

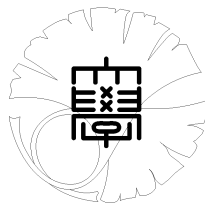
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fractional diffusion equation**

by

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DETERMINATION OF ORDER IN FRACTIONAL DIFFUSION EQUATION

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ABSTRACT. We show formulae of determining the order of fractional derivative in time in the fractional diffusion equation by time history at one fixed spatial point. The proof is based on asymptotics of the solution as $t \rightarrow 0$ or $t \rightarrow \infty$. The order is important for evaluating the anomaly of the diffusion in heterogeneous medium.

§1. Introduction.

Recently anomalous diffusion phenomena have attracted great attention, which show different aspects from the classical diffusion. For example, Adams and Gelhar [1] pointed that observation data in the saturated zone of an actual aquifer deviate from simulated results by the classical advection-diffusion equation. An anomalous diffusion is interpreted as slow diffusion, and is characterized by the long-tailed

profile in spatial distribution of densities as the time passes. Also see Berkowitz, Cortis, Dentz and Scher [3].

For the anomalous diffusion, a microscopic model was proposed by the continuous-time random walk. That is, let $x(t)$, $t > 0$ be the probability density function of location of particle at time t , and let us assume that the mean square displacement grows as

$$(1.1) \quad \langle x^2(t) \rangle \sim t^\alpha,$$

where $\alpha > 0$ is a constant (e.g., Metzler and Klafter [7], Sokolov, Klafter and Blumen [11]). The case $\alpha = 1$ corresponds to the classical diffusion, and the transport phenomenon exhibits sub-diffusion for $\alpha < 1$, while super-diffusion for $\alpha > 1$. Thus the determination of α is needed for suitable simulation of the anomalous diffusion and there are many column experiments on reactive flow in heterogeneous media (e.g., Hatano and Hatano [6]). On the other hand, the anomalous diffusion subject to (1.1) can be described by a macroscopic model (e.g., [7], [11]) which is called the fractiocal diffusion equation:

$$(1.2) \quad \partial_t^\alpha u(x, t) = \mu \Delta u(x, t) + \sum_{j=1}^d \mu_j \frac{\partial u}{\partial x_j}(x, t), \quad x \in \Omega,$$

where $\Omega \subset \mathbb{R}^d$, $\mu > 0$, $\mu_j \in \mathbb{R}$, and we set

$$\partial_t^\alpha u(x, t) = \frac{1}{\Gamma(1 - \alpha)} \int_0^t (t - s)^{-\alpha} \frac{\partial u}{\partial s}(x, s) ds$$

where $\Gamma(1 - \alpha)$ is the gamma function. Then $u(x, t)$ describes the probability of finding a particle at location x and time t .

In this paper, we establish formulae of determining $0 < \alpha < 1$ by observation data of solution u to (1.2). Our formulae may give easy way for determining α , e.g., by experiments in the flow cells or columns.

§2. Main result.

Consider

$$(2.1) \quad \begin{cases} D_t^\alpha u(x, t) = (Lu)(x, t) \equiv \sum_{i,j=1}^d \frac{\partial}{\partial x_i} \left(a_{ij}(x) \frac{\partial u}{\partial x_j} \right) + c(x)u(x, t), & x \in \Omega, 0 < t < T, \\ \partial_L u(x, t) + \sigma(x)u(x, t) = 0, & x \in \partial\Omega, 0 < t < T, \\ u(x, 0) = a(x), & x \in \Omega. \end{cases}$$

