the error equation (2.19), which gives $\mu_k(\delta u, v_k)_X = (P, v_k)_X$ due to (5.1). Hence, the solution δu of (2.19) is represented as $\delta u = \sum\limits_k a_k v_k$, $a_k = (P, v_k)_X/\mu_k$. Then, it is easily seen that $\psi = \sum\limits_k a_k\varphi_k$, $\psi^* = \sum\limits_k a_k\varphi_k^*$ are the solutions to (5.5), (5.6), respectively. The completeness of the system $\{\varphi_k\}, \{\varphi_k^*\}, \{v_k\}$ gives the convergence of the corresponding series in W_0, W_1, X. This ends the proof.

From (5.8), we have the representation for the Fourier coefficients $(\delta u)_k$ of the error δu:

$$(\delta u)_k = (\delta u, v_k)_X = a_k = \frac{1}{\mu_k}(R_1\xi_1 + R_2\xi_2 + R_3\xi_3, v_k)_X. \tag{5.9}$$

Note that

$$(R_1\xi_1, v_k)_X = \alpha(\xi_1, v_k)_X. \tag{5.10}$$

By definition of R_2, R_3,

$$(R_2\xi_2, v_k)_X = (\theta^*|_{t=0}, v_k)_X, \quad (R_3\xi_3, v_k)_X = (\theta_1^*|_{t=0}, v_k)_X,$$

where θ^* is the solution of (2.15) for $g = \xi_2$, and θ_1, θ_1^* are the solutions of (2.16)–(2.17) for $h = \xi_3$. From (2.15) and (5.2) we get

$$(\theta^*|_{t=0}, v_k)_X = (\xi_2, \varphi_k)_Y.$$

Hence,

$$(R_2\xi_2, v_k)_X = (\xi_2, \varphi_k)_Y. \tag{5.11}$$

Analogously, from (2.17) and (5.2),

$$(\theta_1^*|_{t=0}, v_k)_X = (-\theta_1, \varphi_k)_Y.$$

Further, (2.16) and (5.3) give

$$(\theta_1, -\varphi_k)_Y = (\theta_1|_{t=0}, \varphi_k^*|_{t=0})_X + (\xi_3, \varphi_k^*)_Y = (\xi_3, \varphi_k^*)_Y.$$

Hence,

$$(R_3\xi_3, v_k)_X = (\xi_3, \varphi_k^*)_Y. \tag{5.12}$$

From (5.9)–(5.12) we obtain the expression for the Fourier coefficients $(\delta u)_k$ of the error δu of the optimal solution through the errors ξ_1, ξ_2, ξ_3:

$$(\delta u)_k = \frac{\alpha}{\mu_k}(\xi_1, v_k)_X + \frac{1}{\mu_k}(\xi_2, \varphi_k)_Y + \frac{1}{\mu_k}(\xi_3, \varphi_k^*)_Y, \tag{5.13}$$

where $\{\varphi_k, \varphi_k^*, v_k\}$ are the fundamental control functions defined by (5.2)–(5.4).

From (5.13), it is seen that the fundamental control functions play a role of "sensitivity functions"; they are the weight-functions for the corresponding errors ξ_1, ξ_2, ξ_3 in the representation (5.13). Note that the fundamental control functions $\{\varphi_k, \varphi_k^*, v_k\}$ do not depend on the structure of the errors ξ_1, ξ_2, ξ_3 and may be calculated beforehand for each k in need.

Remark 5.2. In the case that $F'(\bar\varphi) = (F'(\bar\varphi))^* = -A$ is a t-independent self-adjoint operator, under the conditions of Section 4, it is easily seen that the fundamental control functions $\varphi_k, \varphi_k^*, v_k$ defined by (5.2)–(5.4) coincide with the functions $\psi_{(k)}w_k, \psi_{(k)}^*w_k, w_k$, respectively, where w_k are the eigenfunctions of A, and $\psi_{(k)}, \psi_{(k)}^*$ are given by (4.8). In this case, the representation (5.13) is nothing else then (4.14).

In more general case, when $Y_{obs} \neq Y$, $C \neq E$, we may also define the control functions $\varphi_k, \varphi_k^*, v_k$ as the solutions to the system:

$$\begin{cases} \dfrac{\partial \varphi_k}{\partial t} - F'(\bar\varphi)\varphi_k &= 0, \ t \in (0,T), \\ \varphi_k|_{t=0} &= v_k, \end{cases} \tag{5.14}$$

$$\begin{cases} -\dfrac{\partial \varphi_k^*}{\partial t} - (F'(\bar\varphi))^*\varphi_k^* &= -C^*C\varphi_k, \ \ t \in (0,T) \\ \varphi_k^*|_{t=T} &= 0, \end{cases} \tag{5.15}$$

$$\alpha v_k - \varphi_k^*|_{t=0} = \mu_k v_k. \tag{5.16}$$

It may be easily verified that in this case the error relationship (5.13) changes to

$$(\delta u)_k = \frac{\alpha}{\mu_k}(\xi_1, v_k)_X + \frac{1}{\mu_k}(\xi_2, C\varphi_k)_{Y_{obs}} + \frac{1}{\mu_k}(\xi_3, \varphi_k^*)_Y. \tag{5.17}$$

