

Observability of the Doi Orientation Tensor Model

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Abstract

We apply the observability rank condition to the two-dimensional Doi orientation tensor model to investigate the observability of liquid crystalline polymers under imposed shear or extensional flows. Here the observability means the ability of determining the orientation tensor from the time history of the observations of the birefringence. The Doi model under shear or extensional flow is observable almost everywhere. In other words, all components of the orientation tensor can be determined from the observation of the birefringence provided that the points formed by the two components of the orientation tensor do not lie on certain curves in the plane. We also run simulations using the unscented Kalman filter (UKF) to reconstruct the orientation tensor from observations without and with noises. The UKF gives good estimates for the orientation tensor both in the absence and in the presence of observation noises.

1 Introduction

Observability of a dynamic system is a very useful subject in control theory [3]. It means the ability to determine uniquely the state of the system from observable quantities [5, 8]. In practice, noise may occur in both the observations and the system dynamics. If the system is not observable, then it is hopeless to get an accurate estimate of the state or to guide the system to a desirable final state. So from a practical point of view, it is important to investigate the observability of a dynamical system.

In this work we extend our previous study on the observability of viscoelastic fluids [8] to the observability of the Doi orientation tensor model in liquid

crystalline polymers. We impose the velocity field and assume monodomain structure. We further assume the birefringence is measured in experiments, which is consistent with light scattering measurements. Our goal is to infer the full orientation tensor from measurements, if possible. To do so, we apply the observability rank condition to investigate the short time local observability of the Doi orientation tensor model under imposed extensional or shear flow.

The outline of this paper is as follows. We present a brief overview of the observability of dynamical systems and the observability rank condition in Section 2. In section 3 we focus on the analysis of the observability of the Doi orientation tensor model under shear or extensional flow. We carry out some numerical experiments where the performance of the unscented Kalman filter is examined both in the case of zero observation noise and in the case of Gaussian observation noise in Section 4. We summarize our work in Section 5.

2 Observability rank condition of dynamical systems

For reader's convenience, we quickly recall the observability of dynamical systems and observability rank condition [8].

Consider a dynamical system without control input:

$$\dot{x} = f(x), \quad x \in R^n \quad (1)$$

$$y = h(x), \quad y \in R^p \quad (2)$$

$$x(0) = x^0, \quad (3)$$

where x is the state variable, y is the quantity that can be observed experimentally. Functions f and h are assumed to be sufficiently smooth. The state x is not observed directly but the output y is. We would like to know whether it is possible to determine the initial state x^0 from the output history $y(0 : \infty)$ where the symbol $y(0 : T)$ denotes the trajectory $t \rightarrow y(t)$ with $0 \leq t < T$. If the map $x^0 \rightarrow y(0 : \infty)$ is one to one, then one can reconstruct x^0 from $y(0 : \infty)$ mathematically and the system (1)-(2) is called *observable*. Since $x(t)$ can be treated as the initial state for evolutions after time t , the observability indicates that $x(t)$ can be reconstructed from $y(0 : \infty)$ as well.

Other definitions of observability are also possible. The most useful and easiest to measure one is *short time local observability*. A system is *short time locally observable* if for every $T > 0$, the map $x^0 \rightarrow y(0 : T)$ is locally one

to one. Mathematically speaking, *locally one to one* means that for each x^0 , there is a neighborhood $U(x^0)$ such that if $x^1 \in U(x^0)$, then the output from x^1 and the output from x^0 are different. Now we recall a sufficient condition for the short-time local observability [5].

We begin with some notations. Note that from (2) and (3) we have $y(0) = h(x^0)$ and thus

$$\frac{dy}{dt}(0) = \frac{\partial h}{\partial x}(x^0)f(x^0) \tag{4}$$

using the chain rule and (1). The right hand side of (4) is called the Lie derivative of the function h by the vector field f :

$$L_f(h)(x) = \frac{\partial h}{\partial x}(x)f(x). \tag{5}$$

Since the Lie derivative is another function from R^n to R^p , one can repeat the process of taking the Lie derivative:

$$\begin{aligned} L_f^2(h)(x) &= L_f(L_f(h))(x) = L_f\left(\frac{\partial h}{\partial x}(x)f(x)\right) \\ L_f^k(h)(x) &= L_f(L_f^{k-1}(h))(x). \end{aligned}$$