Here $\Omega \subset \mathbb{R}^d$ is a bounded domain with smooth boundary $\partial\Omega$, $\nu(x) = (\nu_1(x), \dots, \nu_d(x))$ denotes the unit outward normal vector to $\partial\Omega$ at x , and $a_{ij} = a_{ji}$, $1 \leq i, j \leq d$ are of $C^1(\bar{\Omega})$, $c \in C(\bar{\Omega})$, $c(x) \leq 0$ for $x \in \Omega$, $\sigma \in C^\infty(\partial\Omega)$, ≥ 0 , $\neq 0$ on $\partial\Omega$, there exists a constant $\nu > 0$ such that

$$\sum_{i,j=1}^d a_{ij}(x)\xi_i\xi_j \geq \nu \sum_{j=1}^d \xi_j^2, \quad x \in \Omega, \xi_1, \dots, \xi_d \in \mathbb{R},$$

and we set

$$\partial_L v(x) = \sum_{i,j=1}^d a_{ij}(x) \frac{\partial v}{\partial x_j}(x) \nu_i(x), \quad x \in \partial\Omega.$$

Inverse Problem. Let $x_0 \in \Omega$ be fixed. Determine $\alpha \in (0, 1)$ from observation data

$$u(x_0, t) \quad \text{for small } t \text{ or large } t.$$

Theorem.

(i) We assume that

$$(2.2) \quad a \in C_0^\infty(\Omega), \quad La(x_0) \neq 0.$$

Then

$$\alpha = \lim_{t \rightarrow 0} \frac{t \frac{\partial u}{\partial t}(x_0, t)}{u(x_0, t) - a(x_0)}.$$

(ii) We assume that

$$(2.3) \quad a \in C_0^\infty(\Omega), \quad a \geq 0 \text{ or } \leq 0, \neq 0 \text{ on } \bar{\Omega}.$$

Then

$$\alpha = - \lim_{t \rightarrow \infty} \frac{t \frac{\partial u}{\partial t}(x_0, t)}{u(x_0, t)}.$$

Remark. (i) gives an identification formula for the order α by data near $t = 0$, while (ii) is for data for large $t > 0$. The condition $a \in C_0^\infty(\Omega)$ means that $a = 0$ near the boundary $\partial\Omega$ and a is infinitely many times differentiable in Ω . For example we can take a very smooth bell-shaped function as $a(x)$.

As is seen from the proof in section 3, we see the following: for any fixed small $\delta > 0$, there exists a constant $C_0 > 0$ depending on $a_{ij}, c, a, \Omega, \sigma$, such that

$$\left| \left(- \frac{T \frac{\partial u}{\partial t}(x_0, T)}{u(x_0, T)} \right) - \alpha \right| \leq \frac{C_0}{T^\alpha}$$

for any $\alpha \in [0, 1 - \delta]$. This is useful for estimating errors when we approximate α by setting $t = T$:

$$- \frac{T \frac{\partial u}{\partial t}(x_0, T)}{u(x_0, T)}.$$

§3. Proof of Theorem.

Let $L^2(\Omega)$, $H^\ell(\Omega)$, $\ell \in \mathbb{N}$, denote usual Lebesgue space and Sobolev space and let us set

$$(a, b) = \int_{\Omega} a(x)b(x)dx, \quad \|a\| = (a, a)^{\frac{1}{2}}.$$

Let $\{\varphi_n\}_{n \in \mathbb{N}}$ be the set of all the eigenfunctions of L with the boundary condition $\partial_L u + \sigma u = 0$; that is, $L\varphi_n = -\lambda_n\varphi_n$, $\varphi_n \neq 0$, and $\partial_L\varphi_n(x) + \sigma(x)\varphi_n(x) = 0$ for $x \in \partial\Omega$. We number the eigenvalues with multiplicities as

$$\lambda_1 \leq \lambda_2 \leq \dots,$$

and we choose φ_n such that $(\varphi_n, \varphi_n) = 1$ and $(\varphi_n, \varphi_m) = 0$ if $n \neq m$. Then we can prove

$$\lambda_n > 0, \quad n \in \mathbb{N}.$$

In fact, $\lambda_n \geq 0$ can be first proved as follows. Let $Lu = -\lambda_n u$, $\partial_L u + \sigma u = 0$ and $u \neq 0$. Then, multiplying $Lu = \lambda_n u$ by u and integrating by parts, and using the boundary condition, we obtain