6 Singular vectors and error sensitivity analysis

Consider the error equation (2.19). Under the hypotheses of Theorem 3.1, we may rewrite (2.19) as

$$\delta u = H^{-1}R_1\xi_1 + H^{-1}R_2\xi_2 + H^{-1}R_3\xi_3. \tag{6.1}$$

Suppose that the errors ξ_1, ξ_2, ξ_3 do not correlate and the following relation is satisfied:

$$\|\delta u\|_X^2 = \|T_1\xi_1\|_X^2 + \|T_2\xi_2\|_X^2 + \|T_3\xi_3\|_X^2, \tag{6.2}$$

where $T_i = H^{-1}R_i$. From (6.2),

$$\|\delta u\|_X^2 = (T_1^*T_1\xi_1, \xi_1)_X + (T_2^*T_2\xi_2, \xi_2)_{Y_{obs}} + (T_3^*T_3\xi_3, \xi_3)_Y, \tag{6.3}$$

where $T_1^* : X \to X$, $T_2^* : X \to Y_{obs}$, $T_3^* : X \to Y$ are the adjoints to T_i, $i = 1, 2, 3$.

Each summand in (6.3) determines the impact given by the correspoding error ξ_i. We have

$$(T_1^*T_1\xi_1, \xi_1)_X \le \|T_1^*T_1\|\|\xi_1\|_X^2, \quad (T_2^*T_2\xi_2, \xi_2)_{Y_{obs}} \le \|T_2^*T_2\|\|\xi_2\|_{Y_{obs}}^2,$$

$$(T_3^*T_3\xi_3, \xi_3)_Y \le \|T_3^*T_3\|\|\xi_3\|_Y^2, \tag{6.4}$$

and the i-th inequality becomes an equality when ξ_i is the singular vector of T_i corresponding to the largest singular value $\sigma_{max}^2 = \|T_i^*T_i\|$. The values $r_i = \sqrt{\|T_i^*T_i\|}$ may be considered as *sensitivity coefficients* which clearly demonstrate the measure of influence of the corresponding error upon the optimal solution. The higher the relative sensitivity coefficient, the more effectual is the error in question.

As above, we assume that the Hessian H defined by (2.11)–(2.13) is positive and has a complete orthonormal system in X of eigenfunctions v_k corresponding to the eigenvalues μ_k: $Hv_k = \mu_k v_k$, $\quad (v_k, v_l)_X = \delta_{kl}$, $k, l = 1, 2, \ldots$

Consider the operator T_1. Since $T_1 = H^{-1}R_1 = \alpha H^{-1} = T_1^*$, the singular vectors of T_1 are the eigenvectors v_i of the Hessian H, and the corresponding sensitivity coefficient is equal to

$$r_1 = \sqrt{\|T_1^*T_1\|} = \frac{\alpha}{\mu_{\min}}, \tag{6.5}$$

where $\mu_{\min}$ is the lower spectrum bound of H.

For the operator $T_2 : Y_{obs} \to X$ the following statement is valid.

Lemma 6.1. *The singular values σ_k^2 and the corresponding orthonormal (right) singular vectors $w_k \in Y_{obs}$ of the operator T_2 are defined by the formulas:*

$$\sigma_k^2 = \frac{\mu_k - \alpha}{\mu_k^2}, \quad w_k = \frac{1}{\sqrt{\mu_k - \alpha}} C\varphi_k, \tag{6.6}$$

where μ_k are the eigenvalues of the Hessian H, and φ_k are the fundamental control functions defined by (5.14)*. The left singular vectors of T_2 coincide with the eigenvectors v_k of H:*

$$T_2 T_2^* v_k = \sigma_k^2 v_k, \quad k = 1, 2, \ldots$$

Proof. Since $T_2 = H^{-1}R_2$, then $T_2T_2^* = H^{-1}R_2R_2^*H^{-1}$. To determine R_2^*, consider the inner product $(R_2 g, p)_X, g \in Y_{obs}, p \in X$. From (2.14)–(2.15),

$$(R_2 g, p)_X = (\theta^*|_{t=0}, p)_X = (C^* g, \phi)_Y = (g, R_2^* p)_{Y_{obs}},$$

where $R_2^* p = C\phi$, and ϕ is the solution to the problem

$$\left\{ \begin{array}{rcl} \dfrac{\partial \phi}{\partial t} - F'(\bar{\varphi})\phi & = & 0, \ t \in (0, T), \\ \phi|_{t=0} & = & p. \end{array} \right. \tag{6.7}$$