A set of functions $g_1(x), \dots, g_k(x)$ is said to *separate points* if given any pair of two points x^0 and x^1 , there is at least one $g_i(x)$ such that $g_i(x^0) \neq g_i(x^1)$. If $g_1(x), \dots, g_k(x)$ separate points, then the map $x \rightarrow (g_1(x), \dots, g_k(x))$ is one to one. Mathematically, if the functions $L_f^j(h)(x)$, $j = 0, \dots, k$, locally separate points in R^n for some k , then the system is short time locally observable. A sufficient condition for this to happen is that the so-called *one forms*

$$dh_i(x), \dots, dL_f^k(h_i)(x), \quad i = 1, \dots, p$$

span n dimensions at every x where

$$dh_i(x) = \sum_{j=1}^n \frac{\partial h_i}{\partial x_j}(x)dx_j = \left(\frac{\partial h_i}{\partial x_1}, \dots, \frac{\partial h_i}{\partial x_n}\right). \tag{6}$$

Now we introduce the definition of observability rank condition (ORC).

Definition 2.1 *The system (1)-(2) satisfies the observability rank condition at x^0 if there exists a k such that $\{dL_f^j(h_i) : j = 0, \dots, k; i = 1, \dots, p\}$ has rank n . The system (1)-(2) satisfies the observability rank condition if it satisfies it at every $x \in R^n$ (note k may vary with x).*

For linear systems, observability rank condition (ORC) leads to global short-time observability as well. For nonlinear systems, ORC is a sufficient condition of short-time local observability. In addition, ORC is almost a necessary condition for short-time local observability. It has been shown Hermann *Krenner that if the ORC is violated on an open subset of \mathbb{R}^n* , then the system (1)-(2) is not short time, locally observable.

In the next section we would like to apply the observability rank condition to investigate the observability of the Doi orientation tensor model in the study of liquid crystalline polymers.

3 The Doi orientation tensor model

The Doi orientation tensor model for rodlike liquid crystalline polymers in a solvent is well-known for its capability to describe both the isotropic and nematic phases and phase transition between them [6]. A fundamental part of this model is the single molecule orientation distribution function. Interactions between molecules are represented by a mean-field potential (so-called Maier-Saupe potential). The rodlike molecules are also subject to Brownian force due to the fact that they interact with other rodlike molecules and with the flow.

Basically, the model is a microscopic Smoluchowski equation or Fokker-Planck type equation for the dynamics of the orientational distribution function coupled with a macroscopic hydrodynamic equation [1]. The Smoluchowski equation describes the convection, rotation and diffusion of the rodlike molecules. The full Doi orientation tensor theory is developed after the kinetic Smoluchowski equation is projected onto a second-moment description using various closure rules. The major element in this tensor theory is the second-moment tensor \mathbf{Q} which describes the orientational distribution of the ensemble of rodlike macromolecules. The orientation tensor is traceless and symmetric. The physical and practical significance of the orientation tensor is that it is the basis for micro-scale light scattering measurements of primary axes (“directors”), degrees of molecular alignment (“birefringence”), and normal and shear stress measurements.

Here we restrict our attention to two-dimensional monodomain structure. The study of two-dimensional liquid crystal polymers has been physically inspired by monolayer films. Thin films of liquid crystal polymers have been used as alignment layers for liquid crystal displays because of their stability and nonlinear optical properties. A lot of theoretical and experimental studies

have been devoted to the two-dimensional Doi model (for example, see [7] and references therein).

