



Data-driven Learning of Generalized Langevin Equations with State-dependent Memory

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Generalized Langevin Equations

- Following the Zwanzig's projection formalism

$$\begin{cases} \dot{\mathbf{q}} = M^{-1} \mathbf{p} \\ \dot{\mathbf{p}} = -\nabla U(\mathbf{q}) - \int_0^t \mathbf{K}(\mathbf{q}(\tau), t - \tau) \dot{\mathbf{q}}(\tau) d\tau + \mathcal{R}(t). \end{cases}$$

- Standard GLE: **Homogeneous** memory kernel. $\mathbf{K}(\mathbf{q}(\tau), t - \tau) \approx \mathbf{K}(t - \tau)$.
- Not enough for accurately predicting the collective behaviors.

GLE with State-dependent Memory

- The state-dependent GLE model

$$\begin{cases} \dot{\mathbf{q}} = \mathbf{M}^{-1} \mathbf{p} \\ \dot{\mathbf{p}} = -\nabla U(\mathbf{q}) - \int_0^t \phi(\mathbf{q}_t)^T \Theta(t - \tau) \phi(\mathbf{q}_\tau) \mathbf{v}(\tau) d\tau + \phi(\mathbf{q}_t)^T \mathbf{R}(t), \end{cases}$$

where $\langle \mathbf{R}(t), \mathbf{R}(\tau) \rangle = k_B T \Theta(t - \tau)$, $\Theta(t)$ is $\mathbb{R}^{1 \times 1} \rightarrow \mathbb{R}^{n \times n}$, $\phi(\mathbf{q})$ is $\mathbb{R}^{M \times 1} \rightarrow \mathbb{R}^{n \times M}$.

- As a covariance function, $\Theta(-t) = \Theta(t)^T$.

$$\Theta(t > 0) = e^{-\alpha t} \sum_{k=0}^{N_\omega} \tilde{\Theta}_k^S \cos(\omega_k t) + i \tilde{\Theta}_k^A \cos(\omega_k t),$$

where $e^{-\alpha t}$ is a **regularization term**.

Invariant Density Distribution

- **Proposition: Invariant distribution:** $\rho_{\text{eq}}(\mathbf{q}, \mathbf{p}) \propto \exp\left\{-\left[U(\mathbf{q}) + \mathbf{p}^T \mathbf{M}^{-1} \mathbf{p}/2\right]/k_B T\right\}$
- **Prof:** For simplify, we assume $\Theta(t) = \Theta(t)^T$, $\tilde{\Theta}_k^S = \Gamma_k^T \Gamma_k$.

$$\Theta(t) = \sum_{k=0}^{N_\omega} \begin{pmatrix} \Gamma_k \\ 0 \end{pmatrix}^T e^{-\alpha t} \begin{pmatrix} \cos(\omega_k t) I & \sin(\omega_k t) I \\ -\sin(\omega_k t) I & \cos(\omega_k t) I \end{pmatrix} \begin{pmatrix} \Gamma_k \\ 0 \end{pmatrix} = \sum_{k=0}^{N_\omega} \begin{pmatrix} \Gamma_k \\ 0 \end{pmatrix}^T \exp\left(\begin{pmatrix} -\alpha I & \omega_k I \\ -\omega_k I & -\alpha I \end{pmatrix} t\right) \begin{pmatrix} \Gamma_k \\ 0 \end{pmatrix},$$

- Recall that $\langle \mathbf{R}(t), \mathbf{R}(\tau) \rangle = k_B T \Theta(t - \tau)$, rewrite the noise term into

$$\mathbf{R}(t) = \sum_{k=0}^{N_\omega} \begin{pmatrix} \Gamma_k \\ 0 \end{pmatrix}^T \mathbf{R}_k(t), \quad \langle \mathbf{R}_k(t), \mathbf{R}_k(\tau) \rangle = k_B T \exp\left(\begin{pmatrix} -\alpha I & \omega_k I \\ -\omega_k I & -\alpha I \end{pmatrix} (t - \tau)\right)$$