From definition of the Hessian H by (2.11)–(2.13), it is easily seen that $R_2 R_2^* = H - \alpha E$. Then,

$$T_2 T_2^* = H^{-1}(H - \alpha E)H^{-1} = H^{-2}(H - \alpha E).$$

Hence, the eigenvectors v_k of H are the eigenvectors of $T_2T_2^*$ which are the left singular vectors of T_2, with

$$\sigma_k^2 = \frac{\mu_k - \alpha}{\mu_k^2}.$$

The right singular vectors w_k of T_2 satisfy the equation

$$T_2^* T_2 w_k = \sigma_k^2 w_k, \quad k = 1, 2, \ldots$$

and are defined by

$$w_k = \frac{1}{\sigma_k} T_2^* v_k.$$

Due to (5.14)–(5.16),

$$w_k = \frac{1}{\sigma_k} R_2^* H^{-1} v_k = \frac{1}{\sigma_k \mu_k} R_2^* v_k = \frac{1}{\sqrt{\mu_k - \alpha}} C\varphi_k$$

and

$$(w_k, w_l)_{Y_{obs}} = \frac{1}{\sqrt{\mu_k - \alpha}} \frac{1}{\sqrt{\mu_l - \alpha}} (C\varphi_k, C\varphi_l)_Y =$$
$$= \frac{\mu_k - \alpha}{\sqrt{(\mu_k - \alpha)(\mu_l - \alpha)}} (v_k, v_l)_X = \delta_{kl}.$$

Therefore, w_k satisfy (6.6) and form an orthonormal system in Y_{obs}. The lemma is proved.

Corollary 6.1. The sensitivity coefficient $r_2 = \sqrt{\|T_2^* T_2\|}$ is defined by the formula:

$$r_2 = \max_k \frac{\sqrt{\mu_k - \alpha}}{\mu_k}. \tag{6.8}$$

The equality $(T_2^* T_2 \xi_2, \xi_2)_{Y_{obs}} = r_2^2 \|\xi_2\|^2_{Y_{obs}}$ holds if $\xi_2 = w_{k_0}$, where w_{k_0} is the singular vector of T_2 corresponding to the largest singular value $\sigma^2_{k_0}$.

Remark 6.1. The proof of Lemma 6.1 was done for the case $\mu_k > \alpha$. If $\mu_k = \alpha$, the singular value of T_2 equals zero, v_k is still the left singular vector, and $C\varphi_k = 0$.

Consider now the operator $T_3 = H^{-1} R_3$. To determine the sensitivity coefficient $r_3 = \sqrt{\|T_3^* T_3\|}$, we need to derive R_3^*. For $h \in Y, p \in X$, we have from (2.16)–(2.18):

$$(R_3 h, p)_X = (\theta_1^*|_{t=0}, p)_X = -(C^* C\theta_1, \phi)_Y = -(C\theta_1, C\phi)_{Y_{obs}},$$

where θ_1, θ_1^* are the solutions to (2.16)–(2.17), and ϕ is the solution to (6.7). Further,

$$(R_3 h, p)_X = -(\theta_1, C^* C\phi)_Y = (h, \phi^*)_Y$$

and $R_3^* p = \phi^*$, where ϕ^* is the solution to the adjoint problem:

$$\begin{cases} -\dfrac{\partial \phi^*}{\partial t} - (F'(\bar{\varphi}))^* \phi^* &= -C^* C\phi, \quad t \in (0, T) \\ \phi^*|_{t=T} &= 0. \end{cases} \tag{6.9}$$

The operator $R_3 R_3^* : X \to X$ may be defined as follows: for given $p \in X$ find ϕ as the solution of (6.7), find ϕ^* as the solution of (6.9), and for $h = \phi^*$ find θ_1, θ_1^* as the solutions of (2.16)–(2.17); then, put $R_3 R_3^* = \theta_1^*|_{t=0}$.

Therefore, the operator $T_3 T_3^* = H^{-1} R_3 R_3^* H^{-1}$ is defined by the successive solutions of the following problems (for given $v \in X$):

$$Hp = v, \tag{6.10}$$

$$\begin{cases} \dfrac{\partial \phi}{\partial t} - F'(\bar{\varphi})\phi &= 0, \ t \in (0,T), \\ \phi|_{t=0} &= p, \end{cases} \tag{6.11}$$

$$\begin{cases} -\dfrac{\partial \phi^*}{\partial t} - (F'(\bar{\varphi}))^*\phi^* &= -C^*C\phi, \ \ t \in (0,T) \\ \phi^*|_{t=T} &= 0. \end{cases} \tag{6.12}$$

$$\begin{cases} \dfrac{\partial \theta_1}{\partial t} - F'(\bar{\varphi})\theta_1 &= \phi^*, \ \ t \in (0,T) \\ \theta_1|_{t=0} &= 0, \end{cases} \tag{6.13}$$

$$\begin{cases} -\dfrac{\partial \theta_1^*}{\partial t} - (F'(\bar{\varphi}))^*\theta_1^* &= -C^*C\theta_1, \ \ t \in (0,T) \\ \theta_1^*|_{t=T} &= 0, \end{cases} \tag{6.14}$$

$$Hw = \theta_1^*|_{t=0}, \tag{6.15}$$

then

$$T_3 T_3^* v = w, \tag{6.16}$$

and for the sensitivity coefficient r_3 we have

$$r_3 = \sqrt{\|T_3 T_3^*\|}. \tag{6.17}$$

In some cases the sensitivity coefficient r_3 may be found in the explicit form. To give an example, consider the case of Section 4. Let $Y_{obs} = Y$, $C = E$ (the identity operator), and $F'(\bar{\varphi}) = (F'(\bar{\varphi}))^* = -A$ be a t-independent self-adjoint operator such that A generates an orthonormal basis in X consisting of eigenfunctions v_k: $Av_k = \lambda_k v_k$, $(v_k, v_j)_X = \delta_{kj}$, where λ_k are the corresponding eigenvalues of A. Then the eigenfunctions of the Hessian H coincide with the eigenfunctions v_k, and the eigenvalues μ_k are defined by (4.9). In this case, the following statement is valid.

