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

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Generalized Langevin Equations

- Following the Zwanzig's projection formalism

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

- 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

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

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

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

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

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

Invariant Density Distribution

- **Proposition**: Invariant distribution: $\rho_{\mathrm{eq}}(\mathbf{q},\mathbf{p}) \propto \exp\left\{-\left[U(\mathbf{q}) + \mathbf{p}^T\mathbf{M}^{-1}\mathbf{p}/2\right]/k_B T\right\}$

- **Prof**: For simplify, we assume $\Theta(t) = \Theta(t)^T$, $\tilde{\Theta}_k^S = \Gamma_k^T\Gamma_k$.

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

- 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

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

- We can rewrite it as

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

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

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

Data-driven Method

- $\dot{\mathbf{p}} + \nabla U(\mathbf{q}) = -\int_0^t \phi(\mathbf{q}_t)^T \Theta(t-\tau)\phi(\mathbf{q}_\tau)\mathbf{v}(\tau)\,\mathrm{d}\tau + \phi(\mathbf{q}_t)^T \mathbf{R}(t)$
- Conditional correlation function: $\left\langle \dot{\mathbf{p}}_t + \nabla U(\mathbf{q}), \mathbf{v}_0^T \middle| \mathbf{q}_0 = \mathbf{q}^* \right\rangle$
- Convolution term: $\left\langle \phi(\mathbf{q}_t)^T \Theta(t-\tau)\phi(\mathbf{q}_\tau)\mathbf{v}(\tau), \mathbf{v}_0^T \middle| \mathbf{q}_0 = \mathbf{q}^* \right\rangle$
- 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

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

Loss Function

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

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

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

Simulation

- Convolution:

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

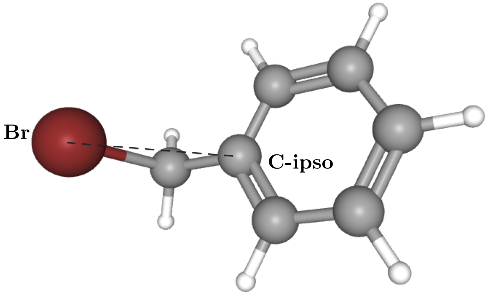
$$\Theta(t) = \mathrm{e}^{-\alpha t} \sum_{k=0}^{N_\omega} \tilde{\Theta}_k \cos(\omega_k t)$$

- Noise:

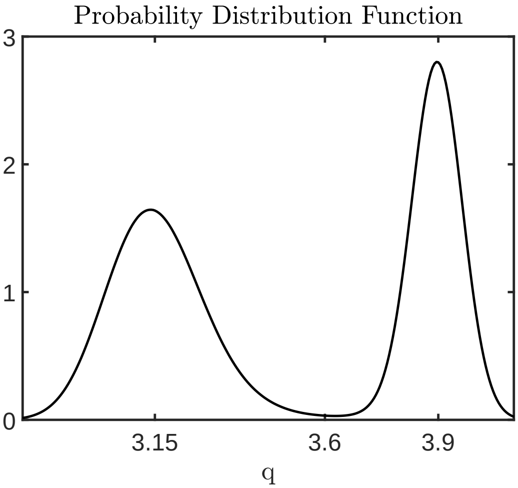
$$\mathbf{R}(t) = \frac{1}{\sqrt{k_B T}} \sum_{k=0}^{2N} \hat{\Theta}_k^{1/2} \left[\cos(\omega_k t)\xi_k + \sin(\omega_k t)\eta_k\right]$$