$$\begin{aligned} -\lambda_n \|u\|^2 &= \int_{\Omega} \left(\sum_{i,j=1}^d \frac{\partial}{\partial x_i} \left(a_{ij} \frac{\partial u}{\partial x_j} \right) + cu \right) u dx \\ &= \int_{\Omega} \left(- \sum_{i,j=1}^d a_{ij} \frac{\partial u}{\partial x_i} \frac{\partial u}{\partial x_j} + cu^2 \right) dx \\ &\quad + \int_{\partial\Omega} (\partial_L u) u dS \\ &= \int_{\Omega} \left(- \sum_{i,j=1}^d a_{ij} \frac{\partial u}{\partial x_i} \frac{\partial u}{\partial x_j} + cu^2 \right) dx - \int_{\partial\Omega} \sigma u^2 dS \leq 0. \end{aligned}$$

Therefore by $u \neq 0$, we see that $\lambda_n \geq 0$. Moreover let $Lu_0 = 0$ in Ω and $\partial_L u_0 + \sigma u_0 = 0$ on $\partial\Omega$. Then by the above equalities, we have

$$\int_{\Omega} \left(- \sum_{i,j=1}^d a_{ij} \frac{\partial u_0}{\partial x_i} \frac{\partial u_0}{\partial x_j} + cu_0^2 \right) dx - \int_{\partial\Omega} \sigma u_0^2 dS = 0,$$

which implies $\nabla u_0 = 0$ in Ω . Hence u_0 is a constant function, and $\int_{\partial\Omega} \sigma u_0^2 dS = 0$.

Since $\sigma \not\equiv 0$ on $\partial\Omega$, we see that $u_0 = 0$. This means that 0 can not be an eigenvalue.

Thus we have proved $\lambda_n > 0$, $n \in \mathbb{N}$.

By $a \in C_0^\infty(\Omega)$, we can see the following:

For any $\ell \in \mathbb{N}$, there exists a constant $C(\ell) > 0$ such that

$$(3.1) \quad |(a, \varphi_n)| \leq \frac{C(\ell)}{|\lambda_n|^\ell}, \quad n \in \mathbb{N}$$

and

$$(3.2) \quad \sum_{n=1}^{\infty} -\lambda_n (a, \varphi_n) \varphi_n(x_0) = La(x_0), \quad \sum_{n=1}^{\infty} (a, \varphi_n) \varphi_n(x_0) = a(x_0).$$

Moreover $L\varphi_n = -\lambda_n \varphi_n$ in Ω implies $\|L^m \varphi_n\| = |\lambda_n|^m$, $m \in \mathbb{N}$. By the regularity of elliptic equation (e.g., Gilbarg and Trudinger [5]), we see that there exists a

constant $C_1 > 0$ such that $\|\varphi_n\|_{H^{2m}(\Omega)} \leq C_1(\|L^m\varphi_n\| + \|\varphi_n\|)$. Here $\|\varphi_n\|_{H^{2m}(\Omega)}$ is the norm in $H^{2m}(\Omega)$ (e.g., Adams [2]). By the Sobolev embedding theorem (e.g., [2]), if $m > \frac{d}{4}$, then there exists a constant $C_2 = C_2(m) > 0$ such that

$$\max_{x \in \overline{\Omega}} |\varphi_n(x)| \leq C_2 \|\varphi_n\|_{H^{2m}(\Omega)} \leq C_1 C_2 (|\lambda_n|^m + 1), \quad n \in \mathbb{N}.$$

Hence there exist constants $\kappa > 0$ and $C_3 > 0$ such that

$$(3.3) \quad |\varphi_n(x_0)| \leq C_3 |\lambda_n|^\kappa, \quad n \in \mathbb{N}.$$