Lemma 6.2. *The singular values σ_k^2 of the operator T_3 are defined by the formula:*

$$\sigma_k^2 = \frac{1}{(2\mu_k\lambda_k)^2}\Big(\frac{1 - e^{-4\lambda_k T}}{2\lambda_k} - 2Te^{-2\lambda_k T}\Big), \tag{6.18}$$

where $\mu_k = \alpha + (1 - e^{-2\lambda_k T})/(2\lambda_k)$. The left singular vectors of T_3 coincide with the eigenvectors v_k, and the corresponding orthonormal right singular vectors $w_k \in Y$ are defined as

$$w_k = \frac{1}{\sigma_k \mu_k}\varphi_k^*, \quad \varphi_k^*(t) = \frac{1}{2\lambda_k} e^{\lambda_k t}(e^{-2\lambda_k T} - e^{-2\lambda_k t})v_k, \tag{6.19}$$

where φ_k^* *are the fundamental control functions satisfying* (5.2)–(5.4).

Proof. Consider the operator $T_3T_3^*$ defined by the formulas (6.10)–(6.17). For $v = v_k$ we get

$$p = \frac{1}{\mu_k}v_k, \quad \phi = \frac{1}{\mu_k}e^{-\lambda_k t}v_k, \quad \phi^* = -\frac{1}{\mu_k}e^{\lambda_k t}\int\limits_t^T e^{-2\lambda_k s}v_k ds,$$

$$\theta_1 = -\frac{1}{\mu_k}e^{-\lambda_k t}\int\limits_0^t e^{2\lambda_k \xi}\int\limits_\xi^T e^{-2\lambda_k s}v_k ds d\xi,$$

$$\theta_1^* = \frac{1}{\mu_k}\int\limits_t^T e^{-\lambda_k(\theta-t)}e^{-\lambda_k\theta}\int\limits_0^\theta e^{2\lambda_k\xi}\int\limits_\xi^T e^{-2\lambda_k s}v_k ds d\xi d\theta,$$

$$w = \frac{1}{\mu_k}\theta_1^*\Big|_{t=0} = \frac{1}{\mu_k^2}\int\limits_0^T e^{-2\lambda_k\theta}\int\limits_0^\theta e^{2\lambda_k\xi}\int\limits_\xi^T e^{-2\lambda_k s}v_k ds d\xi d\theta.$$

Then, from (6.16),

$$T_3T_3^*v_k = \sigma_k^2 v_k, \quad k = 1, 2, \ldots,$$

where

$$\sigma_k^2 = \frac{1}{\mu_k^2}\int\limits_0^T e^{-2\lambda_k\theta}\int\limits_0^\theta e^{2\lambda_k\xi}\int\limits_\xi^T e^{-2\lambda_k s}ds d\xi d\theta =$$

$$= \frac{1}{\mu_k^2}\int\limits_0^T e^{2\lambda_k\xi}\Big(\int\limits_\xi^T e^{-2\lambda_k s}ds\Big)^2 d\xi = \frac{1}{(2\mu_k\lambda_k)^2}\Big(\frac{1-e^{-4\lambda_k T}}{2\lambda_k} - 2Te^{-2\lambda_k T}\Big) > 0.$$

Thus, v_k are the left singular values of T_2 corresponding to the singular values σ_k^2. The right singular vectors of T_3 satisfy the equation

$$T_3^*T_3 w_k = \sigma_k^2 w_k, \quad k = 1, 2, \ldots$$

and are defined by

$$w_k = \frac{1}{\sigma_k}T_3^* v_k.$$

Due to (5.2)–(5.3),

$$w_k = \frac{1}{\sigma_k} R_3^* H^{-1} v_k = \frac{1}{\sigma_k \mu_k} R_3^* v_k = \frac{1}{\sigma_k \mu_k} \varphi_k^*$$

and

$$(w_k, w_l)_Y = \frac{1}{\sigma_k \mu_k} \frac{1}{\sigma_l \mu_l} (\varphi_k^*, \varphi_l^*)_Y = \frac{1}{\sigma_k \mu_k} \frac{1}{\sigma_l \mu_l} (R_3^* v_k, R_3^* v_l)_Y =$$

$$= \frac{1}{\sigma_k \sigma_l} (H^{-1} R_3 R_3^* H^{-1} v_k, v_l)_X = \frac{1}{\sigma_k \sigma_l} (T_3 T_3^* v_k, v_l)_X = \frac{\sigma_k}{\sigma_l} (v_k, v_l)_X = \delta_{kl}.$$

The lemma is proved.

