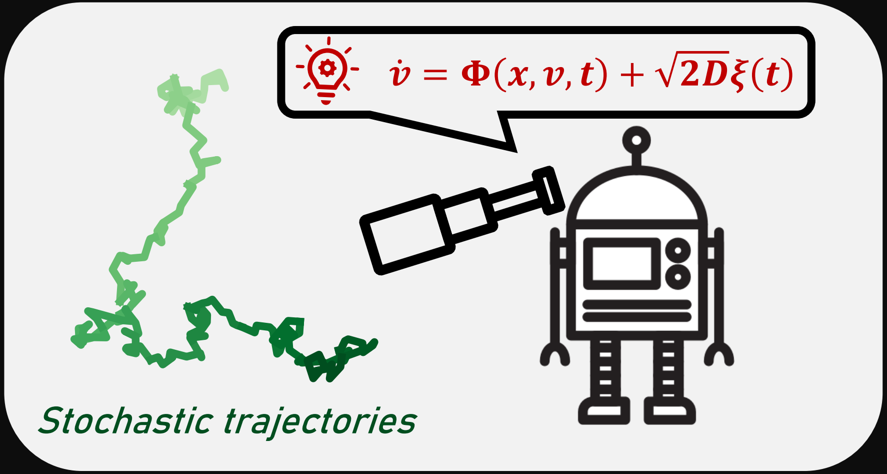
Dynamics Days Asia Pacific 13 in Kyoto

Decoding the Underdamped Langevin Equation from Trajectories via Bayesian Neural Networks



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[1]*Department of Physics and Astronomy, Seoul National University, Korea*

[2]*Department of Santa Fe Institute, USA*

[3]*Department of Physics, Korea Advanced Institute of Science and Technology, Korea*

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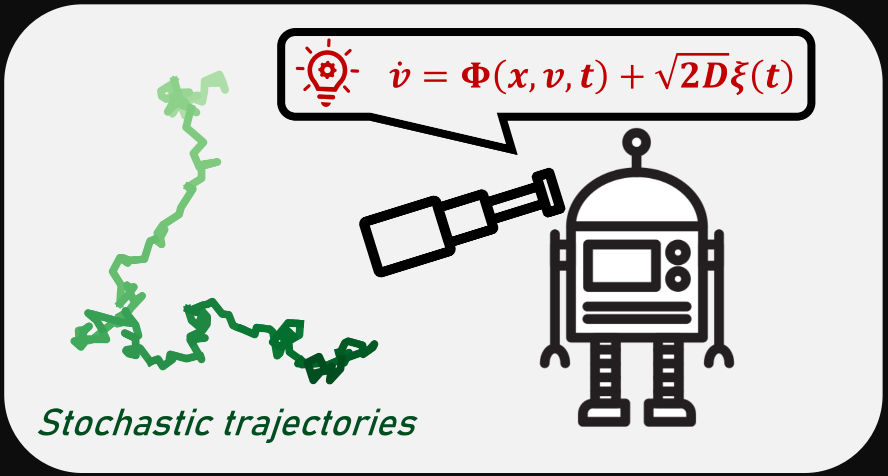

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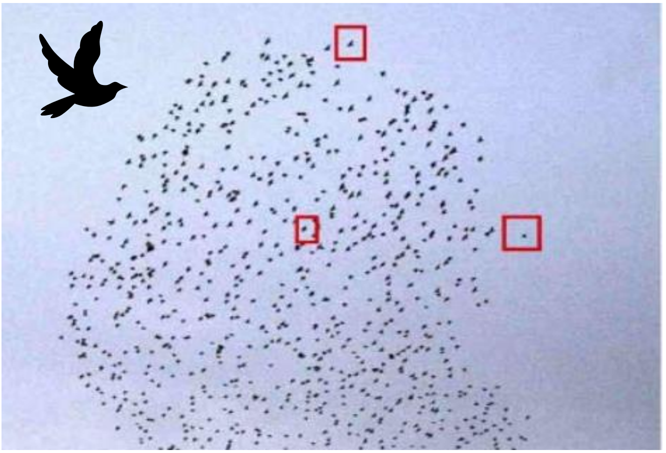
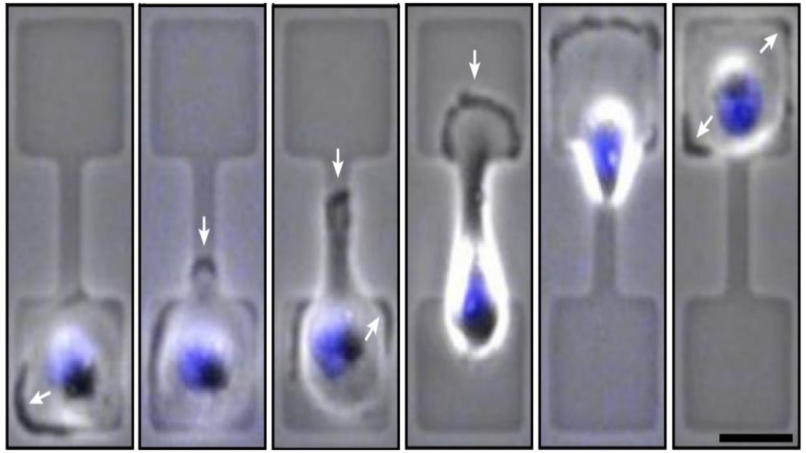
Introduction

| Stochastic dynamics → *Langevin equation*

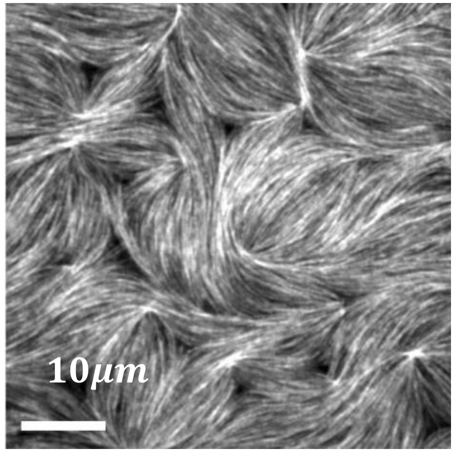
M. Ballerini et al, *Proc. Natl. Acad. Sci. U.S.A.* **105**, 1232-1237 (2008)



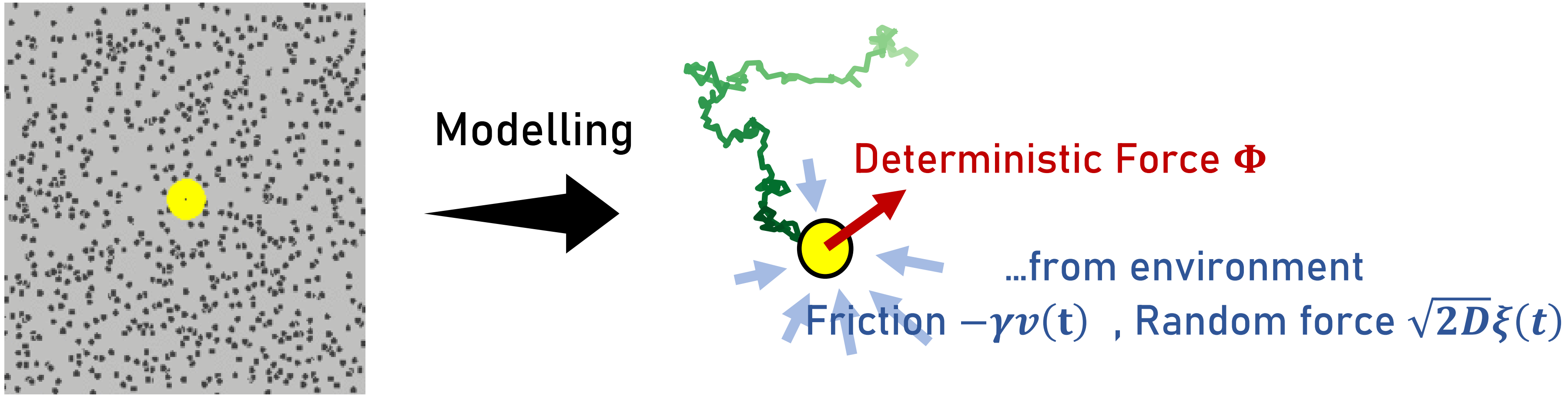
D. B. Bruckner et al, *Nat. Phys.* **15**, 595-601 (2019)