Invariant Density Distribution

- $\dot{\mathbf{p}} = -\nabla U(\mathbf{q}) - \int_0^t \phi(\mathbf{q}_t)^T \Theta(t - \tau) \phi(\mathbf{q}_\tau) \mathbf{v}(\tau) d\tau + \phi(\mathbf{q}_t)^T \mathbf{R}(t)$

- We can rewrite it as

$$\frac{d}{dt} \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \\ \dots \\ \mathbf{z}_{k,1} \\ \mathbf{z}_{k,2} \\ \dots \end{pmatrix} = \begin{pmatrix} 0 & I & \dots & 0 & 0 & \dots \\ -I & 0 & \dots & -\phi(\mathbf{q})^T \Gamma_k^T & 0 & \dots \\ 0 & \dots & \dots & \dots & \dots & \dots \\ 0 & -\Gamma_k \phi(\mathbf{q}) & \dots & -\alpha I & -\omega_k I & \dots \\ 0 & 0 & \dots & \omega_k I & -\alpha I & \dots \\ 0 & \dots & \dots & \dots & \dots & \dots \end{pmatrix} \begin{pmatrix} \nabla U(\mathbf{q}) \\ \mathbf{v} \\ \dots \\ \mathbf{z}_{k,1} \\ \mathbf{z}_{k,2} \\ \dots \end{pmatrix} + \sqrt{2k_B T \alpha} \begin{pmatrix} 0 \\ 0 \\ \dots \\ \dot{\mathbf{W}}_{k,1} \\ \dot{\mathbf{W}}_{k,2} \\ \dots \end{pmatrix}$$

$$\triangleq \mathbf{K} \nabla F(\mathbf{q}, \mathbf{p}, \dots, \mathbf{z}_{k,1}, \mathbf{z}_{k,2}, \dots) + \Lambda \dot{\mathbf{W}}_t,$$

- The **invariant density function** $\rho_{\text{eq}}(\mathbf{q}, \mathbf{p}, \mathbf{z}) = \exp[-F(\mathbf{q}, \mathbf{p}, \mathbf{z})/k_B T]$

Data-driven Method

- $\dot{\mathbf{p}} + \nabla U(\mathbf{q}) = - \int_0^t \phi(\mathbf{q}_t)^T \Theta(t - \tau) \phi(\mathbf{q}_\tau) \mathbf{v}(\tau) d\tau + \phi(\mathbf{q}_t)^T \mathbf{R}(t)$
- Conditional correlation function: $\langle \dot{\mathbf{p}}_t + \nabla U(\mathbf{q}), \mathbf{v}_0^T | \mathbf{q}_0 = \mathbf{q}^* \rangle$
- Convolution term: $\langle \phi(\mathbf{q}_t)^T \Theta(t - \tau) \phi(\mathbf{q}_\tau) \mathbf{v}(\tau), \mathbf{v}_0^T | \mathbf{q}_0 = \mathbf{q}^* \rangle$
- Represent $\phi(\mathbf{q})$ with a set of sparse bases $\psi(\mathbf{q})$, such that $\phi(\mathbf{q}) = \mathbf{H}\psi(\mathbf{q})$
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Data-driven Method