The two-dimensional Doi model is given by [7]

$$\frac{d}{dt}\mathbf{Q} = \boldsymbol{\Omega}\mathbf{Q} - \mathbf{Q}\boldsymbol{\Omega} + a[\mathbf{D}\mathbf{Q} + \mathbf{Q}\mathbf{D}] + a\mathbf{D} - 2a\mathbf{D} : \mathbf{Q}(\mathbf{Q} + \frac{\mathbf{I}}{2}) - 6D_r F(\mathbf{Q}), \quad (7)$$

where \mathbf{Q} is the 2×2 orientation tensor such that

$$\mathbf{Q} = \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix}, \quad Q_{11} = -Q_{22}, \quad Q_{12} = Q_{21};$$

$\boldsymbol{\Omega}$ is the vorticity tensor such that $\boldsymbol{\Omega} = \frac{1}{2}[\nabla\mathbf{v} - \nabla\mathbf{v}^T]$; a is a dimensionless parameter which depends on the molecular aspect ratio; \mathbf{D} is the rate-of-strain tensor $\mathbf{D} = \frac{1}{2}[\nabla\mathbf{v} + \nabla\mathbf{v}^T]$; D_r is the averaged rotary diffusivity or relaxation rate; $F(\mathbf{Q})$ is defined by

$$F(\mathbf{Q}) = (1 - \frac{N}{2})\mathbf{Q} - N\mathbf{Q}^2 + N\mathbf{Q} : \mathbf{Q}(\mathbf{Q} + \frac{\mathbf{I}}{2})$$

and N is a dimensionless concentration of nematic polymers.

3.1 The Doi model under extensional flow

When an extensional flow with rate $\dot{\gamma}$ is imposed to the monodomain of liquid crystalline polymers, the velocity field can be expressed as

$$\mathbf{v} = (\dot{\gamma}(t)\frac{x}{2}, -\dot{\gamma}(t)\frac{y}{2}), \quad (8)$$

and the velocity gradient is

$$\nabla\mathbf{v} = \begin{bmatrix} \frac{\dot{\gamma}(t)}{2} & 0 \\ 0 & -\frac{\dot{\gamma}(t)}{2} \end{bmatrix}. \quad (9)$$

After applying the gradient of the homogeneous extensional flow (9) to the Doi system (7), we obtain

$$\begin{aligned} \dot{Q}_{11} &= -6D_r [(1 - \frac{N}{2})Q_{11} + 2NQ_{11}(Q_{11}^2 + Q_{12}^2)] + a(\frac{1}{2} - 2Q_{11}^2)\dot{\gamma}(t), \\ \dot{Q}_{12} &= -6D_r Q_{12} [(1 - \frac{N}{2}) + 2N(Q_{11}^2 + Q_{12}^2)] - 2aQ_{11}Q_{12}\dot{\gamma}(t). \end{aligned} \quad (10)$$

Using the nematic relaxation time scale $\frac{1}{D_r}$, the flow field and orientation dynamics of (7) can be non-dimensionalized. The key dimensionless parameters

are then the Peclet number $Pe = \dot{\gamma}/D_r$ (the shear rate normalized with respect to nematic relaxation rate) and the dimensionless concentration parameter N . Rescaling time as $\bar{t} = tD_r$, the nematodynamic model (7) in the dimensionless form becomes

$$\begin{aligned}\dot{Q}_{11} &= -6Q_{11} \left[1 - \frac{N}{2} + 2N(Q_{11}^2 + Q_{12}^2)\right] + a\left(\frac{1}{2} - 2Q_{11}^2\right)Pe, \\ \dot{Q}_{12} &= -6Q_{12} \left[1 - \frac{N}{2} + 2N(Q_{11}^2 + Q_{12}^2)\right] - 2aQ_{11}Q_{12}Pe.\end{aligned}\quad (11)$$

More succinctly, the system (11) can be written as

$$\frac{d\vec{x}}{dt} = \vec{f}(\vec{x}),$$

where

$$\begin{aligned}\vec{x} &= \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} Q_{11} \\ Q_{12} \end{bmatrix}, \\ \vec{f}(\vec{x}) &= \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = -6 \left[1 - \frac{N}{2} + 2N(x_1^2 + x_2^2)\right] \vec{x} + aPe \begin{bmatrix} \frac{1}{2} - 2x_1^2 \\ -2x_1x_2 \end{bmatrix}.\end{aligned}\quad (12)$$

In the light scattering experiments one can measure the birefringence, which corresponds to the difference of the two eigenvalues of \mathbf{Q} . Since the two eigenvalues of \mathbf{Q} are $\lambda_{1,2} = \pm\sqrt{Q_{11}^2 + Q_{12}^2}$, their difference is $2\sqrt{Q_{11}^2 + Q_{12}^2}$. For computational convenience, we assume the observation is $h \equiv Q_{11}^2 + Q_{12}^2 = x_1^2 + x_2^2$.