D. S. Seara et al, *Nat. Commun.* **9**, 370 (2007)



Stochastic dynamics = Deterministic force $\boldsymbol{\Phi}$ + Random force $\sqrt{2D}\xi$



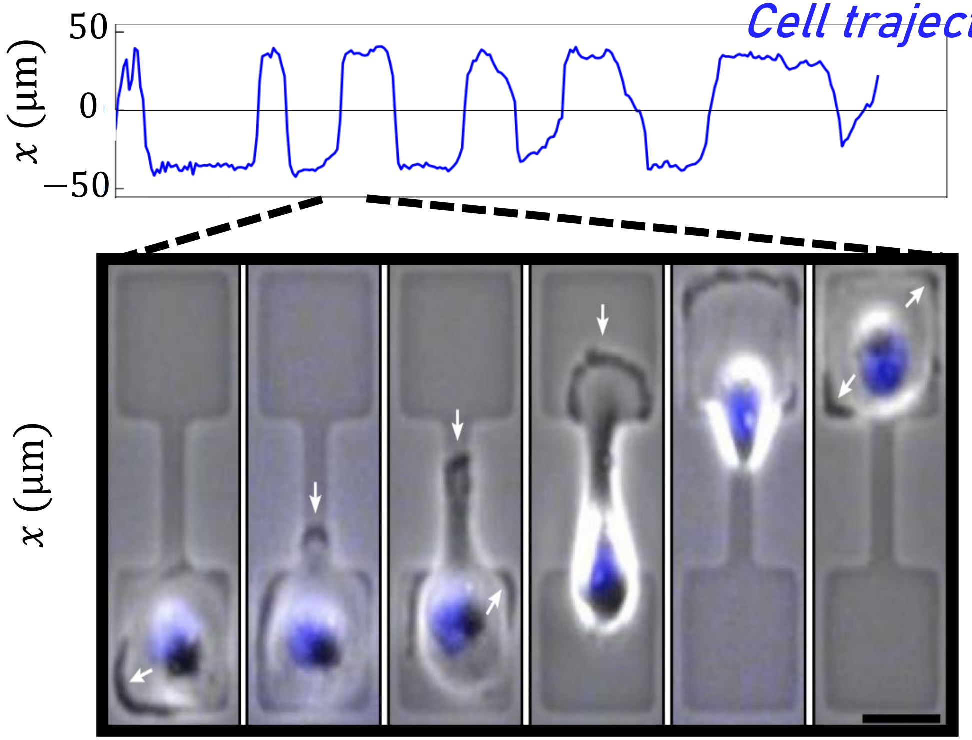
Introduction

| Advantages of Langevin equation inference

Cell migration in two-state confinements

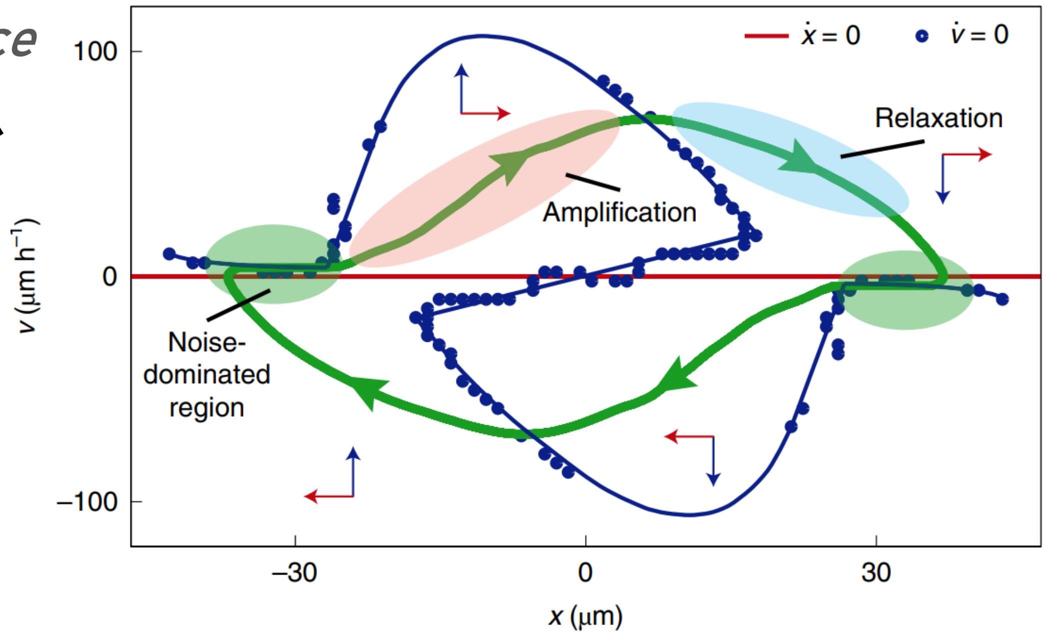
D. B. Bruckner et al., *Nat. Phys.* 15, 595 (2019)

