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The Parameter Identification Model and Its Optimal Property in Dynamics Equations*

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Abstract In this paper, a mathematical model with respect to optimal identification of the parameters is established. The identifiability of the dynamics problem is proved. At last the necessary conditions of the optimality are given.

1. Introduction

There are some parameters in many evolution equations, such as $a_{10}, a_{11}, a_{12}, a_{20}, a_{21}, a_{22}$ in 2-dimensional Volterra model [1]; birthrate, natural death rate, incidence of a disease death rate, lifelong immunity rate in the dynamics of infectious disease [2,3]. Obviously, these parameters related to the practical states of applying model such as time and place. These mathematical models which descripte dynamics developing process do not have practical value and theory significance until these parameters are determined according to concrete practice. Consequently, identifying these parameters is very importance. But it is short of the study of the identification problem at present[4]. With respect to the dynamics equations of oil and gas generation[5], this paper firstly establishes a mathematical model with regard to the optimal identification of the parameters with activation energy and frequency factor. Secondly, applies the continuity of functional to prove the identifiability of this problem. At last proves that the solution of this dynamics equations is weak Gâteaux differentiable and gives the necessary conditions of an optimality of this optimal identification problem.

2. Optimal identification problem

In the early 1970's, B.P.Tissot gave a mathematical model of generating process of oil and gas as follows:

$$\text{DES}: \quad \dot{x}_i = -k_i(t)x_i(t) \quad i = 1, \ldots, 6 \quad t \in I = [0, T_0] \tag{1}$$

$$\dot{x}_8(t) = k_7(t)x_7(t) \tag{2}$$

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$$\sum_{i=1}^{8} x_i(t) = \sum_{i=1}^{8} x_{0i} = g_0 \tag{3}$$

$$x_i(0) = x_{0i} \quad i = 1, \ldots, 8 \tag{4}$$

where $x_i(t), i = 1, \ldots, 6$, are the contents of i-th bonding kerogen at time $t \in I$, $x_7(t)$ is the content of liquid hydrocarbon (i.e., petroleum) generated by kerogen thermol degradation, and $x_8(t)$ is the content of nature gas generated by liquid hydrocarbon at time t. Therefore above variables should save for

$$0 \leq x_i(t) < 1, \quad i = 1, \ldots, 8 \tag{5}$$

The initial values of these variables save for

$$0 < x_{0i} < 1, \quad i = 1, \ldots, 6, \quad x_{07} = x_{08} = 0, \quad 0 < g_0 < 1 \tag{6}$$

$T_0 > 0$ is the finish time of kerogen thermol degradation, hence we have:

$$0 \leq x_i(T_0) < 1, \quad i = 1, \ldots, 6 \tag{7}$$

$k_i(t)$ is the degradation rate of i-th bonding kerogen and it satisfies

$$k_i(t) = A_i exp(-E_i/(R \times T(t))) \tag{8}$$

where frequency factor $A_i \in L_a = [10^5, 10^{35}]$ and activation energy $E_i \in L_e = [35, 350]$ are undetermined constants, R is positive constant and $T(t)$ is stratigraphic temprature at time t. Following from geography, $T(t)$ has the property:

Property 1 *The stratigraphic temprature $T(t)$ at time t is monotone increasing linear function of $t \in I$, and $T(t) > 0$, $t \in I$.*
According to formula (8), Property 1 and the existence and uniqueness of solution for initial values problem of ordinary differential equations, we know that the solution for initial value problem of ordinary differential equation DES formed by formulae (1)–(4) exists and unique. See [6].

Theorem 1 *If $x_7(t) \geq 0$, $\forall t \in I$, then under the initial conditions (6),the solution with components $x_i(t)$, $i = 1, \ldots, 8$ of problem DES satisfy the formula (5).*

Proof From formula (8) and Property 1 we have

$$k_i(t) > 0, \quad t \in I, \quad i = 1, \ldots, 7 \tag{9}$$

Then according to formulae (6), (1) and for t small enough, we have

$$x_i(t) > 0, \quad \dot{x}_i(t) < 0, \quad i = 1, \ldots, 6$$

Since T_0 is the finish time of kerogen thermol degradation, it is clear that $x_i(t) \geq 0$, $i = 1, \ldots, 6$ whenever $0 \leq t \leq T_0$. Hence, we have $\dot{x}_i(t) \leq 0$, $i = 1, \ldots, 6$, $\forall t \in I$. Therefore, $x_i(t)$, $i = 1, \ldots, 6$ is monotone decreasing function of $t \in I$, and

$$0 \leq x_i(T_0) \leq x_i(t) \leq x_i(0) < 1, \quad i = 1, \ldots, 6. \tag{10}$$

