Topography and Force Estimation in Atomic Force Microscopy by State and Parameter Estimation

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Introduction – AFM AM Loop

[Diagram of AFM AM Loop]

- Function generator
- Lock-in amplifier
- Phase
- Amplitude
- Setpoint
- Sample
- xyz-scanner
- PID controller
- z
- Setpoint
- Cantilever
- Laser
- Photo detector
- Piezo
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Introduction – AFM AM Loop

- Sensor
- Controller
- Piezo actuator
- Output image
- Sample height
- Tip-sample interaction force
- Cantilever response
- Setpoint
- Amplitude estimation
- Cantilever response
- Force $F$
- Sample height
- $D$
- $\theta$
- $\text{Output image}$
- $\text{Amplitude estimation}$
- $\text{Sensor}$
- $\text{Controller}$
- $\text{Piezo actuator}$
- $\text{Sample height}$
- $\text{Tip-sample interaction force}$
- $\text{Cantilever response}$
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Introduction – AFM AM Loop

Setpoint

Amplitude estimation

Sensor

Cantilever response

Tip-sample interaction force

Controller

Piezo actuator

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Introduction – AFM AM Loop
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Introduction – AFM AM Loop

- **Amplitude estimation**
- **Controller**
- **Piezo actuator**
- **Output image**
- **Sample height**
- **Tip-sample interaction force**
- **Cantilever response**
- **State and parameter estimator**
- **Setpoint**
- **Sensor**
Introduction

— We will employ observers to directly estimate the topography
  • By considering the cantilever dynamics and interaction force
— Two observers were designed for the same purpose:
  • A nonlinear observer with well-defined exponential stability results.
  • An extended Kalman Filter for comparison.
Outline

Introduction

System Modeling

Observer Design

Simulation Results

Conclusion and Further Work
System Modeling

- $G$: Cantilever model from applied force, to tip deflection.
  - Second order harmonic oscillator.
- $F_{ts}$: Tip-sample interaction force: Modeled by Lennard-Jones potential.
System Modeling – Lennard-Jones potential

\[ F_{ts}(D) = k_1 \left[ \frac{\sigma^2}{D^2} - \frac{1}{30} \frac{\sigma^8}{D^8} \right] \] (1)
System Modeling – State-space form

System can be expressed as an extended state-space model suitable for the state- and parameter estimator.

\[
\begin{bmatrix}
\dot{x} \\
\dot{\phi}
\end{bmatrix} =
\begin{bmatrix}
A & E \\
0 & 0
\end{bmatrix}
\begin{bmatrix}
x \\
\phi
\end{bmatrix} +
\begin{bmatrix}
B \\
0
\end{bmatrix} u +
\begin{bmatrix}
0 \\
1
\end{bmatrix} d
\]

(2)

\[
A =
\begin{bmatrix}
0 & 1 \\
-\omega_0^2 & -2\zeta\omega_0
\end{bmatrix},
B = E =
\begin{bmatrix}
0 \\
\frac{1}{m}
\end{bmatrix},
C =
\begin{bmatrix}
1 & 0
\end{bmatrix}
\]

(3)
System Modeling – State-space form

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where

— the state \(x \triangleq (x_1, x_2)^T\) represent the cantilever deflection and the deflection velocity
— the Lennard-Jones force \(F_{ts}\) has been introduced as a state \(\phi\)
— \(d\) is the time-derivative of \(\phi\)
— and the input \(u\) is the driving force of the cantilever.
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Nonlinear Observer

Based on Håvard F. Grip’s article: “Estimation of States and Parameters for linear systems with nonlinearily parameterized perturbations” (2011).

Structure of the state- and parameter estimator. From (Grip et al., 2011).
Nonlinear Observer – Modified High-Gain Observer

Observes the state \((\hat{x}, \hat{\phi})\) as if the parameter estimate \(\hat{\theta}\) is perfectly known.

\[
\dot{\hat{x}} = A\hat{x} + Bu + E\hat{\phi} + K_x(\varepsilon)(y - C\hat{x})
\]

\[
\dot{\hat{\theta}} = -\frac{\partial g}{\partial \theta} \hat{\theta} - \frac{\partial g}{\partial x} K_x(\varepsilon)(y - C\hat{x}) + K_\phi(\varepsilon)(y - C\hat{x})
\] (4)

\[
\hat{\phi} = g(\hat{x}_1, \hat{\theta}) + z
\]

— Need to determine \(K_x(\varepsilon), K_\phi(\varepsilon)\) such that the error dynamics of the observer are input-to-state stable.
Nonlinear Observer – Modified High-Gain Observer

Observes the state \((\hat{x}, \hat{\phi})\) as if the parameter estimate \(\hat{\theta}\) is perfectly known.

\[
\dot{\hat{x}} = A\hat{x} + Bu + E\hat{\phi} + K_x(\varepsilon)(y - C\hat{x}) \\
\dot{\hat{\phi}} = g(\hat{x}_1, \hat{\theta}) + z
\]

Need to determine \(K_x(\varepsilon), K_\phi(\varepsilon)\) such that the error dynamics of the observer are input-to-state stable.