Cell trajectory



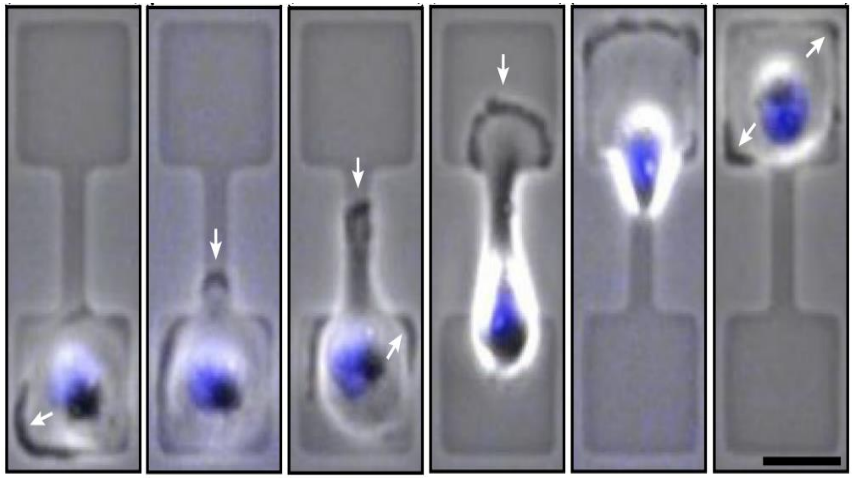
Inference

Drift field in xv-plane



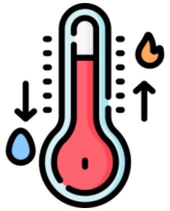
Introduction

| Advantages of Langevin equation inference



$$\dot{x}(t) = v(t)$$

$$\dot{v}(t) = \Phi(x, v, t) + \sqrt{2D(x, v, t)}\xi(t)$$

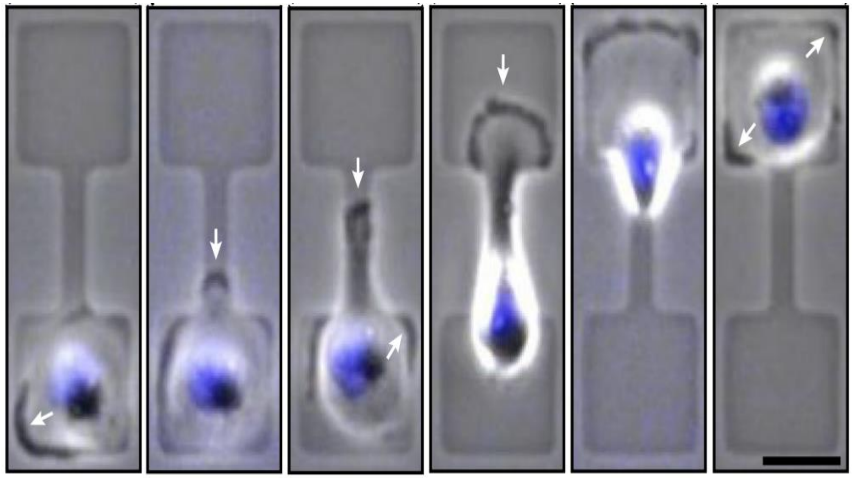


Calculate thermodynamic quantities

$$\boldsymbol{W(t), Q(t), \Delta S(t), \ldots}$$

Introduction

| Advantages of Langevin equation inference



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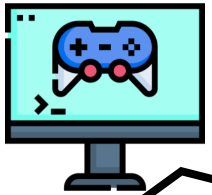
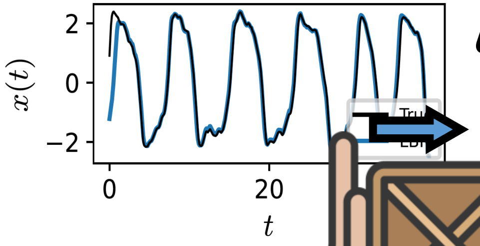
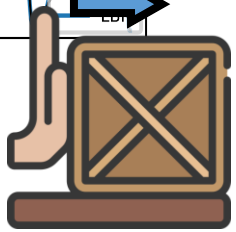


Emulate the system

even in different environment



Generate more trajectories?

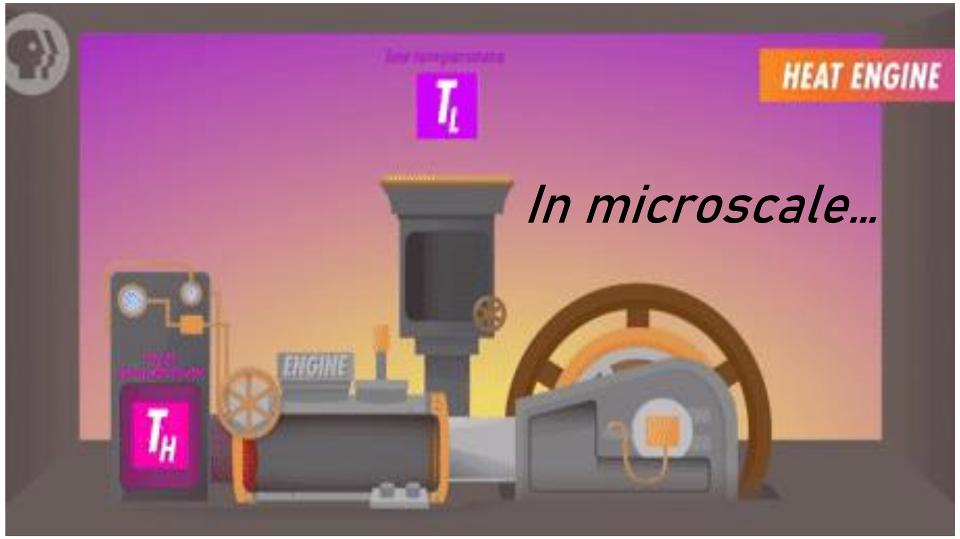


Additional force?

Different temperature?

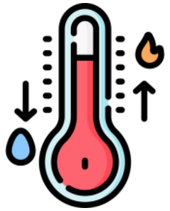
Introduction

| Advantages of Langevin equation inference



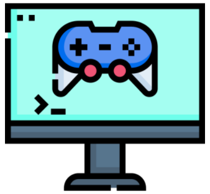
$$\dot{x}(t) = v(t)$$

$$\dot{v}(t) = \Phi(x, v, t) + \sqrt{2D(x, v, t)}\xi(t)$$



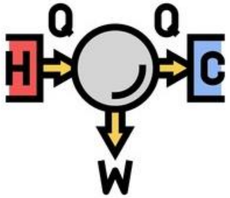
Calculate thermodynamic quantities

$\boldsymbol{W(t), Q(t), \Delta S(t), \ldots}$



Emulate the system

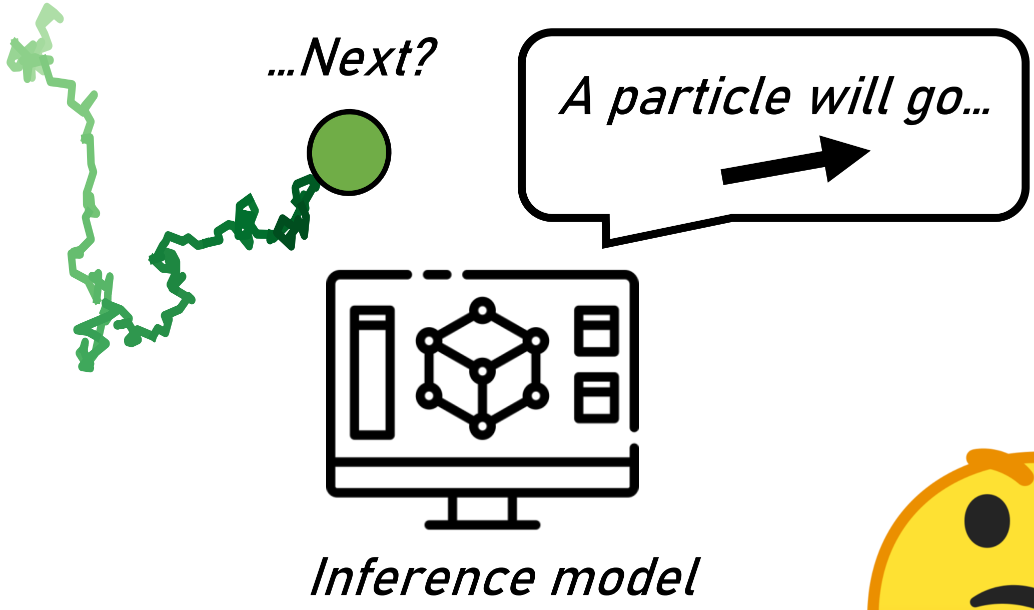
even in different environment



Design more efficient heat engine

Introduction

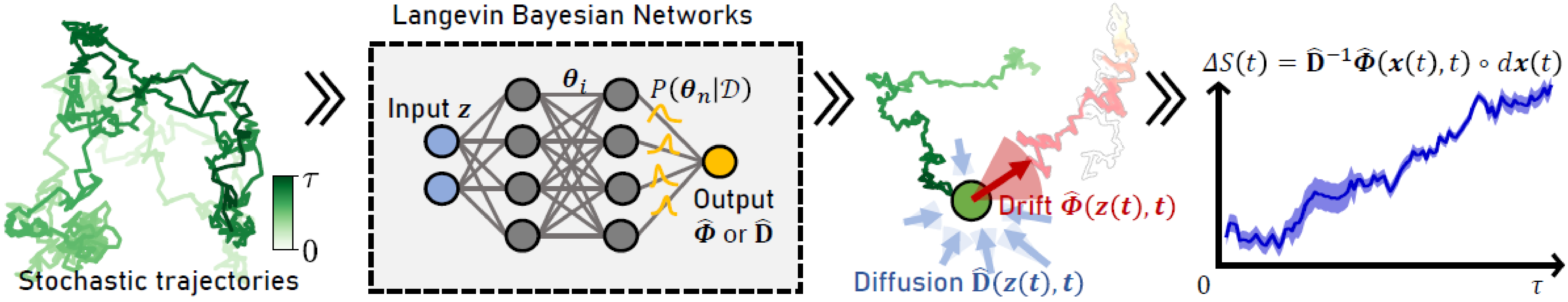
| Can you trust the prediction of an inference model?