Corollary 6.2. Under the hypotheses of Lemma 6.1, the sensitivity coefficient $r_3 = \sqrt{\|T_3^* T_3\|}$ is defined by the formula:

$$r_3 = \max_k \frac{1}{2\mu_k \lambda_k} \sqrt{\frac{1 - e^{-4\lambda_k T}}{2\lambda_k} - 2T e^{-2\lambda_k T}}. \tag{6.20}$$

The equality $(T_3^* T_3 \xi_3, \xi_3)_Y = r_3^2 \|\xi_3\|_Y^2$ holds if $\xi_3 = w_{k_0}$, where w_{k_0} is the singular vector of T_3 corresponding to the largest singular value $\sigma_{k_0}^2$.

For more general cases, the algorithm (6.10)–(6.17) may be used for computing r_3 numerically.

7 Application to the data assimilation in hydrology

Consider the following initial-boundary value problem for the quasilinear parabolic equation arisen in the soil water movement:

$$\begin{cases} \dfrac{\partial \theta}{\partial t} = \dfrac{\partial}{\partial z} D(\theta) \dfrac{\partial \theta}{\partial z} - \dfrac{\partial K(\theta)}{\partial z}, & t \in (0, T), \; z \in (0, Z), \\ \theta|_{t=0} = u(z), \; \theta|_{z=0} = \theta_0(t), \; \theta|_{z=Z} = \theta_1(t), \end{cases} \tag{7.1}$$

where $\theta = \theta(t, z)$ is the volumetric water content (soil wetness), $D(\theta)$ the diffusion coefficient, $K(\theta)$ the hydraulic conductivity, Z the soil depth, T the time interval, and $u(z), \theta_0(t), \theta_1(t)$ are prescribed functions. The coefficients $D(\theta)$ and $K(\theta)$ are defined by the formulas [7]:

$$K(\theta) = K_s \left(\frac{\theta}{\theta_s} \right)^\eta, \quad D(\theta) = K(\theta) \frac{\partial h}{\partial \theta}, \tag{7.2}$$

where h is the soil water pressure head related to the water content by $\theta = \theta_s(1 + (hh_g^{-1})^n)^{\frac{2}{n}-1}$, K_s and θ_s are the hydraulic conductivity and the water content profile at natural saturation, respectively, n and η are the so-called shape parameters linked to the soil texture, and h is the scale parameter depending on the soil structural properties [7]. In this model, the soil water movement is supposed to be isotermal and one-dimensional, whereas the influence of swelling and shrinking of soil porous material is not taken into consideration. (For more details, we refer to [7], [29].)

Consider the functional

$$S(u) = \frac{\alpha}{2}\int_0^Z (u(z) - u_0(z))^2 dz + \frac{1}{2}\int_0^T (I_{cal}(t) - I_{obs}(t))^2 dt, \tag{7.3}$$

where $\alpha \geq 0$, $I_{cal}(t) = \int_0^Z (\theta(t,z) - \theta_{ini})dz$ is the cumulative infiltration, and θ_{ini}, u_0, I_{obs} are prescribed functions, $I_{obs}(t)$ being the observed cumulative infiltration.

It is easily seen that the functional (7.3) takes the form (1.2) if we put

$$X = L_2(0,Z),\ \ Y_{obs} = L_2(0,T),\ \ C\theta = \int_0^Z \theta(t,z)dz,\ \ \varphi_{obs} = I_{obs} + \int_0^Z \theta_{ini}dz.$$

Then, the data assimilation problem may be written in the form (1.3) and is formulated as follows: find u and θ such that they satisfy (7.1) and the functional (7.3) on the set of solutions of (7.1) takes its minimal value.

The solvability of such problems for quasilinear parabolic equations was studied in [13], [14]. In this paper, we study numerically the sensitivity of the optimal solution to the errors of the input data according to the above-formulated theoretical approach. For numerical solution of the data assimilation problem we used the algorithm developed in [21], based on the gradient method, finite differencing in space, and the leap-frog differencing in time. The unconstrained minimization algorithm of the quasi-Newton limited memory type with stopping criteron either on the number of iterations or on the gradient norm of the cost function was used [21].

First, using the observed cumulative infiltration $I_{obs}(t)$ from [21] (see Fig.1), we solved the data assimilation problem (1.3) for $\alpha = 0$, $K_s = 5.37641 \times 10^{-3} m/s$, $\theta_s = 0.31361 cm^3/cm^3$, $h_g = -15.83975m$, $\eta = 4.97411$, $n = 3.25759$, $\theta_0 = 0.30254 cm^3/cm^3$, $\theta_1 = 0.28738 cm^3/cm^3$, $\theta_{ini} = 9.18441 \times 10^{-2} cm^3/cm^3$, $T = 3600s$, $Z = 1m$.

The decay of the gradient norm of the functional (7.2) with iterations of the minimization procedure for various α is shown in Fig.2, and the resulted simulated cumulative infiltration for $\alpha = 0.001$ is presented in Fig.1. Figure 2 shows the convergence of the identification process, and Figure 1 demonstrates the fact that the optimal initial value function as well as possible adjusts the cumulative infiltrations.