Since $x_7(t) \geq 0, \ \forall t \in I$, it follows from formula (9) that

$$\dot{x}_8(t) = k_7(t) \times x_7(t) \geq 0, \quad \forall t \in I$$

i.e., $x_8(t)$ is monotone increasing function of t. Hence $0 = x_{08} = x_8(0) \leq x_8(t), \quad \forall t \in I$. Since $0 < g_0 = \sum_{i=1}^{8} x_i(t) < 1$ and $x_i(t) \geq 0, \quad i = 1, \ldots, 8, \quad \forall t \in I$. This completes the proof.

Let

$$B = \begin{pmatrix} -k_1(t) & 0 & \ldots & 0 \\ 0 & -k_2(t) & \ldots & 0 \\ \ldots & & \ldots & \\ k_1(t) & k_2(t) & \ldots & -k_7(t) \end{pmatrix} \tag{11}$$

$B \in L(H)$ where $L(H)$ is a bounded linear oprator space from H ($H = R^7$, a Hilbert space) to H. Solve $x_8(t)$ from formula (3) and substitute it into (1),(2). Let $x(t) = [x_1(t), \ldots, x_7(t)]^T \in C^1(I, H), \quad x_0 = [x_{01}, \ldots, x_{07}]^T \in R^7$. The model can not response the generating process of oil and gas truely until the solution of problem DES satisfies formula (5). Therefore, marshaling the model, we obtain

$$\begin{aligned} \text{DES1}: \quad & \dot{x} = B \times x \\ & x(0) = x_0 \\ & 0 < x_{0i} < 1, \quad i = 1, \ldots, 6, \quad x_{07} = 0, \quad g_0 = \textstyle\sum_{i=1}^{7} x_{0i} < 1 \\ & x_7(t) \geq 0, \quad g_0 - \textstyle\sum_{i=1}^{7} x_i(t) \geq 0, \quad t \in I \end{aligned}$$

From Theorem 1, the solution of DES1 satisfies (5). Assuming that

$$q_a = [A_1, \ldots, A_7]^T \in L_a^7, \quad q_e = [E_1, \ldots, E_7]^T \in L_e^7, Q = \{q : q = [q_a^T, q_e^T]^T \in L_a^7 \times L_e^7\}$$

It is easy to know from (8) and (11) that for any $q \in Q$ there is unique operator $B \in L(H)$, denoted by $B(q)$ or B. Set $P_b = \{B(q) : q \in Q\} \subset L(H)$. Since $Q \subset R^7 \times R^7$ is bounded closed set, so it is compact. Moreover, mapping $q \to B(q)$ is continuous for any $t \in I$. So P_b is a compact subset of $L(H)$. The solution of DES1 is exist and unique for any $q \in Q$ (or $B \in P_b$) following from DES, denoted by $x(t, B)$ or $x(B)$. The chief grounds of numerical analogue in oil and gas generating process is the function obtained by the observed data:

$$y(t) = [y_1(t), \ldots, y_7(t)]^T \in C^1(I, H)$$

Thus the main task of analogue is to find a operator $B \in P_b$ such that $J(B) = 1/2 \int_I ||x(t, B) - y(t)||_H^2 dt$ is minimal. Denote the identification problem by OI, i.e.,

$$\begin{aligned} \text{OI}: \quad & \min \quad J(B) = 1/2 \times \int_I ||x(t, B) - y(t)||_H^2 dt \\ & s.t. \quad x(t, B) \text{is the solution of DES1}, \quad B \in P_b \end{aligned}$$

3. Identifiability

The identifiability of problem OI is equivalent to the existence of the optimal solution of problem OI. Therefore, we prove the Lemma first.

Lemma 1 *Assuming that* $g(t,x) = 1/2 \times \|x - y\|_H^2$. *If* $y \in C^1(I,H)$, *then function* $t \to g(t,x)$ *is measurable for any* $x \in C^1(I,H)$ *and* $\forall t \in I$, $x \to g(t,x)$ *is continuous in* H. *Moreover, if* $x(t,B)$, $B \in P_b$, *is the solution of DES1 , then mapping* $B \to J(B)$ *is continuous in* P_b.