How sure are you,,,?

Method

| Design the *Langevin Bayesian Networks* (LBN)



Accurate Inference of Langevin equation

& Providing *the prediction uncertainty*

Introduction

| Description of Stochastic process

Overdamped Langevin equation

$$\dot{x}(t) = \Phi(x,t) + \sqrt{2D(x,t)}\xi(t)$$

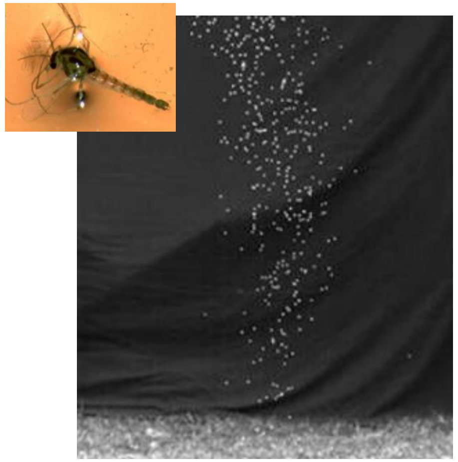
- ✓ *State variable: Position $x(t)$*
- ✓ *Molecular-scale*

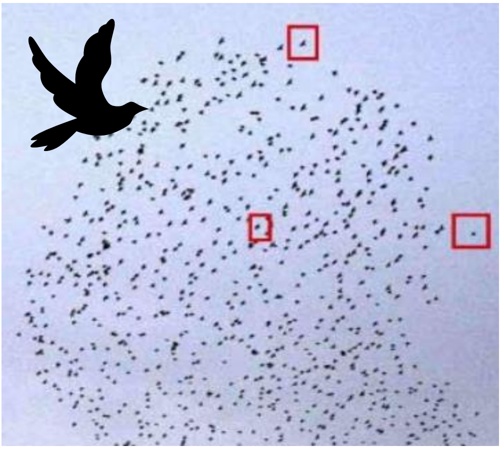
Our topic!

Underdamped Langevin equation

$$\dot{x}(t) = v(t)$$
$$\dot{v}(t) = \Phi(x,v,t) + \sqrt{2D(x,v,t)}\xi(t)$$

- ✓ *State variable: Position $x(t)$, Velocity $v(t)$*
- ✓ *Larger scales*





Result

| Tested Stochastic Systems

	System	Drift field $\boldsymbol{\Phi}$ and Diffusion matrix $\mathbf{D}$
Synthetic	(OLE) Nonlinear force field	$\Phi_\mu(x) = F_\mu(x) = -\sum_\nu A_{\mu\nu}x_\nu + \alpha x_\mu e^{x_\mu^2}$ $D_{\mu\nu} = T\delta_{\mu\nu} - \sqrt{T}\delta_{\mu,\nu+1} + \sqrt{T}\delta_{\mu,\nu-1}$
	(OLE) Inhomogeneous diffusion matrix	$F_\mu(x) = -\sum_\nu A_{\mu\nu}x_\nu$, $\Phi_\mu(x) = -\sum_\nu A_{\mu\nu}x_\nu - \alpha T x_\mu e^{-x_\mu^2/2}$ $D_{\mu\nu}(x) = T\left(1 + \alpha e^{-x_\mu^2/2}\right)\delta_{\mu\nu}$
Challenge	(OLE) Stochastic HH model	*This margin is too narrow to contain it…*
Synthetic	(ULE) Nonlinear force field & Inhomogeneous diffusion matrix	$\Phi_\mu(x,v) = k\left(1 - x_\mu^2\right)v_\mu - x_\mu$ $D_{\mu\nu}(x) = T\delta_{\mu\nu}$ *or* $D_{\mu\nu}(x) = \left(T_0 + T_x x_\mu^2 + T_v v_\mu^2\right)\delta_{\mu\nu}$
Challenge	(ULE) Brownian Carnot engine (non-stationary)	*This margin is too narrow to contain it…*

Refer to our paper in arXiv for the overdamped case ☺

Result

| (OLE) Stochastic Hodgkin-Huxley neuron model

- *The Hodgkin-Huxley model* describes the dynamics of action potentials in neurons and has extremely complicated drift fields... $(x_1 \equiv V,\ x_2 \equiv n, x_3 \equiv m,\ x_4 \equiv h)$.

$$\dot{x}_1(t) = C_m\left(-g_K x_2^4(x_1 - E_K) - g_{Na} x_3^3 x_4 (x_1 - E_{Na}) - g_L(x_1 - E_L)\right) + I_{ext}$$

$$\dot{x}_i(t) = \alpha_i(x_1)(1 - x_i) - \beta_i(x_1)x_i + T\xi_i(t) \quad (i = 2, 3, 4)$$