Result

\[
K_x(\varepsilon) = \begin{bmatrix} 4.0\varepsilon^{-1} \\ 5.04\varepsilon^{-2} \end{bmatrix} \\
K_\phi(\varepsilon) = 4.0\omega_0^2\varepsilon^{-1} + 10.08\zeta\omega_0\varepsilon^{-2} + 2.08\varepsilon^{-3}
\]
Nonlinear Observer – Parameter Estimator

Need to find an update law

\[
\dot{\hat{\theta}} = u_\theta(\nu, \hat{x}, \hat{\phi}, \hat{\theta})
\]

such that the origin of the error dynamics

\[
\hat{\theta} = -u_\theta(\nu, \hat{x}, \hat{\phi}, \theta - \hat{\theta})
\]

is uniformly exponentially stable whenever \( \hat{x} = x \) and \( \hat{\phi} = \phi \).
Nonlinear Observer – Parameter Estimator

Need to find an update law

\[ \dot{\hat{\theta}} = u_\theta(\nu, \hat{x}, \phi, \hat{\theta}) \]  

(7)

such that the origin of the error dynamics

\[ \dot{\tilde{\theta}} = -u_\theta(\nu, \hat{x}, \phi, \theta - \tilde{\theta}) \]  

(8)

is uniformly exponentially stable whenever \( \hat{x} = x \) and \( \hat{\phi} = \phi \).

Assumption 6

There exist a differentiable function \( V_u: \mathbb{R}_{\geq 0} \times (\Theta - \Theta) \rightarrow \mathbb{R}_{\geq 0} \) and positive constants \( a_1, \ldots, a_4 \) such that for all \( (t, \tilde{\theta}) \in \mathbb{R}_{\geq 0} \times (\Theta - \Theta) \),

\[
\begin{align*}
 a_1 \left\| \tilde{\theta} \right\|^2 & \leq V_u(t, \tilde{\theta}) \leq a_2 \left\| \tilde{\theta} \right\|^2 \\
 \frac{\partial V_u}{\partial t}(t, \tilde{\theta}) - \frac{\partial V_u}{\partial \tilde{\theta}}(t, \tilde{\theta})u_\theta(\nu, x, \phi, \theta - \tilde{\theta}) & \leq -a_3 \left\| \tilde{\theta} \right\| \\
 \left\| \frac{\partial V_u}{\partial \tilde{\theta}}(t, \tilde{\theta}) \right\| & \leq a_4 \left\| \tilde{\theta} \right\|
\end{align*}
\]

Furthermore, the update law (7) ensures that if \( \hat{\theta}(0) \in \Theta \), then for all \( t \geq 0 \), \( \hat{\theta} \in \Theta \).
Nonlinear Observer – Parameter Estimator

Need to find an update law
\[ \dot{\hat{\theta}} = u_\theta(\nu, \hat{x}, \hat{\phi}, \hat{\theta}) \] (7)
such that the origin of the error dynamics
\[ \hat{\theta} = -u_\theta(\nu, \hat{x}, \hat{\phi}, \theta - \tilde{\theta}) \] (8)
is uniformly exponentially stable whenever \( \hat{x} = x \) and \( \hat{\phi} = \phi \).

Assumption 6 satisfied by the following update law:
\[ u_\theta(\nu, \hat{x}, \hat{\phi}, \hat{\theta}) = \text{Proj} \left( \Gamma M(\nu, \hat{x}, \hat{\theta})(\hat{\phi} - g(\nu, \hat{x}, \hat{\theta})) \right) \] (9)
\[ M = \frac{1}{2} M_{\text{max}} \left[ \tanh(M_{\text{rate}}(\hat{D} - D_M)) + 1 \right] \] (10)
Nonlinear Observer – Assumptions

— Bounded topography, well defined input signal and time-derivative
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— Operation in noncontact mode – allows the force profile to be represented by a monotonic function
Nonlinear Observer – Assumptions

— Bounded topography, well defined input signal and time-derivative
— Operation in noncontact mode – allows the force profile to be represented by a monotonic function
— Known Lennard-Jones parameters
  • Parameters appear linearly in Lennard-Jones function ⇒ Method can easily be extended to simultaneously determine these.
Nonlinear Observer – Stability Theorem

Theorem 1 (Abbreviated)

If all assumptions are satisfied and \( \hat{\theta}(0) \in \Theta \), there exists \( 0 < \varepsilon^* \leq 1 \) such that for all \( 0 < \varepsilon \leq \varepsilon^* \), the origin of the error dynamics of the observer and parameter estimator is exponentially stable.
Outline

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Simulation Results

Conclusion and Further Work
Simulation Results

Topography estimate with output noise.
Simulation Results

Estimated interaction force $\phi$ with noise.

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Introduction

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Simulation Results

Conclusion and Further Work
Conclusion

— New dynamic mode imaging method.
— Cantilever dynamics and interaction force "inverted" to estimate topography.
— Avoids bandwidth-limiting amplitude estimation.
— Exponentially stable observer.
Further Work

— Experimental results.
— Include estimation of Lennard-Jones parameters.
— Use observer in feedback loop for control.
— Proper analysis of closed-loop bandwidth.
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Questions?
References