The Lie bracket is

$$\begin{aligned}L_{\vec{f}}\vec{h} &= \frac{\partial \vec{h}}{\partial x_i}(\vec{x})f_i(\vec{x}) = \left[\frac{\partial h}{\partial x_1}, \frac{\partial h}{\partial x_2} \right] \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} \\ &= [2x_1, 2x_2] \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = 2(x_1 f_1 + x_2 f_2) \\ &= -12x_1^2 + 6Nx_1^2 - 24Nx_1^4 - 48Nx_1^2x_2^2 + aPex_1 \\ &\quad - 4aPex_1^3 - 12x_2^2 + 6Nx_2^2 - 24Nx_2^4 - 4aPex_1x_2^2\end{aligned}\quad (13)$$

After some algebra, one has

$$\begin{aligned}\det \left(\frac{\partial}{\partial \vec{x}} \begin{bmatrix} \vec{h} \\ L_{\vec{f}}\vec{h} \end{bmatrix} \right) &= \det \begin{bmatrix} 2x_1 & 2x_2 \\ c_1 & c_2 \end{bmatrix} \\ &= 2aPex_2(4x_1^2 + 4x_2^2 - 1),\end{aligned}\quad (14)$$

where

$$\begin{aligned}
 c_1 &= -24x_1 + 12Nx_1 - 96Nx_1^3 - 96Nx_1x_2^2 + aPe - 12aPex_1^2 - 4aPex_2^2, \\
 c_2 &= -96Nx_1^2x_2 - 24x_2 + 12Nx_2 - 96Nx_2^3 - 8aPex_1x_2.
 \end{aligned}
 \tag{15}$$

So if $x_1^2 + x_2^2 \neq 1/4$ and $x_2 \neq 0$, then the determinant is nonsingular and consequently the observability rank condition (ORC) is satisfied. In other words, if the two components of the orientation tensor \mathbf{Q} satisfies the conditions $Q_{11}^2 + Q_{12}^2 \neq 1/4$ and $Q_{12} \neq 0$, then the Doi model under extensional flow is short time locally observable.

In Figure 1 we plot the two curves described by $x_2 = 0$ and $x_1^2 + x_2^2 = 1/4$, respectively in the $x_1 - x_2$ plane.. The Doi model under extensional flow is short time, locally observable as long as the point (Q_{11}, Q_{12}) does not lie on these two dashed curves.

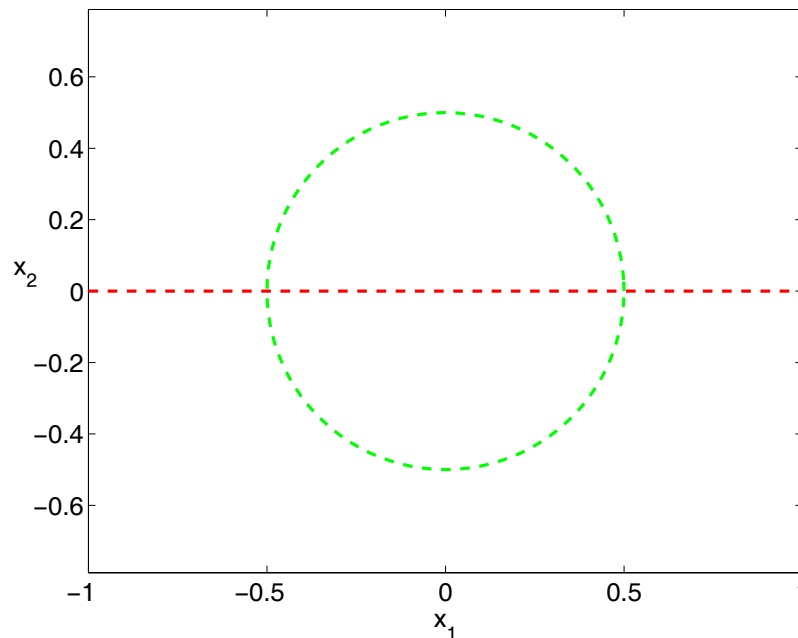


Figure 1: The curves where the determinant in (14) vanishes. The Doi model under extensional flow is observable for all components Q_{11} and Q_{12} of the orientation tensor when the point (Q_{11}, Q_{12}) doesn't lie on these curves.