where

$$\alpha_2(x_1) = 0.01(10 - x_1)/(\exp[-(x_1 - 10)/10] - 1)$$

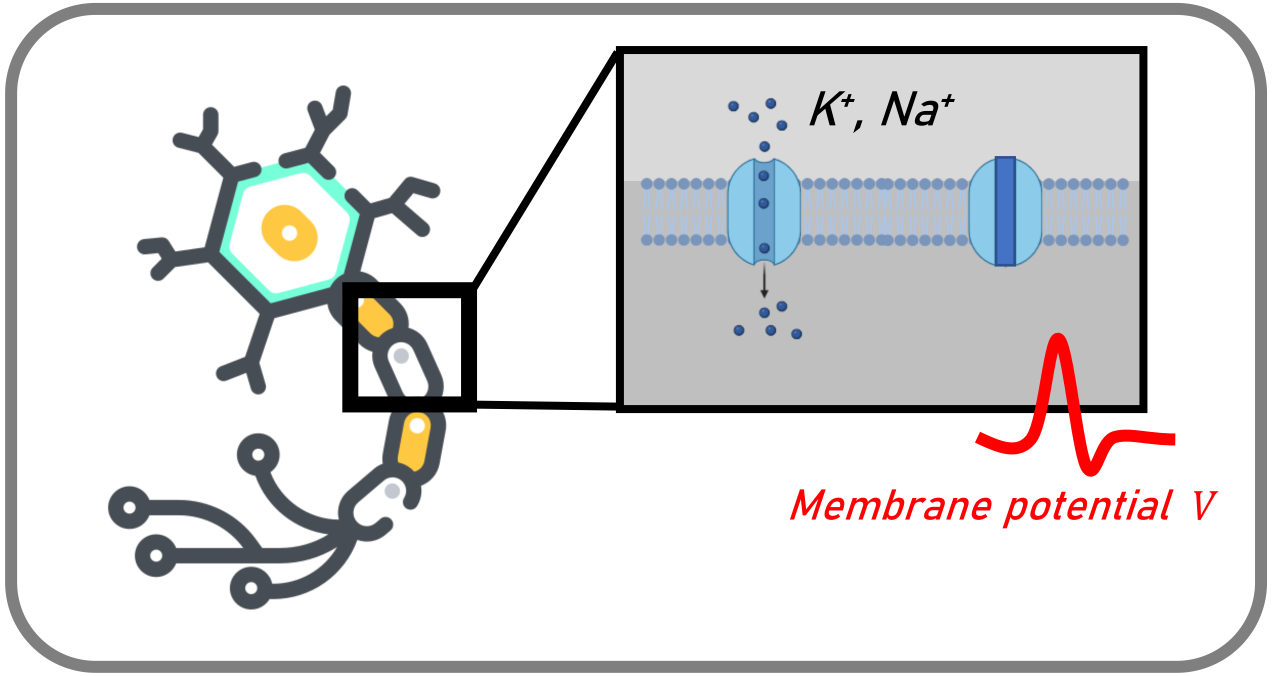
$$\beta_2(x_1) = 0.125 \exp[-x_1/80]$$

$$\alpha_3(x_1) = 0.1(25 - x_1)/(\exp[-(x_1 - 25)/10] - 1)$$

$$\beta_3(x_1) = 4 \exp[-x_1/18]$$

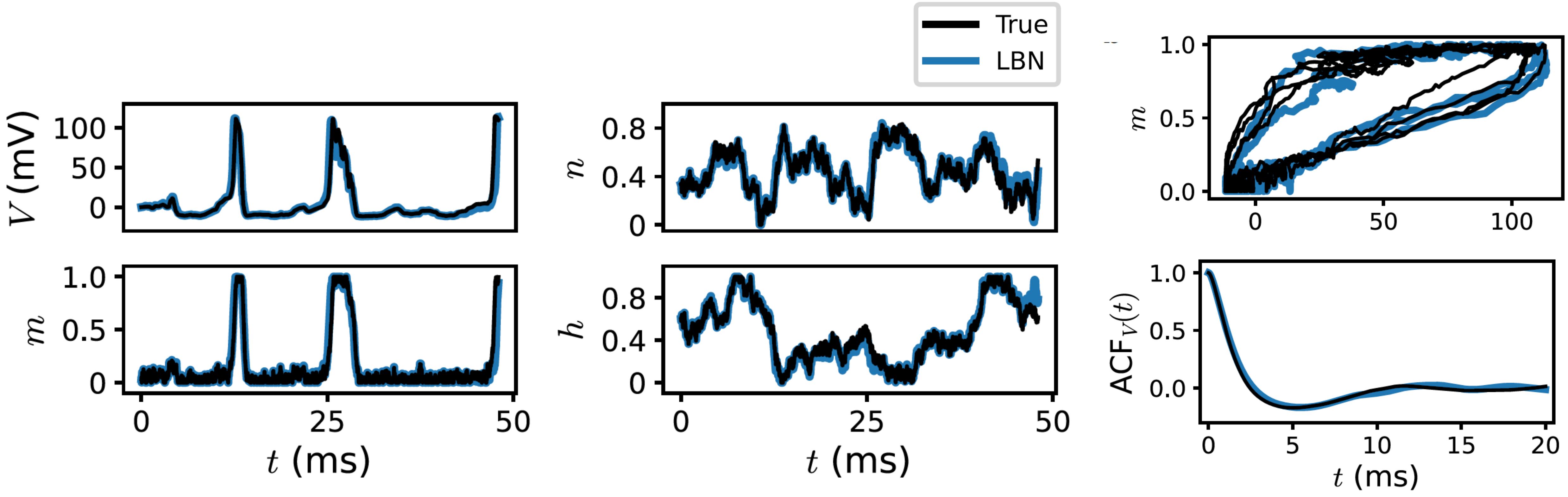
$$\alpha_4(x_1) = 0.07 \exp[-x_1/20]$$

$$\beta_4(x_1) = 1/(\exp[-(x_1 - 30)/10] + 1)$$



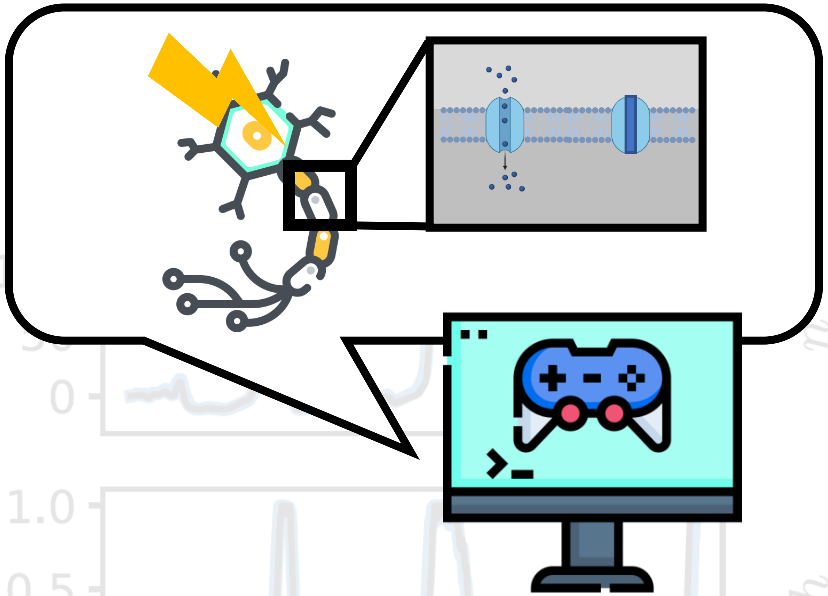
Result

| (OLE) Stochastic Hodgkin-Huxley neuron model