Proof The first two results is immediately from the definition of $g(t,x)$ and $y \in C^1(I,H)$. We only prove that mapping $B \to J(B)$ is continuous for any $B \in P_b$. Let $\{B^n\} \in P_b$, and suppose $B^n \to B^0$. Clearly $B^0 \in P_b$, and hence the system

$$\begin{cases} \dot{x} = B^0 \times x \\ x(0) = x_0 \end{cases}$$

has a unique solution x^0. Similarly, corresponding to each B^n, the system

$$\begin{cases} \dot{x} = B^n \times x \\ x(0) = x_0 \end{cases}$$

has a unique solution x^n. Defining $z^n = x^n - x^0$, one observe that z^n is the solution of the system

$$\begin{cases} \dot{z}^n = B^n \times z^n + (B^n - B^0)x^0 \\ z(0) = 0 \end{cases} \tag{12}$$

Scalar multiplying the first equation of (12) on either side by z^n and using the elementary inequality $ab \le a^2/(2\varepsilon) + \varepsilon b^2/2$ for all $a, b \in R$, $\varepsilon > 0$, one can easily verify (using $\varepsilon = \alpha$) that

$$\|z^n(t)\|_H^2 + \alpha \int_0^t \|z^n(\theta)\|_H^2 d\theta \le \alpha \int_0^t \|z^n(\theta)\|_H^2 d\theta + 1/\alpha \int_0^t \|(B^n - B^0)x^0\|_H^2 d\theta \tag{13}$$

Let

$$\phi^n(t) = \|z^n(t)\|_H^2 + \alpha \int_0^t \|z^n(\theta)\|_H^2 d\theta$$

It follows from the above inequality (13) that

$$\phi^n(t) \le \alpha \int_0^t \phi^n(\theta) d\theta + 1/\alpha \int_0^t \|(B^n - B^0)x^0\|_H^2 d\theta \tag{14}$$

Using Gronwall's Lemma, one concludes that

$$\phi^n(t) \le (exp(\alpha T^0))1/\alpha \int_0^t \|(B^n - B^0)x^0\|_H^2 d\theta$$

for all $t \in I$. Since $\|x^0\|_H < 7$, $B^n \to B^0$, it is clear that $\|(B^n - B^0)x^0\|_H \to 0$. Hence by Lebesgue dominated convergence theorem it follows that $\phi^n(t) \to 0$ as $n \to \infty$ uniformly on I. Thus one may conclude from (13) that $x^n \to x^0$ in $C^1(I,H)$ for all $t \in I$. Let $J(B^n) = \int_I g(t,x^n)dt$ and $J(B^0) = \int_I g(t,x^0)dt$ where x^n and x^0 are the solutions of DES1 corresponding to B^n and B^0 respectively. Since, for all $t \in I$, $x \to g(t,x)$ is continuous on H, we have

$$g(t,x^0(t)) = \lim_{n\to\infty} g(t,x^n(t)) \quad \text{on } I$$

and consequently

$$\int_I g(t,x^0(t))dt = \lim_{n\to\infty} \int_I g(t,x^n(t))dt$$

Clearly, this is equivalent to

$$J(B^0) = \lim_{n\to\infty} J(B^n)$$

This completes the Lemma.

Theorem 2 *Under the assumption of Lemma 1, there exists a* $B^0 \in P_b$ *such that* $J(B^0) \le J(B)$ for all $b \in P_b$.

Proof Define $v = \inf\{J(B), B \in P_b\}$. Since $g(t,x) \ge 0$, $(t,x) \in I \times H$, the infimum is well defined and $v \ge 0$. Let $\{B^k\}$ be a minimizing sequence from P_b, i.e., $\lim_k J(B^k) = v$. Then by the compactness of P_b, there exists $\{B^{k_l}\} \subset \{B^k\}$, still relabeled as $\{B^k\}$ and a $B^0 \in P_b$ such that $B^k \to B^0$. Since $B \to J(B)$ is continuous, we have

$$v \le J(B^0) = \lim_k J(B^k) = v$$

Hence $J(B^0) = v$, implying that $J(.)$ attains its infimum on P_b. This completes the theorem.

4. The necessary conditions of optimality

For the proof of necessary conditions of optimality, we shall make use of Gâteaux differential of $x(B)$ with respect to the oprator B where $x(B)$ is the solution of DES1 corresponding to $B \in P_b$. Indeed, we show that the Gâteaux differential of x at B_0 in the direction B, defined by:

$$\hat{x}(B_0, B) = w - \lim_\varepsilon (x(B_0 + \varepsilon B) - x(B_0))/\varepsilon$$

exists and that it is the solution of a related differential equation.