3.2 The Doi model under shear flow

The velocity field of a shear flow with rate $\dot{\gamma}$ is described by

$$\mathbf{v} = \dot{\gamma}(t)(y, 0) \quad (16)$$

The rate-of-strain tensor is

$$\mathbf{D} = \frac{1}{2}[\nabla\mathbf{v} + (\nabla\mathbf{v})^T] = \frac{\dot{\gamma}(t)}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \quad (17)$$

We non-dimensionalize the flow field and orientation dynamics using the nematic relaxation time scale $1/D_r$. The dimensionless parameters consist of the Peclet number $Pe = \dot{\gamma}(t)/D_r$ which is the shear rate normalized with respect to nematic relaxation rate, and the dimensionless concentration parameter N . From now on, we work in dimensionless time $\bar{t} = tD_r$.

The nematodynamic Doi model (7) in component form is

$$\begin{aligned} \dot{Q}_{11} &= -6Q_{11} \left[1 - \frac{N}{2} + 2N(Q_{11}^2 + Q_{12}^2)\right] + (Q_{12} - 2aQ_{11}Q_{12})Pe, \\ \dot{Q}_{12} &= -6Q_{12} \left[1 - \frac{N}{2} + 2N(Q_{11}^2 + Q_{12}^2)\right] + (-Q_{11} + \frac{a}{2} - 2aQ_{12}^2)Pe. \end{aligned} \quad (18)$$

Introducing

$$\vec{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} Q_{11} \\ Q_{12} \end{bmatrix},$$

the system (18) has the simple form

$$\begin{aligned} \frac{d\vec{x}}{dt} &= \vec{f}(\vec{x}), \\ \vec{f}(\vec{x}) &= \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = -6 \left[1 - \frac{N}{2} + 2N(x_1^2 + x_2^2)\right] \vec{x} + Pe \begin{bmatrix} x_2 - 2ax_1x_2 \\ -x_1 + \frac{a}{2} - 2ax_2^2 \end{bmatrix}. \end{aligned} \quad (19)$$

As before, assume the the observation is related to the birefringence and has the form $h \equiv Q_{11}^2 + Q_{12}^2 = x_1^2 + x_2^2$.

The Lie bracket is

$$\begin{aligned} L_{\vec{f}}\vec{h} &= \frac{\partial\vec{h}}{\partial x_i}(\vec{x})f_i(\vec{x}) = \left[\frac{\partial h}{\partial x_1}, \frac{\partial h}{\partial x_2} \right] \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} \\ &= [2x_1, 2x_2] \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = 2(x_1 f_1 + x_2 f_2) \\ &= -12x_1^2 + 6Nx_1^2 - 24Nx_1^4 - 48Nx_1^2x_2^2 - 4aPex_1^2x_2 \\ &\quad -12x_2^2 + 6Nx_2^2 - 24Nx_2^4 + x_2 a Pe - 4aPex_2^3. \end{aligned} \quad (20)$$

It follows that

$$\det \left(\frac{\partial}{\partial \vec{x}} \begin{bmatrix} \vec{h} \\ L_{\vec{f}} \vec{h} \end{bmatrix} \right) = \det \begin{bmatrix} 2x_1 & 2x_2 \\ d_1 & d_2 \end{bmatrix} = -2a Pe x_1 (4x_1^2 + 4x_2^2 - 1), \quad (21)$$

where

$$\begin{aligned} d_1 &= -24x_1 + 12Nx_1 - 96Nx_1^3 - 96Nx_1x_2^2 - 8a Pe x_1x_2, \\ d_2 &= -96Nx_1^2x_2 - 4a Pe x_1^2 - 24x_2 + 12Nx_2 - 96Nx_2^3 + a Pe - 12a Pe x_2^2. \end{aligned} \quad (22)$$

Therefore, if $x_1 \neq 0$ and $x_1^2 + x_2^2 \neq 1/4$, then the matrix is nonsingular and the ORC is satisfied. Said differently, if $Q_{11} \neq 0$ and $Q_{11}^2 + Q_{12}^2 \neq 1/4$, then the Doi model under shear flow is short time locally observable.