Moreover

$$(3.4) \quad |\lambda_n| \leq C_4 n^{\frac{2}{d}}$$

(e.g., Courant and Hilbert [4]). Therefore, by (3.1) - (3.3), similarly to Sakamoto and Yamamoto [10], by the Fourier method, we can prove

$$(3.5) \quad u(x_0, t) = \sum_{n=1}^{\infty} (a, \varphi_n) \varphi(x_0) E_{\alpha,1}(-\lambda_n t^\alpha), \quad 0 < t < T,$$

where the series is convergent in $C[0, T]$. Here the Mittag-Leffler function is defined as follows:

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)}, \quad \alpha > 0, \beta > 0, z \in \mathbb{C}$$

(e.g., Podlubny [8]). Therefore

$$(3.6) \quad \begin{aligned} \frac{\partial u}{\partial t}(x_0, t) &= \sum_{n=1}^{\infty} (a, \varphi_n) \varphi(x_0) \frac{d}{dt} E_{\alpha,1}(-\lambda_n t^\alpha) \\ &= \sum_{n=1}^{\infty} -\lambda_n (a, \varphi_n) \varphi(x_0) t^{\alpha-1} E_{\alpha,\alpha}(-\lambda_n t^\alpha), \quad 0 < t < T \end{aligned}$$

(e.g., formula (1.83) on p.22 in [8]). On the other hand,

$$\begin{aligned} E_{\alpha,\alpha}(-\lambda_n t^\alpha) &= \sum_{k=0}^{\infty} \frac{(-\lambda_n t^\alpha)^k}{\Gamma((k+1)\alpha)} = \frac{1}{\Gamma(\alpha)} + t^\alpha \left(\frac{E_{\alpha,\alpha}(-\lambda_n t^\alpha) - \Gamma(\alpha)^{-1}}{t^\alpha} \right) \\ &\equiv \frac{1}{\Gamma(\alpha)} + t^\alpha r_n(t), \end{aligned}$$

where $r_n(t)$ is continuous at $t = 0$ and $\lim_{t \rightarrow 0} r_n(t)$ exists. Hence

$$\frac{\partial u}{\partial t}(x_0, t) = \left(\sum_{n=1}^{\infty} -\lambda_n(a, \varphi_n) \varphi(x_0) \right) \frac{t^{\alpha-1}}{\Gamma(\alpha)} + \left(\sum_{n=1}^{\infty} -\lambda_n(a, \varphi_n) \varphi(x_0) r_n(t) \right) t^{2\alpha-1},$$

and

$$(3.7) \quad \begin{aligned} \lim_{t \rightarrow 0} t^{1-\alpha} \frac{\partial u}{\partial t}(x_0, t) &= \frac{1}{\Gamma(\alpha)} \left(\sum_{n=1}^{\infty} -\lambda_n(a, \varphi_n) \varphi(x_0) \right) \\ &+ \lim_{t \rightarrow 0} t^{\alpha} \left(\sum_{n=1}^{\infty} -\lambda_n(a, \varphi_n) \varphi(x_0) r_n(t) \right). \end{aligned}$$

By [8] (formula (1.148) on p.35), we have

$$\begin{aligned} |r_n(t)| &= \left| \sum_{k=1}^{\infty} \frac{(-\lambda_n)^k t^{\alpha(k-1)}}{\Gamma((k+1)\alpha)} \right| = |\lambda_n| \left| \sum_{k=0}^{\infty} \frac{(-\lambda_n t^{\alpha})^k}{\Gamma(k\alpha + 2\alpha)} \right| \\ &= |\lambda_n| |E_{\alpha, 2\alpha}(-\lambda_n t^{\alpha})| \leq |\lambda_n|, \quad t \geq 0, n \in \mathbb{N}. \end{aligned}$$