Lemma 2 *Let $x(B)$ denote the solution of DES1 corresponding to $B \in P_b$. then at each point $B^0 \in P_b$, the function $B \to x(B)$ has a weak Gateaux differential in the direction $B - B^0$, denoted $\hat{x}(B^0, B - B^0)$, and it is the solution of the problem*

$$\begin{cases} \dot{e} - Be = (B - B^0) \times x(B^0) \\ e(0) = 0 \end{cases} \tag{15}$$

Proof Let $B^0, B \in P_b$, From the definition of Q and P_b we know that for any $\varepsilon \in (0,1]$, there exists $q^\varepsilon \in Q$ such that $B(q^\varepsilon) = B^\varepsilon = B^0 + \varepsilon(B - B^0) \in P_b$. Define

$$\phi^\varepsilon = (x(B^\varepsilon) - x(B^0))/\varepsilon \in C^1(I,H)$$

Then using the differential equation DES1, one obtains:

$$\begin{cases} \dot{\phi}^{\varepsilon} - B^{\varepsilon}\phi^{\varepsilon} = (B - B^0)x(t, B^0) \\ \phi^{\varepsilon}(0) = 0 \end{cases}$$

Since $x(t, B) \in C^1(I, H)$ for any $B \in P_b, t \in I$, and $I \subset R$ is a closed bounded set. $P_b \in L(H)$ is compact set. So $\{\phi^{\varepsilon} : \varepsilon \in (0, 1]\}$ is contained in a closed subset of $C^1(I, H)$. Hence from every sequence $\{\phi^n = \phi^{\varepsilon_n}, \quad \varepsilon_n \in (0, 1], \quad \varepsilon_n \to 0\}$, there exists a subsequence $\{\phi^{n_k}\}$, still relabeled as $\{\phi^n\}$ and a ϕ^0 such that $\phi^n \to \phi^0$ in $C^1(I, H)$. Hence the Gâteaux differential of x exists and it is given by $\hat{x}(B^0, B - B^0) = \phi^0$. It remains to show that ϕ^0 is a solution of (15).
Since $\phi^0 \in L_2(I, H), \quad \dot{\phi}^0 \in L_2(I, H)$, it is clear that $\phi^0 \in C(I, H)$, $\phi^0(0)$ is well defined and $\phi^n(0) = 0$ for all n. Hence ϕ^0 satisfies the differential equation (15) and one may identify ϕ^0 as e. This completes the proof.

With the help of above Lemma, we prove the following necessary conditions for the optimality of the operator B.

Theorem 3 *Let* $y(t) \in C^1(I, H), \quad g(B) = 1/2\|x(t, B) - y(t)\|_H^2$

$$OI: \quad \min \quad J(B) = \int_I g(B)dt$$
$$s.t. \quad x(t, B) \textit{ is the solution of DES1}, B \in P_b$$

If B^0 is the best approximation for the unknown operator, then

$$\int_I \langle (B - B^0)x(t, B^0), z\rangle dt \geq 0$$

for all $B \in P_b$, where z is the solution of the adjoint equation

$$\begin{cases} -\dot{z} - B^* z = x(t, B^0) - y(t) \\ z(T^0) = 0 \end{cases} \tag{16}$$

and $x(t, B^0)$ is the solution of DES1 corresponding to $B^0 \in P_b$.

Proof Since $B \to x(t, B)$ is weak Gâteaux differentialable on P_b, it follows that J as defined above also has a Gâteaux differential. Then in order that J attains its minimum at $B^0 \in P_b$ (whose existence is assured by the previous sections), it is necessary that

$$J'_{B^0}(B - B^0) = \int_I \langle \hat{x}(B^0, B - B^0), x(t, B^0) - y(t)\rangle dt \geq 0 \tag{17}$$

for all $B \in P_b$, where $\hat{x}$ is the Gâteaux differential as given in Lemma 2. The inequality can be further simplified by introducing the so called adjoint variable z, which is the solution of the following equation:

$$\begin{cases} -\dot{z} - B^* z = x(t, B^0) - y(t) \\ z(T_0) = 0 \end{cases}$$

Obviously, (16) has a solution.

Utilizing (16) into the above inequality and integrately by parts, one obtains:

$$\int_I \langle (B - B^0)x(t, B^0), z\rangle dt \geq 0$$

This completes the proof.

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动力学方程组中参数识别模型及其优化性质

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摘 要

本文建立了动力学方程组中参数优化识别的数学模型.这是个含有动态约束的泛函极小化问题.应用线性算子的连续性,证明了该问题最优解的存在性,即参数的可识别性.最后依据弱Gateaux 微分,给出并证明达到最优解的一个必要条件.