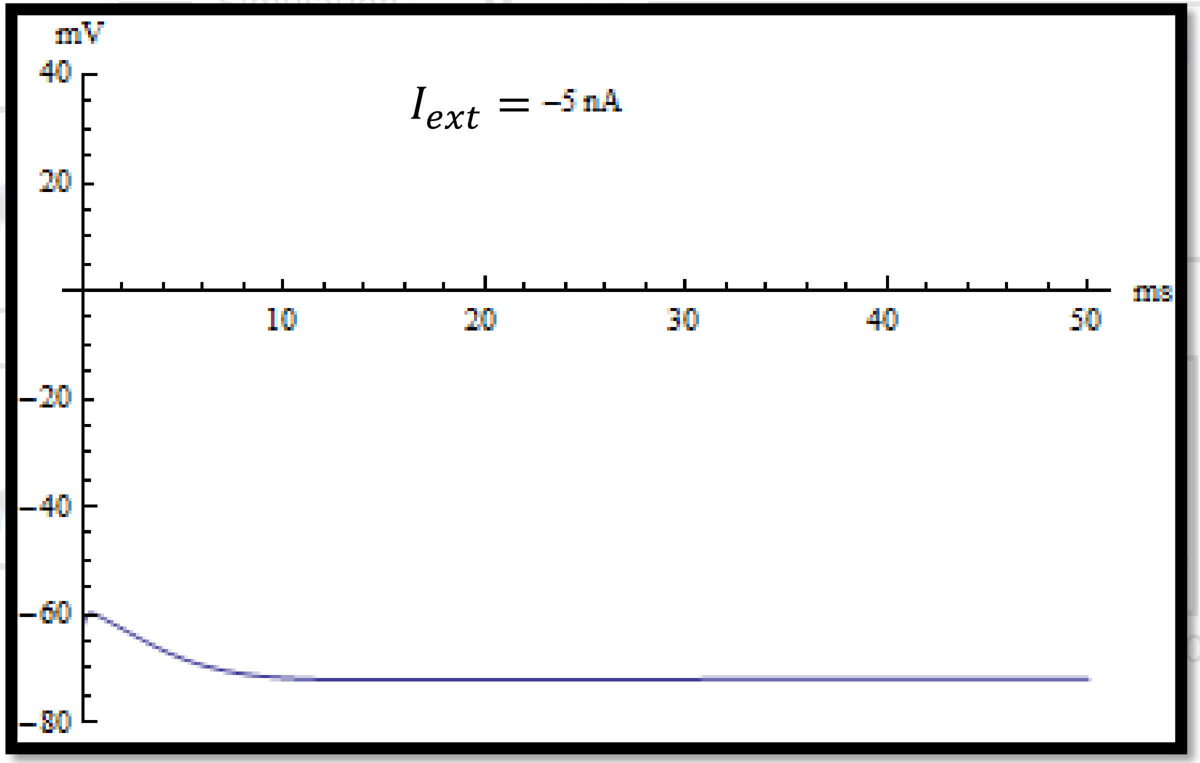
Result

| (OLE) Stochastic Hodgkin-Huxley neuron model



Can we emulate the neuron model

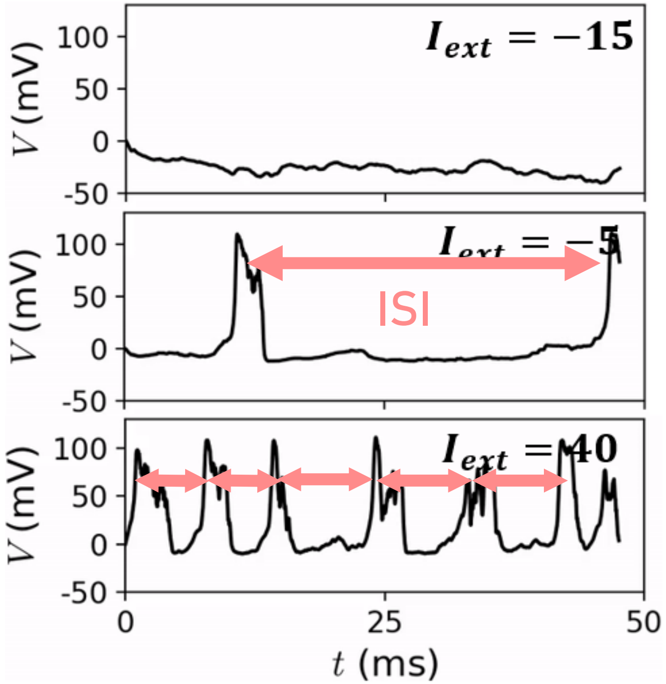
even beyond the training region…?

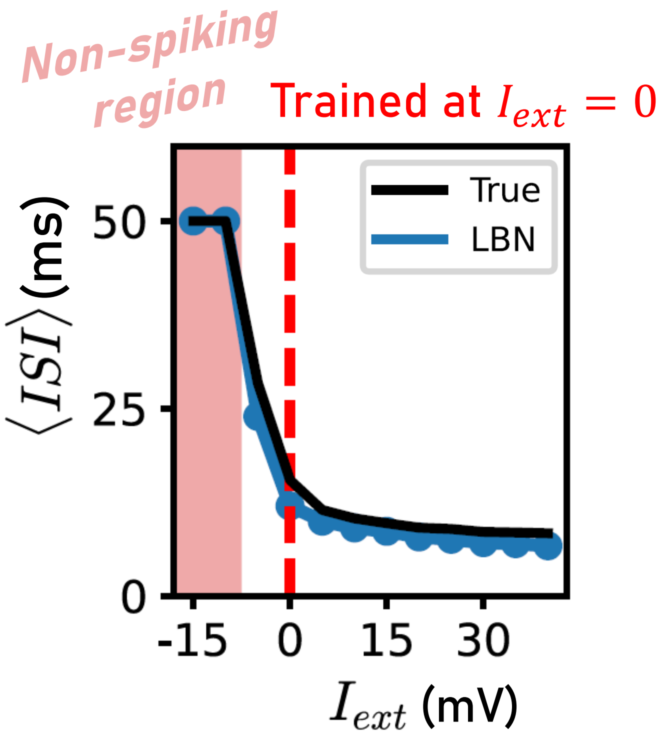


Result

| (OLE) Stochastic HH model, *beyond training range*

Generated from LBN…!





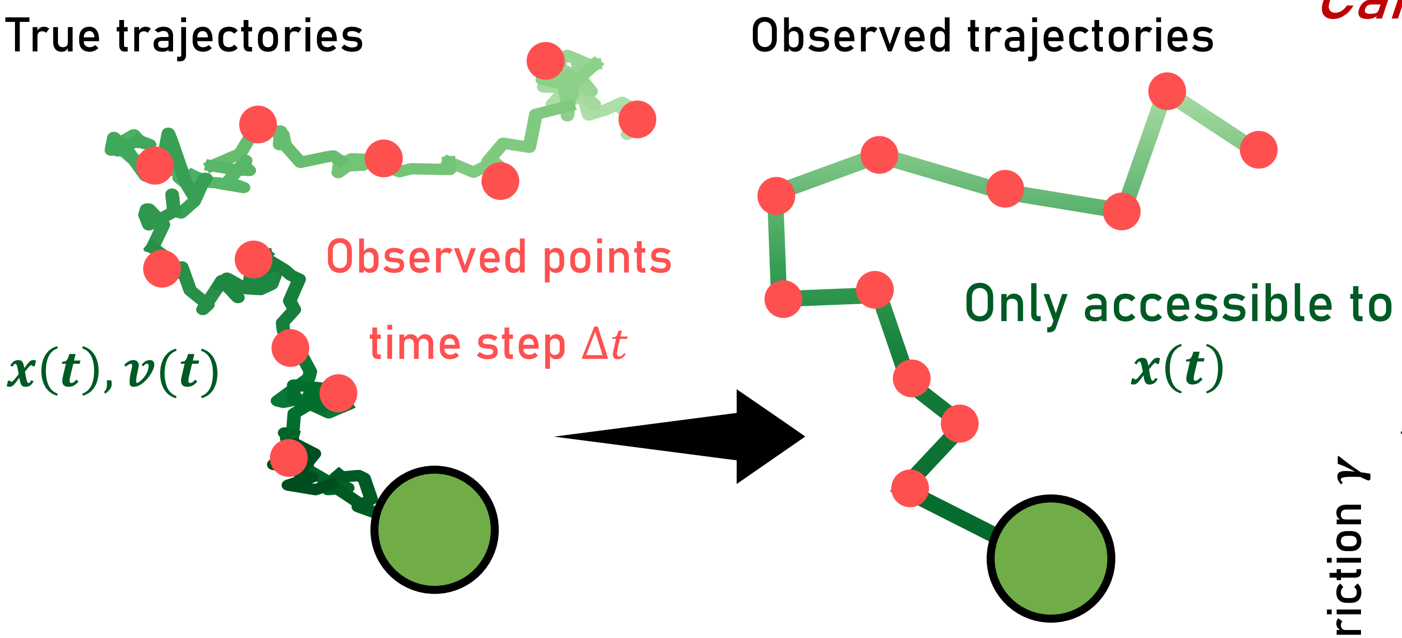
ISI = Inter-spike intervals

Method

| Derivation of Estimators for *Underdamped Systems*

- A Langevin equation (*Underdamped*)