- $\dot{\mathbf{p}} + \nabla U(\mathbf{q}) = - \int_0^t \phi(\mathbf{q}_t)^T \Theta(t - \tau) \phi(\mathbf{q}_\tau) \mathbf{v}(\tau) d\tau + \phi(\mathbf{q}_t)^T \mathbf{R}(t)$
- Conditional correlation function: $\langle \dot{\mathbf{p}}_t + \nabla U(\mathbf{q}), \mathbf{v}_0^T | \mathbf{q}_0 = \mathbf{q}^* \rangle$
- Convolution term: $\text{Tr} \left[\Theta(t - \tau) \mathbf{H} \langle \psi(\mathbf{q}_\tau) \mathbf{v}(\tau) \mathbf{v}_0^T \psi(\mathbf{q}_t)^T | \mathbf{q}_0 = \mathbf{q}^* \rangle \mathbf{H}^T \right]$
- Represent $\phi(\mathbf{q})$ with a set of sparse bases $\psi(\mathbf{q})$, such that $\phi(\mathbf{q}) = \mathbf{H}\psi(\mathbf{q})$
- $\langle \psi(\mathbf{q}_\tau) \mathbf{v}(\tau) \mathbf{v}_0^T \psi(\mathbf{q}_t)^T | \mathbf{q}_0 = \mathbf{q}^* \rangle$ can be **pre-compute**

Loss Function

$$g(t; \mathbf{q}^*) = \langle \dot{\mathbf{p}}_t + \nabla U(\mathbf{q}_t), \mathbf{q}_0^T | \mathbf{q}_0 = \mathbf{q}^* \rangle$$

$$C_{\psi, \psi}(t, \tau; \mathbf{q}^*) = \langle \psi(\mathbf{q}_\tau) \mathbf{v}(\tau) \mathbf{v}_0^T \psi(\mathbf{q}_t)^T | \mathbf{q}_0 = \mathbf{q}^* \rangle$$

$$\text{loss}(\mathbf{q}^*, \mathbf{t}) = \left\| g(t; \mathbf{q}^*) + \int_0^t \text{Tr} [\Theta(t - \tau) \mathbf{H} C_{\psi, \psi}(t, \tau; \mathbf{q}^*) \mathbf{H}^T] d\tau \right\|_2^2$$

Simulation

- Convolution:

$$\dot{\mathbf{p}} = -\nabla U(\mathbf{q}) - \phi(\mathbf{q}_t)^T \int_0^t \Theta(t - \tau) \phi(\mathbf{q}_\tau) \mathbf{v}(\tau) d\tau + \phi(\mathbf{q}_t)^T \mathbf{R}(t)$$

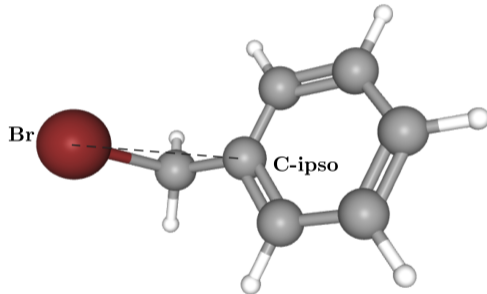
$$\Theta(t) = e^{-\alpha t} \sum_{k=0}^{N_\omega} \tilde{\Theta}_k \cos(\omega_k t)$$

- Noise:

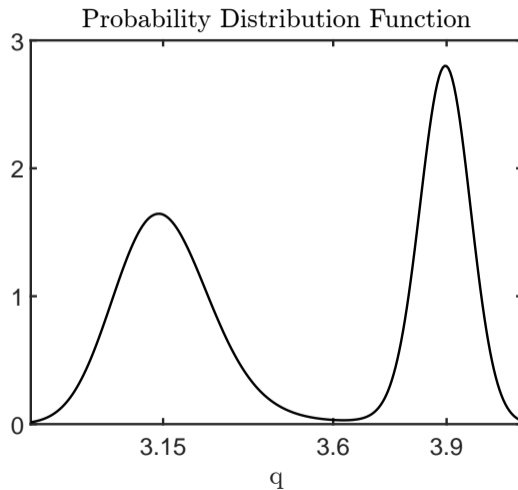
$$\mathbf{R}(t) = \frac{1}{\sqrt{k_B T}} \sum_{k=0}^{2N} \hat{\Theta}_k^{1/2} [\cos(\omega_k t) \xi_k + \sin(\omega_k t) \eta_k]$$

Numerical Result: Full Model

- A Benzyl bromide molecule in water.
- \mathbf{q} is the distance between the bromine atom and the ipso-carbon atom.
- $U(\mathbf{q})$ is evaluated from the PDF.