We plot the two curves described by $x_1 = 0$ and $x_1^2 + x_2^2 = 1/4$, respectively in the $x_1 - x_2$ plane in Figure 2. The Doi model under shear flow is short time, locally observable as long as the point (Q_{11}, Q_{12}) does not lie on these two curves.

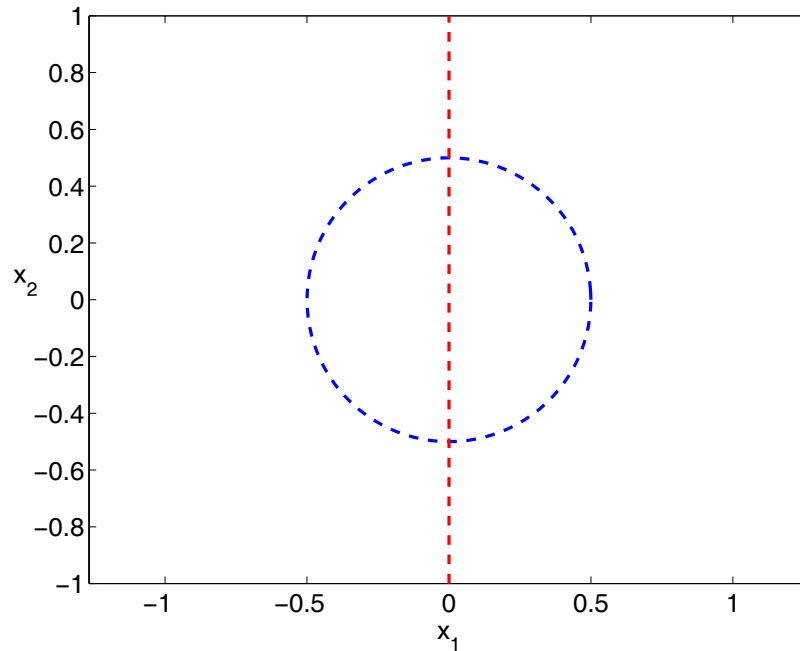


Figure 2: The curves where the determinant in (21) becomes zero. The Doi model under shear flow is observable for all components Q_{11} and Q_{12} of the orientation tensor when the point (Q_{11}, Q_{12}) doesn't lie on these curves.

4 Unscented Kalman filtering (UKF) of the Doi model

The observability of a dynamic system, as studied above, provides the mathematical possibility of recovering the state of the system from observable quantity. However, the concept of observability itself does not provide the mechanism to practically extract the state from observations. In contrast, Kalman filter is a widely used tool to estimate the state using observation data for systems with observability.

Now we want to investigate the performance of the unscented Kalman filtering [4] in recovering the orientation tensor from the observed birefringences. We refer the readers to the original paper by Julier, Uhlmann and Durrant-Whyte [4] for a complete description of the unscented Kalman filtering. UKF is a popular choice when the state transition and observation models are highly nonlinear. However, a rigorous proof on its convergence is still open. In this section we will examine two cases: (1) the observation is noiseless and (2) the observation is polluted by Gaussian noise. We select the Doi model under shear flow as the testbed. Similar results are obtained for the Doi model under extensional flow which are omitted here.

To examine UKF for a non-steady state solution of the Doi model under shear flow, we add an external force

$$\begin{bmatrix} 0.1 \sin(t) \\ 0.1 \cos(t) \end{bmatrix} \quad (23)$$

to the right-hand side of equation (11). We remark that the observability study in the previous section is still valid here.

We start the system of Doi model under extensional flow (11) with the external force (23) at some initial condition $\vec{x}(0)$ and the filter at a different initial condition $\vec{\hat{x}}(0)$. We solve the system equations without noise to get state $\vec{x}(0 : \infty)$ and observation $h(0 : \infty)$ trajectories. In the case of observations with no noise, we pass the noise free observation trajectory to the filter and the filter yields a state estimate trajectory $\vec{\hat{x}}(0 : \infty)$. The estimation error $\vec{x}(t) - \vec{\hat{x}}(t)$ is the difference between the state of the system (which is not directly measurable) and the estimate state produced by the filter from the observation. The filter is said to be convergent if the estimation error goes to zero as $t \rightarrow \infty$ for any $\vec{x}(0)$ and $\vec{\hat{x}}(0)$.