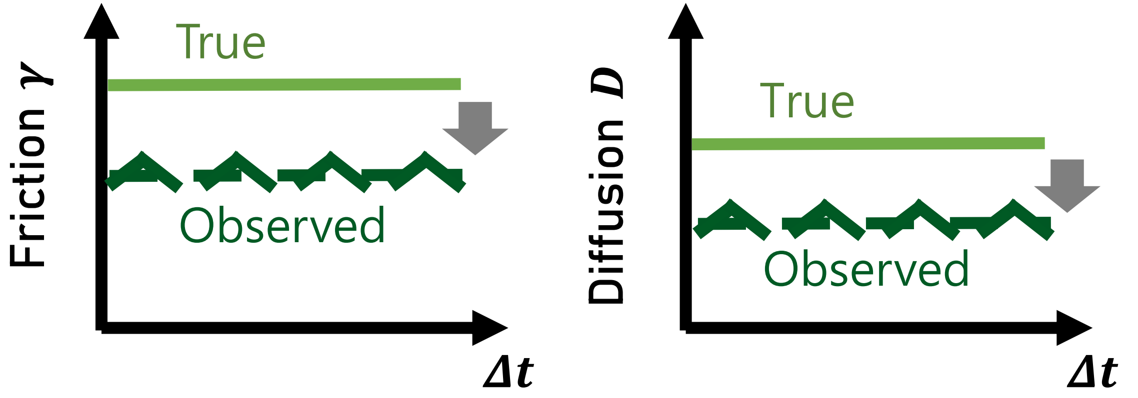
(Ito) $\Delta x(t) = v(t)\Delta t \qquad \Delta v(t) = \Phi(x,v,t)\Delta t + \sqrt{2D(x,v,t)}\Delta W(t)$



Cannot directly measure the velocity v

➡ **Estimated velocity**

$$\hat{\boldsymbol{v}}(\boldsymbol{t}) \equiv \frac{\boldsymbol{\Delta x(t)}}{\boldsymbol{\Delta t}}$$



Method

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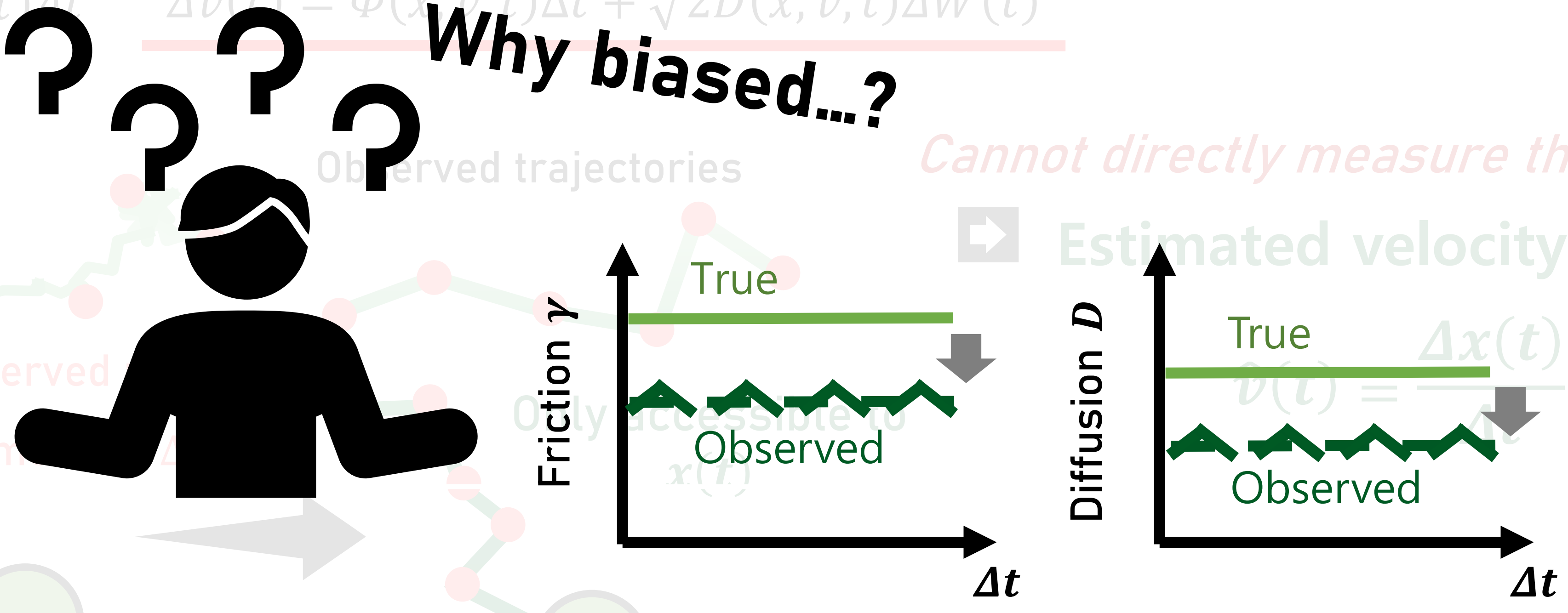


Method

| Discrepancy b/w True and Observed Dynamics

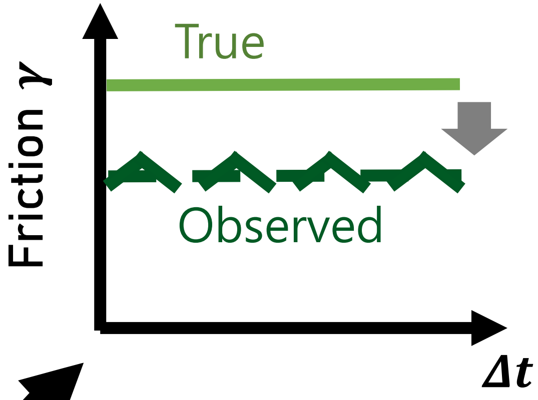
(Ito) $\Delta x(t) = v(t)\Delta t$

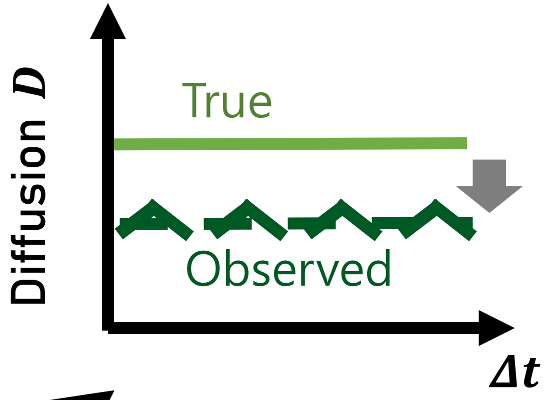
$\Delta v(t) = \boldsymbol{\Phi}(\boldsymbol{x},\boldsymbol{v},\boldsymbol{t})\Delta t + \sqrt{2\boldsymbol{D}(\boldsymbol{x},\boldsymbol{v},\boldsymbol{t})}\Delta W(t)$

$\boldsymbol{x}(\boldsymbol{t}), \hat{\boldsymbol{v}}(\boldsymbol{t})$

$\Delta x(t) = \hat{v}(t)\Delta t$

$\Delta \hat{v}(t) = \widehat{\boldsymbol{\Phi}}(\boldsymbol{x},\hat{\boldsymbol{v}},\boldsymbol{t})\Delta t + \sqrt{2\widehat{\boldsymbol{D}}(\boldsymbol{x},\hat{\boldsymbol{v}},\boldsymbol{t})\Delta \widehat{W}(t)}$





Observed drift field

$$\widehat{\boldsymbol{\Phi}}(\boldsymbol{x},\hat{\boldsymbol{v}},\boldsymbol{t}) = \boldsymbol{\Phi}(\boldsymbol{x},\boldsymbol{v},\boldsymbol{t}) - \frac{1}{3}\boldsymbol{D}(\boldsymbol{x},\boldsymbol{v},\boldsymbol{t})\partial_{\boldsymbol{v}} \ln \boldsymbol{P}(\boldsymbol{x},\boldsymbol{v},\boldsymbol{t})$$

and

Observed diffusion matrix

$$\widehat{\boldsymbol{D}}(\boldsymbol{x},\hat{\boldsymbol{v}},\boldsymbol{t}) = \frac{2}{3}\boldsymbol{D}(\boldsymbol{x},\boldsymbol{v},\boldsymbol{t})$$