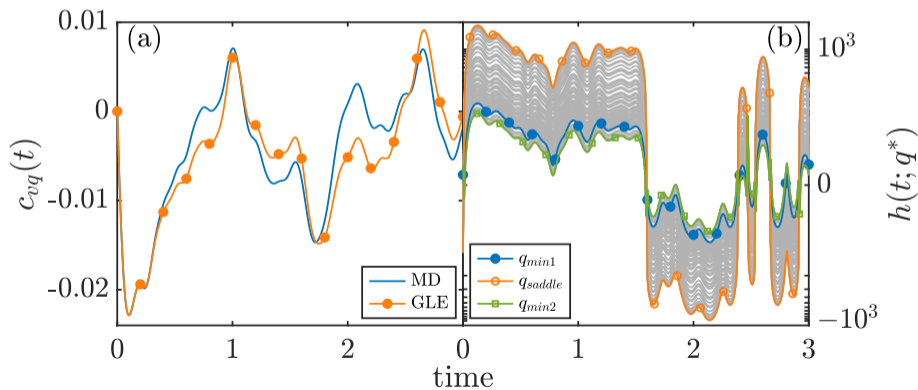


Numerical Result: PDF



Numerical Result: Standard GLE Limit

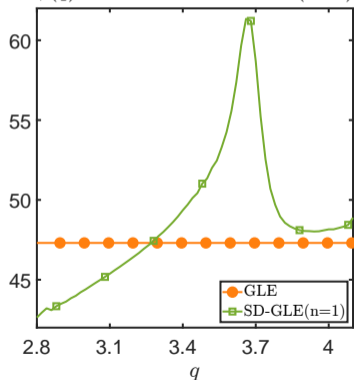
$$h(t; \mathbf{q}^*) = \langle \dot{\mathbf{p}} + \nabla U(\mathbf{q}), \mathbf{q}_0 | \mathbf{q}_0 = \mathbf{q}^* \rangle = - \int_0^t \Theta(t - \tau) \langle \mathbf{v}(\tau), \mathbf{q}_0 | \mathbf{q}_0 = \mathbf{q}^* \rangle d\tau$$



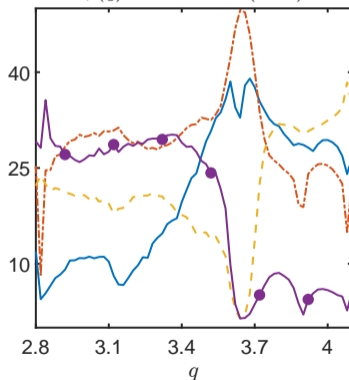
Numerical Result: $\Theta(t)$ and $\phi(\mathbf{q})$

$$\dot{\mathbf{p}} = -\nabla U(\mathbf{q}) - \int_0^t \phi(\mathbf{q}_t)^T \Theta(t - \tau) \phi(\mathbf{q}_\tau) \mathbf{v}(\tau) d\tau + \phi(\mathbf{q}_t)^T \mathbf{R}(t)$$

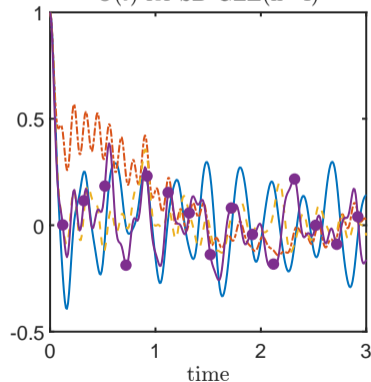
$\phi(q)$ for GLE and SD-GLE($n=1$)