Hence, by (3.1) and (3.3),

$$\begin{aligned} \left| \sum_{n=1}^{\infty} -\lambda_n(a, \varphi_n) \varphi(x_0) r_n(t) \right| &\leq \sum_{n=1}^{\infty} |\lambda_n|^2 |(a, \varphi_n) \varphi(x_0)| \\ &\leq \sum_{n=1}^{\infty} |\lambda_n|^2 \frac{C(\ell)}{|\lambda_n|^{\ell}} C_3 |\lambda_n|^{\kappa}. \end{aligned}$$

By (3.4), we take sufficiently large $\ell \in \mathbb{N}$ to have

$$\max_{0 \leq t \leq T} \left| \sum_{n=1}^{\infty} -\lambda_n(a, \varphi_n) \varphi(x_0) r_n(t) \right| < \infty.$$

Hence, by using (3.2), equation (3.7) yields

$$(3.8) \quad \lim_{t \rightarrow 0} t^{1-\alpha} \frac{\partial u}{\partial t}(x_0, t) = \frac{La(x_0)}{\Gamma(\alpha)}.$$

On the other hand, we have

$$\begin{aligned} E_{\alpha, 1}(-\lambda_n t^{\alpha}) &= 1 - \frac{\lambda_n t^{\alpha}}{\Gamma(\alpha + 1)} + t^{2\alpha} \sum_{k=2}^{\infty} \frac{(-\lambda_n)^k t^{\alpha(k-2)}}{\Gamma(\alpha k + 1)} \\ &= 1 - \frac{\lambda_n t^{\alpha}}{\Gamma(\alpha + 1)} + t^{2\alpha} \lambda_n^2 E_{\alpha, 2\alpha+1}(-\lambda_n t^{\alpha}). \end{aligned}$$

Therefore, using (3.2), we have

$$\begin{aligned} u(x_0, t) &= \sum_{n=1}^{\infty} (a, \varphi_n) \varphi(x_0) + \sum_{n=1}^{\infty} \frac{-\lambda_n (a, \varphi_n) \varphi(x_0)}{\Gamma(\alpha + 1)} t^\alpha \\ &+ t^{2\alpha} \sum_{n=1}^{\infty} \lambda_n^2 E_{\alpha, 2\alpha+1}(-\lambda_n t^\alpha) (a, \varphi_n) \varphi(x_0) = a(x_0) + \frac{La(x_0)}{\Gamma(\alpha + 1)} t^\alpha + t^{2\alpha} \tilde{r}(t). \end{aligned}$$

Here by (3.1), we see that $\sup_{0 \leq t \leq T} |\tilde{r}(t)| < \infty$. Consequently

$$(3.9) \quad \lim_{t \rightarrow 0} t^{-\alpha} (u(x_0, t) - a(x_0)) = \frac{La(x_0)}{\Gamma(\alpha + 1)}.$$

In terms of (3.8) and (3.9), using $La(x_0) \neq 0$ and $\Gamma(\alpha + 1) = \alpha\Gamma(\alpha)$, we have

$$\begin{aligned} & \lim_{t \rightarrow 0} \frac{t \frac{\partial u}{\partial t}(x_0, t)}{u(x_0, t) - a(x_0)} \\ &= \frac{\lim_{t \rightarrow 0} t^{1-\alpha} \frac{\partial u}{\partial t}(x_0, t)}{\lim_{t \rightarrow 0} t^{-\alpha} (u(x_0, t) - a(x_0))} \\ &= \frac{\frac{La(x_0)}{\Gamma(\alpha)}}{\frac{La(x_0)}{\Gamma(\alpha+1)}} = \alpha. \end{aligned}$$

Thus we can complete the proof of (i).