The initial value function u founded was then considered to be the "exact" solution $\bar{u}$ satisfying (1.7) with $\bar{f} = 0$.

Further, we assumed the presence of errors ξ_1, ξ_2, ξ_3 in the corresponding input data u_0, φ_{obs}, f, and analysed the sensitivity coefficients r_1, r_2, r_3 introduced in Section 6. To find r_i, the eigenvalues μ_k of the Hessian H were computed, using the definition of H by (2.11)–(2.13) and the standard Lanczos algorothm [23].

The dependence of the eigenvalues μ_k on their number k for $\alpha = 0.1$ is illustrated by Fig.3. The condition number of the Hessian, which is defined as the ratio of its largest eigenvalue to its smallest, is given for various α in Table 1. It is evident that the Hessian becomes ill-conditioned as soon as α goes to zero.

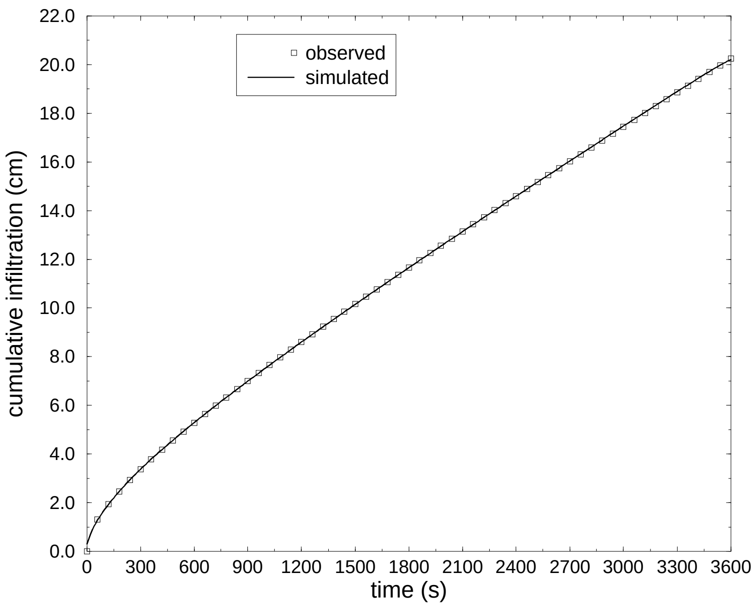

Figure 1: Simulated and observed cumulative infiltration

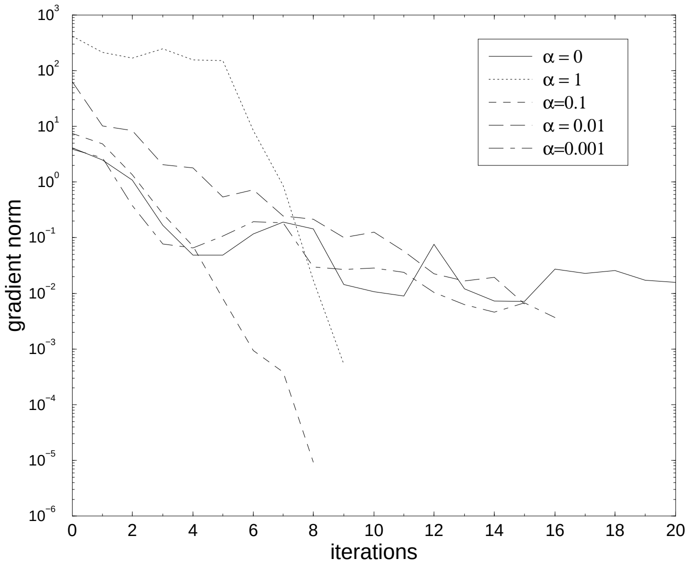

Figure 2: Gradient norm

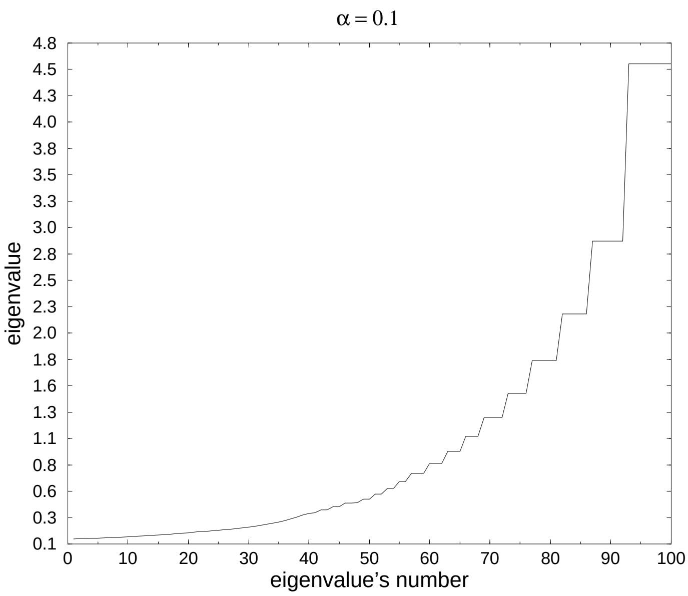

Figure 3: Eigenvalues of the Hessian

To compute the sensitivity coefficients r_1 and r_2, the formulas (6.5) and (6.8) were used. The function $g(k) = \sqrt{\mu_k - \alpha}/\mu_k$ in (6.8) takes its maximum value r_2 for different values of k, depending on α. These values are given in Table 2. The corresponding singular vectors w_k defined by (6.6) are presented in Fig.5. It is seen from Table 2 that the minimal eigenvalue $\mu_{\min}$ of the Hessian gives the maximum value of $g(k)$ if only $\alpha = 0$.