Numerical Result: Full Model

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

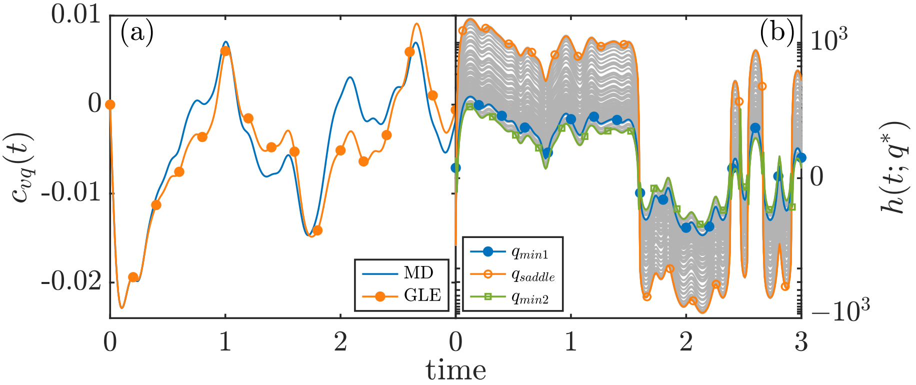


Numerical Result: PDF



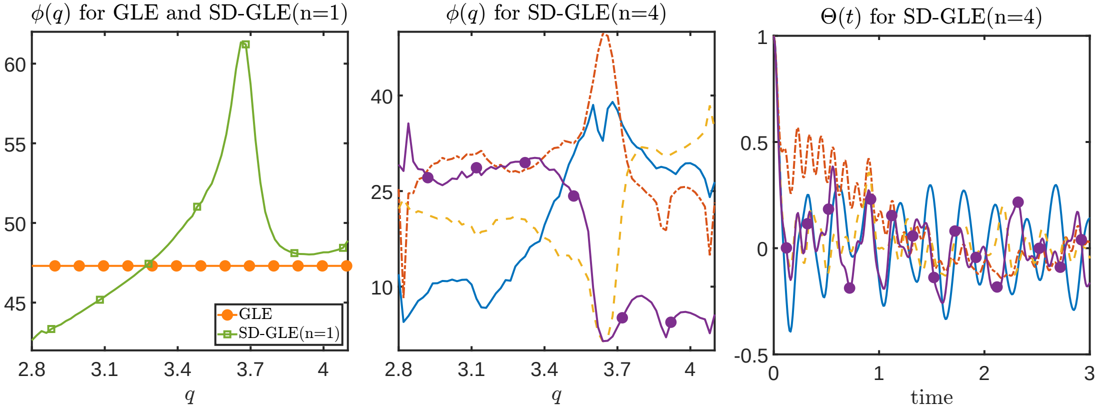
Numerical Result: Standard GLE Limit

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

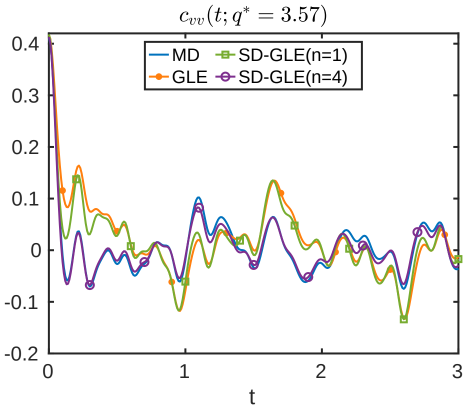


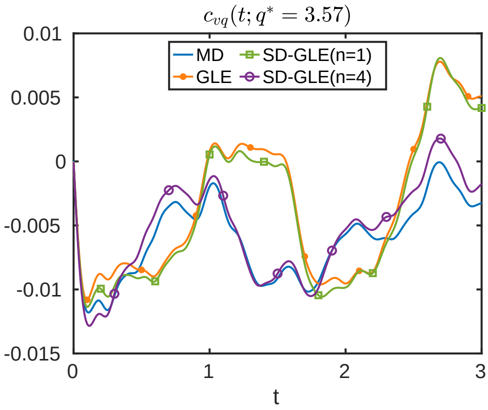
Numerical Result: $\Theta(t)$ and $\phi(\mathbf{q})$

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

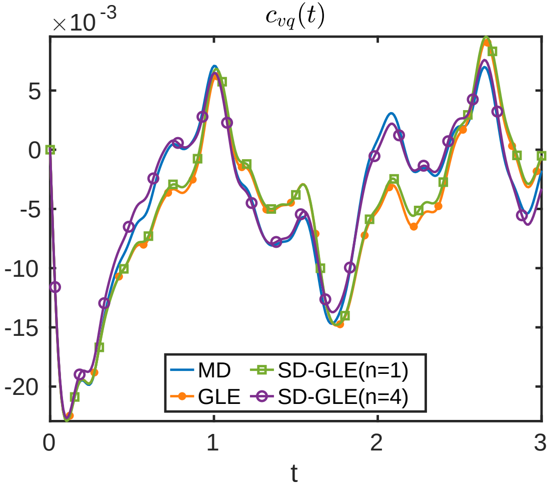


Numerical Result on Saddle Point

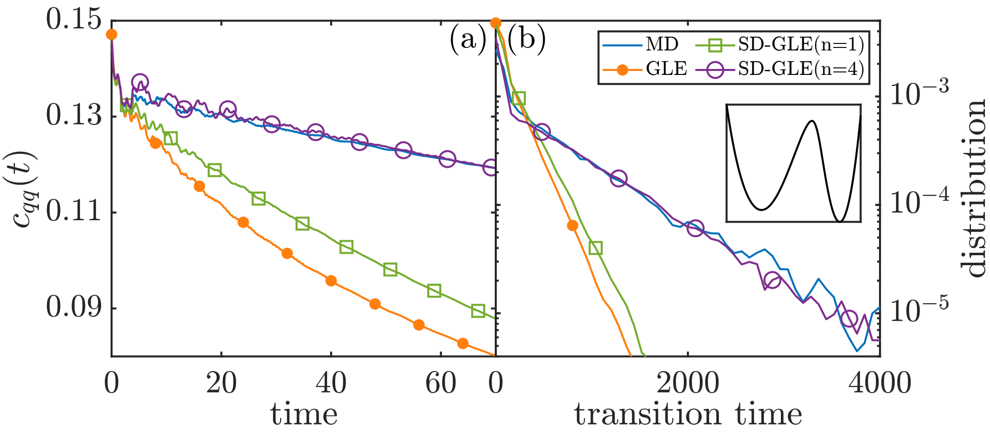




Numerical Result: Standard Correlation Function



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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