In Figure 3 we show the results of UKF for the Doi model under shear flow. The parameters used here are $N = 4.0$, $Pe = 0.01$, and $a = 0.8$. Figure 3(a)

depicts the exact and estimated solutions of the Doi system under shear flow, respectively. Figure 3(b) gives the corresponding filter errors. It implies the convergence of the UKF when there is no noise but only initial estimate error.

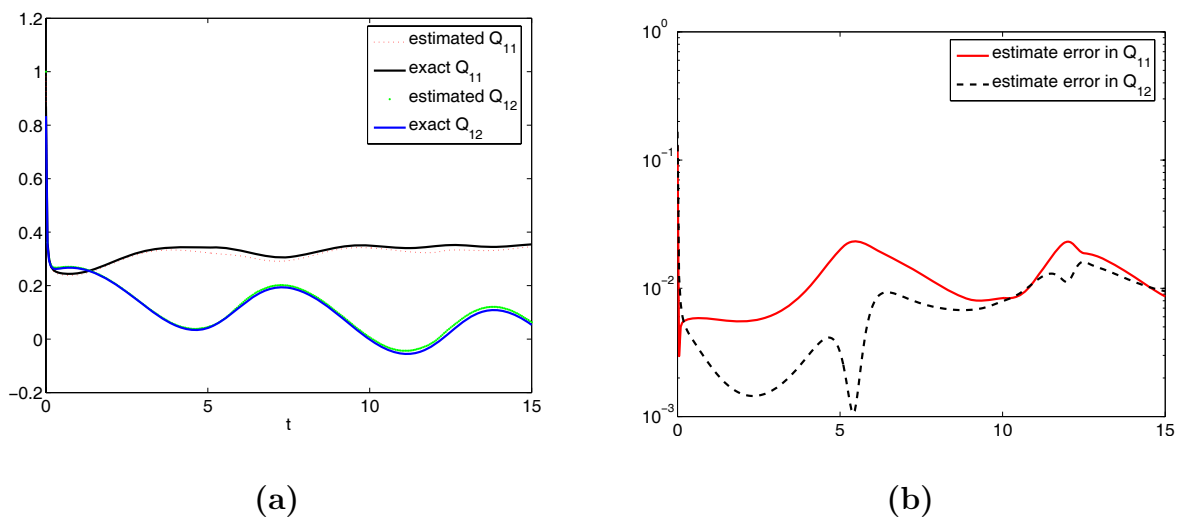


Figure 3: (a) Exact solutions (solid lines) and estimated solutions from UKF (dashed or dotted line) of the Doi model under shear flow with an external force. (b) Corresponding filter errors of UKF in (a).

In practice all observations may be polluted by noises from different sources. Next we check the performance of UKF in the presence of observation noise. We add Gaussian noise to the measurements. Specifically, we assume that the experimental measurement is the true value of the observation plus Gaussian noise:

$$h_{\text{experiment}}(0 : \infty) = h(0 : \infty) + \text{Gaussian noise}.$$

Then we pass the observation with noise $h_{\text{experiment}}(0 : \infty)$ to the filter. The filter outputs an estimated state. Figure 4 depicts the results of UKF for the Doi model under shear flow. Figure 4(a) gives the measurement with noises (the solid line) vs the measurement without noise (dashed line) whereas Figure 4(b) isolates the noise added to the observation. The exact solutions and estimated solutions from UKF are plotted in Figure 4(c) and the corresponding filter errors are given in Figure 4(d). It is clear that UKF yields good estimate even when noises are present in the measurements.

5 Conclusions

We have applied the observability rank condition to the vector fields in the Doi orientation tensor model to investigate the short time local observability of liquid crystalline polymers driven by extensional or shear flow fields. The measurement is assumed to be birefringence of the materials which is consistent with experiments. We have found that the Doi model is observable almost everywhere. That is, one can determine the orientation tensor from the time history of the observations of birefringence when the points formed by the two components of the orientation tensor do not lie on certain curves in the plane.