Next we will prove (ii). In (3.5) and (3.6), we apply the asymptotic behaviour of the Mittag-Leffler function at ∞ (e.g., Theorem 1.4 (pp. 33-34) in [8]):

$$E_{\alpha, 1}(-\eta) = \frac{\eta^{-1}}{\Gamma(1 - \alpha)} + O\left(\frac{1}{\eta^2}\right)$$

and

$$E_{\alpha, \alpha}(-\eta) = -\frac{\eta^{-2}}{\Gamma(-\alpha)} + O\left(\frac{1}{\eta^3}\right)$$

as $\eta \rightarrow \infty$, $\eta > 0$. Therefore

$$\begin{aligned} u(x_0, t) &= \sum_{n=1}^{\infty} (a, \varphi_n) \varphi_n(x_0) \frac{1}{\Gamma(1 - \alpha) \lambda_n t^\alpha} \\ &+ O\left(\frac{1}{t^{2\alpha}}\right) \sum_{n=1}^{\infty} (a, \varphi_n) \varphi_n(x_0) \frac{1}{\lambda_n^2} \end{aligned}$$

and

$$\begin{aligned} \frac{\partial u}{\partial t}(x_0, t) &= \sum_{n=1}^{\infty} (a, \varphi_n) \varphi_n(x_0) \frac{1}{\Gamma(-\alpha) \lambda_n t^{\alpha+1}} \\ &+ O\left(\frac{1}{t^{2\alpha+1}}\right) \sum_{n=1}^{\infty} (a, \varphi_n) \varphi_n(x_0) \frac{1}{\lambda_n^2}. \end{aligned}$$

Since $L\varphi_n = -\lambda_n\varphi_n$ in Ω , noting that $\lambda_n > 0$, we see that

$$\sum_{n=1}^{\infty} \frac{(a, \varphi_n) \varphi_n(x_0)}{\lambda_n} = -(L^{-1}a)(x_0), \quad \sum_{n=1}^{\infty} \frac{(a, \varphi_n) \varphi_n(x_0)}{\lambda_n^2} = (L^{-2}a)(x_0),$$

we obtain

$$u(x_0, t) = \frac{-(L^{-1}a)(x_0)}{\Gamma(1-\alpha)t^\alpha} + O\left(\frac{1}{t^{2\alpha}}\right) (L^{-2}a)(x_0)$$

and

$$\frac{\partial u}{\partial t}(x_0, t) = \frac{-(L^{-1}a)(x_0)}{\Gamma(-\alpha)t^{\alpha+1}} + O\left(\frac{1}{t^{2\alpha+1}}\right) (L^{-2}a)(x_0).$$

Here we can prove

$$(L^{-1}a)(x_0) \neq 0.$$

In fact, we set $b(x) = L^{-1}a(x)$, $x \in \Omega$. Then $Lb(x) = a(x)$, $x \in \Omega$. Without loss of generality, we may assume that $a \geq 0$ on $\bar{\Omega}$. Then $Lb(x) \geq 0$ in Ω . By the strong maximum principle (e.g., Theorem 4.10 (p.109) in Renardy and Rogers [9]), in view of $c \leq 0$ on $\bar{\Omega}$, we see that $\max_{x \in \bar{\Omega}} b(x) < 0$, which means $L^{-1}a(x_0) \neq 0$.

Therefore

$$\begin{aligned} &\frac{t \frac{\partial u}{\partial t}(x_0, t)}{u(x_0, t)} \\ &= \frac{\frac{-(L^{-1}a)(x_0)}{\Gamma(-\alpha)t^{\alpha+1}} + O\left(\frac{1}{t^{2\alpha+1}}\right) (L^{-2}a)(x_0)}{\frac{-(L^{-1}a)(x_0)}{\Gamma(1-\alpha)t^\alpha} + O\left(\frac{1}{t^{2\alpha}}\right) (L^{-2}a)(x_0)} \\ &\longrightarrow \frac{\Gamma(1-\alpha)}{\Gamma(-\alpha)} \end{aligned}$$

as $t \rightarrow \infty$. Since $\Gamma(1-\alpha) = -\alpha\Gamma(-\alpha)$, the proof of (ii) is completed.

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