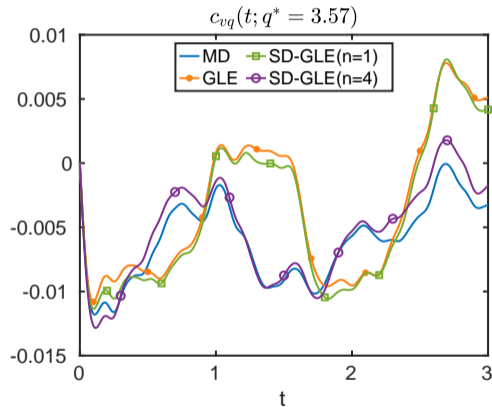
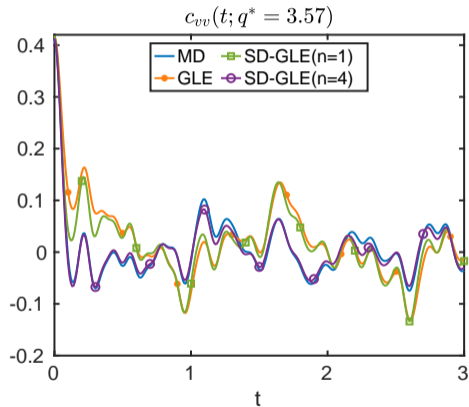
$\phi(q)$ for SD-GLE($n=4$)



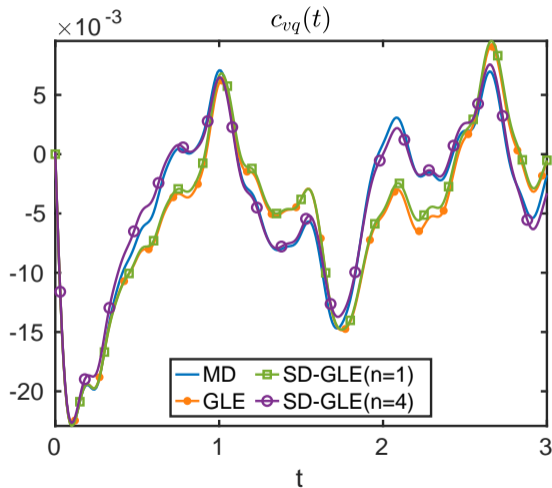
$\Theta(t)$ for SD-GLE($n=4$)



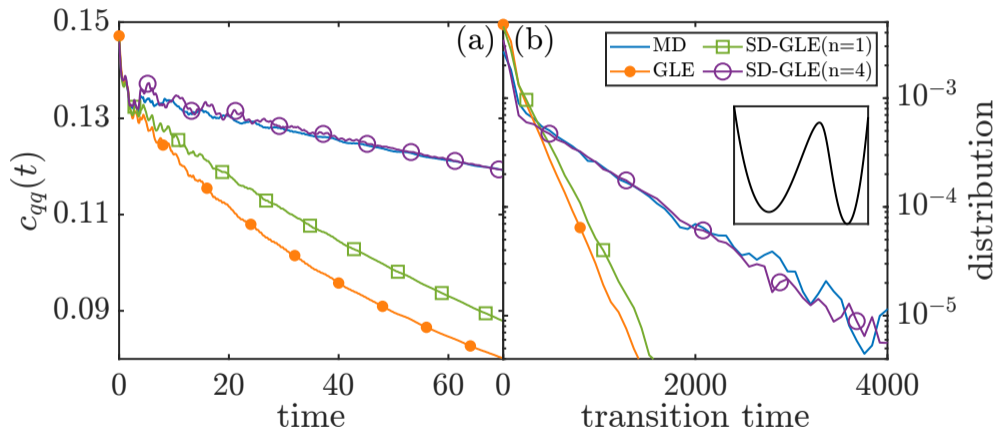
Numerical Result on Saddle Point



Numerical Result: Standard Correlation Function



Numerical Result: Transition Time



Conclusion

- **State-dependent memory kernel** is crucial on the collective behavior.
- Our model has the consistent **density distribution**.
- Only **trajectory samples** are needed to evaluate the model.



Thank You!
Any Questions?

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