Acknowledgment

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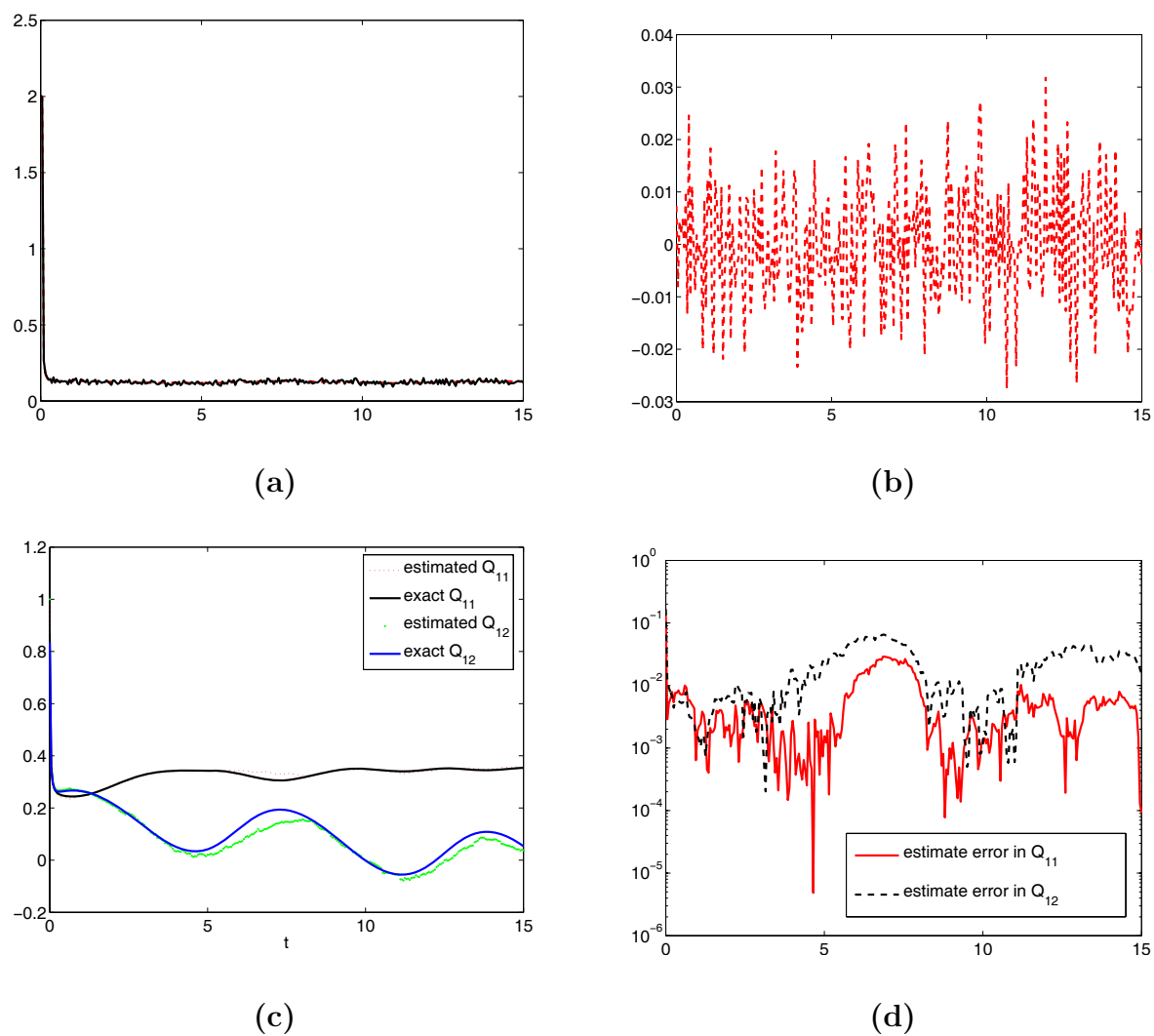


Figure 4: (a) Observation with Gaussian noise (solid line) vs observation without noise (dashed line). (b) The Gaussian noise in (a). (c) Exact solutions (solid lines) and estimated solutions from UKF (symbols) of the Doi model under shear flow with an external force where observations contain Gaussian noise. (d) The corresponding filter errors of (c).