α	0	10^{-3}	10^{-2}	5×10^{-2}	10^{-1}	1
Condition number	1.58×10^{12}	4501.3658	451.0365	91.0073	46.0036	5.5003

Table 1: Condition number of the Hessian

α	0	10^{-3}	10^{-2}	5×10^{-2}	10^{-1}	0.75	1
k_0	1	2	7	18	28	60	66
r_2	5.942×10^5	14.838	4.998	2.235	1.581	0.577	0.499

Table 2: Sensitivity coefficient r_2 and the relative values $k_0 = arg \max_k \frac{\sqrt{\mu_k - \alpha}}{\mu_k}$

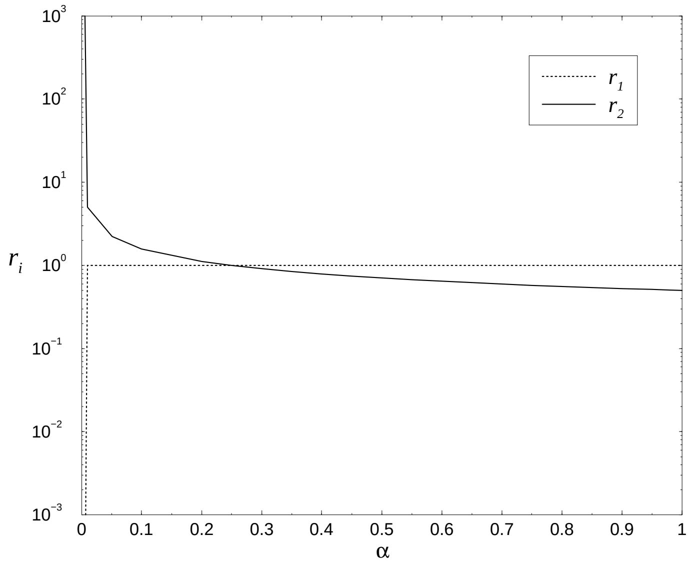

Figure 4: Sensitivity coefficients r_1 and r_2

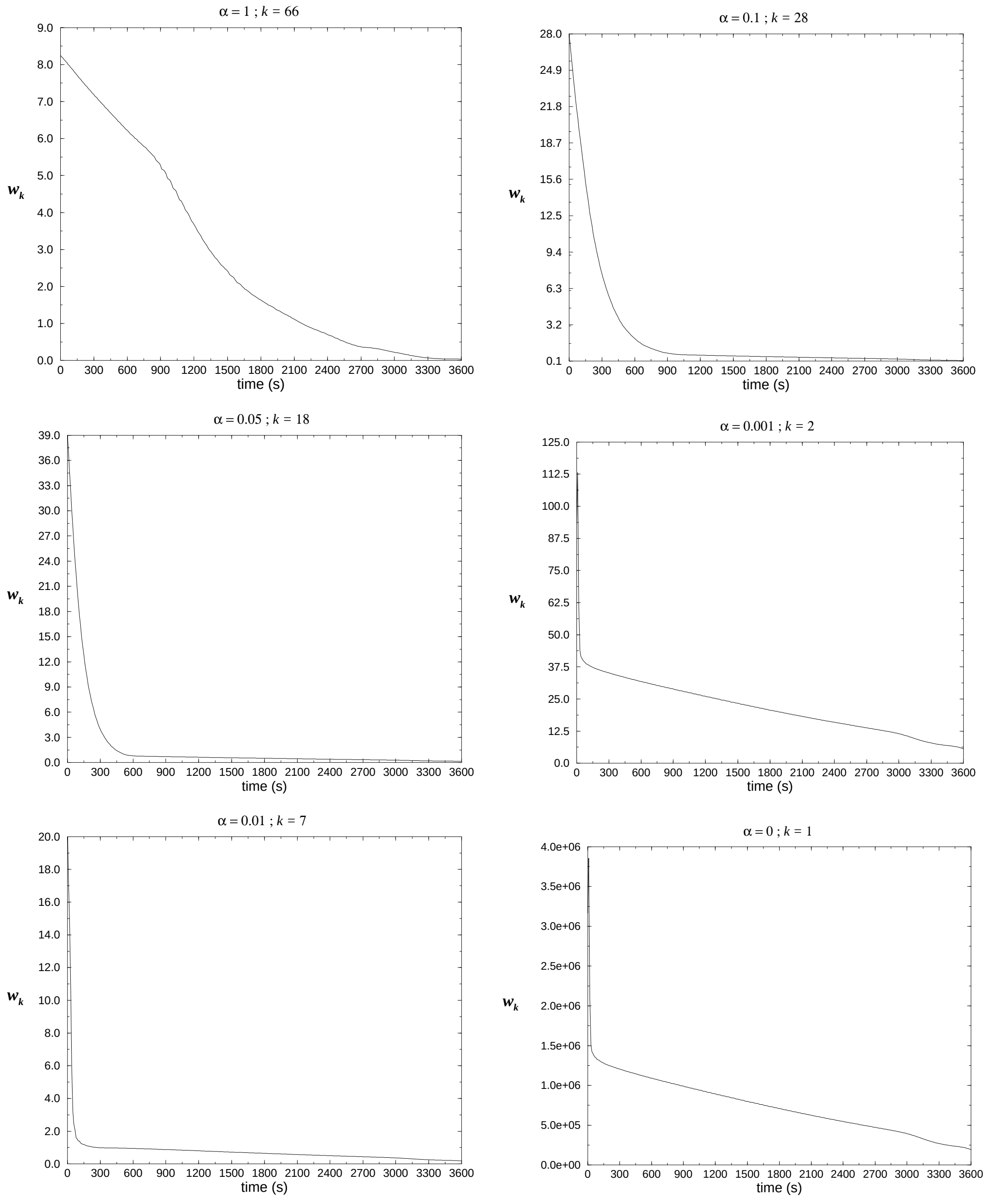

Figure 5: Singular vectors $\quad w_k = \dfrac{C\varphi_k}{\sqrt{\mu_k - \alpha}}$

The dependence of the sensitivity coefficients r_1 and r_2 on α is illusrtated by Fig.4. From Fig.4, the sensitivity coefficient r_1 is small and r_2 is large if α goes to zero. If α goes to 1, the coefficient r_1 also goes to 1, and r_2 is decreasing, being less than r_1. It is seen from Fig.4 that there exist an α such that $r_1 = r_2$. In the case under consideration, we have $\alpha \approx 0.25$.

To compute the sensitivity coefficient r_3, the algorithm (6.10)–(6.11) was used. The dependence of r_3 on the regularization parameter α is illustrated by Fig.6 in comparison with the coefficients r_1 and r_2. The behaviour of r_3 is similar to that of r_2, and, in the case under consideration, r_2 is larger then r_3 for all α. It means that the optimal solution is more sensitive to variations of the observation errors.

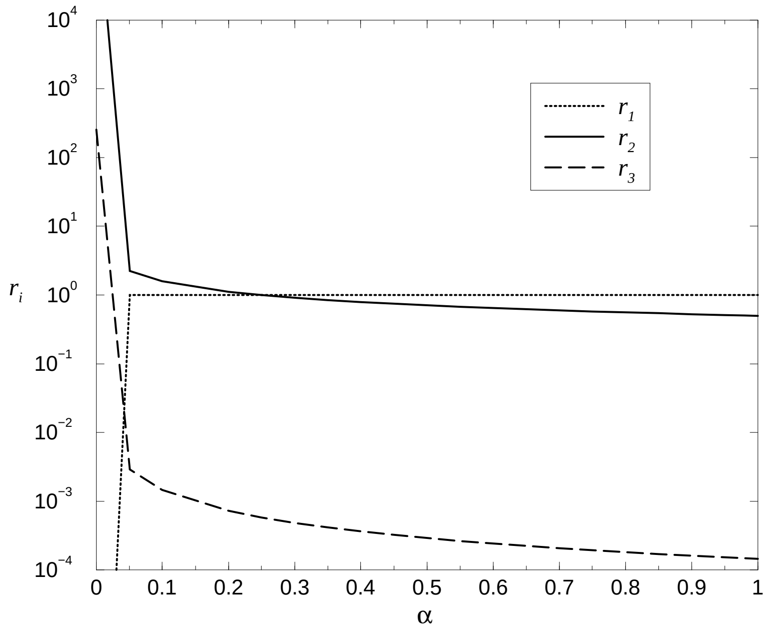

Figure 6: Sensitivity coefficients r_i, $i = 1, 2, 3$

8 Summary and concluding remarks

The error of the optimal initial-value function in data assimilation may be expressed through the errors of the input data using the Hessian of the misfit functional. The sensitivity of the optimal solution to the input errors is determined by the value of the sensitivity coefficients which are the norms of the specific response operators relating the error of the input to the error of the optimal initial-value function. The maximum error growth for the output is given by the singular vectors of the corresponding response operator. In some cases, singular vectors are the fundamental control functions which form complete orthonormal systems in specific functional spaces and may be used for error analysis.

The sensitivity coefficients depend on the regularization parameter α. With α increasing, the output regularization error increases, whereas the sensitivity to the observation and model errors decreases. If α goes to zero, the output regularization error vanishes, however, the sensitivity to the observation and model errors is increasing due to the fact that the Hessian of the cost functional is ill-conditioned.

From numerical experiments, the optimal solution is more sensitive to the observation errors then to the model errors. Therefore, the effect of the observation errors in data assimilation is of more significance and should be taken into account when solving the problem.

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