It is necessary to develop *new unbiased estimators…!*

Method

| Discrepancy b/w True and Observed Dynamics

Observed drift field

$$\widehat{\boldsymbol{\Phi}}(\boldsymbol{x},\widehat{\boldsymbol{v}},\boldsymbol{t}) = \boldsymbol{\Phi}(\boldsymbol{x},\boldsymbol{v},\boldsymbol{t}) - \frac{1}{3}\boldsymbol{D}(\boldsymbol{x},\boldsymbol{v},\boldsymbol{t})\boldsymbol{\partial}_{\boldsymbol{v}} \ln \boldsymbol{P}(\boldsymbol{x},\boldsymbol{v},\boldsymbol{t})$$

and

Observed diffusion matrix

$$\widehat{\boldsymbol{D}}(\boldsymbol{x},\widehat{\boldsymbol{v}},\boldsymbol{t}) = \frac{2}{3}\boldsymbol{D}(\boldsymbol{x},\boldsymbol{v},\boldsymbol{t})$$

Example] *1D Harmonic potential*

True
$$\begin{cases} \dot{x}(t) = v(t) \\ \dot{v}(t) = -\gamma v(t) - kx(t) + \sqrt{2D}\xi(t) \end{cases}$$

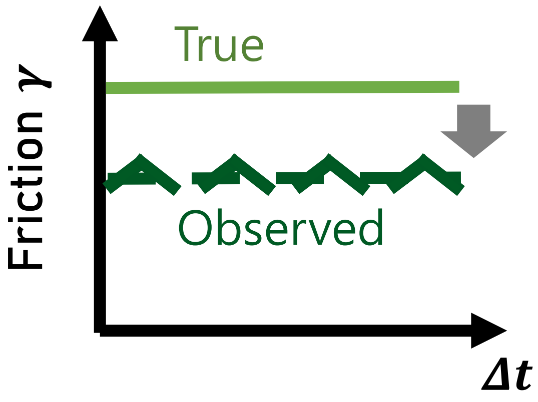
Boltzmann dist.

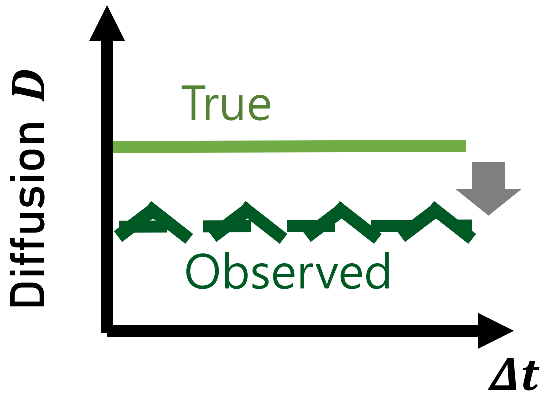
$$P_{eq}(x,v) \propto \exp\left[-\frac{1}{T}\left(\frac{1}{2}v^2 + \frac{1}{2}kx^2\right)\right]$$

$= E$ (energy)

$$-\frac{1}{3}\boldsymbol{D}(\boldsymbol{x},\boldsymbol{v},\boldsymbol{t})\boldsymbol{\partial}_{\boldsymbol{v}} \ln \boldsymbol{P}(\boldsymbol{x},\boldsymbol{v},\boldsymbol{t}) = \frac{1}{3}\boldsymbol{\gamma}$$

Observed
$$\begin{cases} \dot{x}(t) = v(t) \\ \dot{\hat{v}}(t) = -\frac{2}{3}\gamma\hat{v}(t) - kx(t) + \sqrt{\frac{4D}{3}}\xi(t) \end{cases}$$





Method

| Discrepancy b/w True and Observed Dynamics

(Ito) $\Delta x(t) = v(t)\Delta t$

$$\Delta v(t) = \boldsymbol{\Phi}(\boldsymbol{x}, \boldsymbol{v}, \boldsymbol{t})\Delta t + \sqrt{2\boldsymbol{D}(\boldsymbol{x}, \boldsymbol{v}, \boldsymbol{t})}\Delta W(t)$$

$\boldsymbol{x(t)}, \boldsymbol{\hat{v}(t)}$

$$\Delta x(t) = \hat{v}(t)\Delta t$$

$$\Delta \hat{v}(t) = \widehat{\boldsymbol{\Phi}}(\boldsymbol{x}, \hat{\boldsymbol{v}}, \boldsymbol{t})\Delta t + \sqrt{2\widehat{\boldsymbol{D}}(\boldsymbol{x}, \hat{\boldsymbol{v}}, \boldsymbol{t})\Delta \widehat{W}(t)}$$

Observed drift field

$$\widehat{\boldsymbol{\Phi}}(\boldsymbol{x}, \hat{\boldsymbol{v}}, \boldsymbol{t}) = \boldsymbol{\Phi}(\boldsymbol{x}, \boldsymbol{v}, \boldsymbol{t}) - \frac{1}{3}\boldsymbol{D}(\boldsymbol{x}, \boldsymbol{v}, \boldsymbol{t})\boldsymbol{\partial_v} \ln \boldsymbol{P}(\boldsymbol{x}, \boldsymbol{v}, \boldsymbol{t})$$

and

Observed diffusion matrix

$$\widehat{\boldsymbol{D}}(\boldsymbol{x}, \hat{\boldsymbol{v}}, \boldsymbol{t}) = \frac{2}{3}\boldsymbol{D}(\boldsymbol{x}, \boldsymbol{v}, \boldsymbol{t})$$

Diffusion estimator

$$\boldsymbol{D}(x, v, t) = \frac{3}{2}\left\langle \frac{\Delta\hat{v}(t)\Delta\hat{v}(t)^{\mathrm{T}}}{2\Delta t} \right\rangle_{\boldsymbol{x}(t),\hat{v}(t)}$$

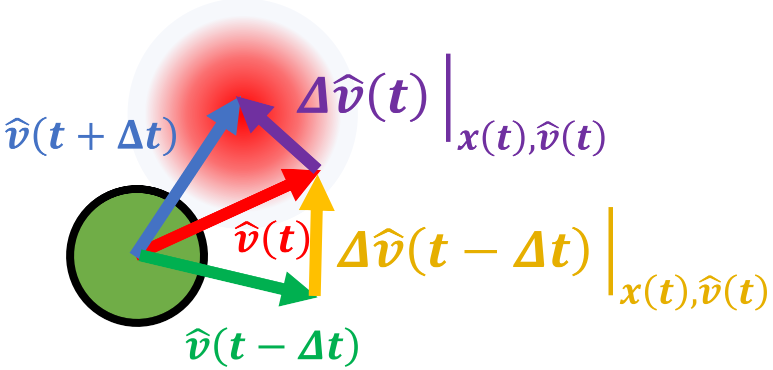
Method

| Reconstruct underlying Langevin dynamics

- Observed Langevin equation

The correction arises from random force

$$\Delta x(t) = \hat{v}(t)\Delta t\,, \quad \Delta\hat{v}(t) = \Phi(x,v,t)\Delta t - \underline{\tfrac{1}{3}D(x,v,t)\partial_v \ln P(x,v,t)\,\Delta t} + \sqrt{\tfrac{4}{3}D(x,v,t)}\Delta\widehat{W}(t)$$



$$\langle\Delta\hat{v}(t)\rangle_{x(t),\hat{v}(t)} = \left[\Phi(x,v,t) - \tfrac{1}{3}D(x,v,t)\partial_v \ln P(x,v,t)\right]\Delta t$$

$$\langle\Delta\hat{v}(t-\Delta t)\rangle_{x(t),\hat{v}(t)} = \left[\Phi(x,v,t) - \tfrac{5}{3}D(x,v,t)\partial_v \ln P(x,v,t)\right]\Delta t$$

Much affected by random force

$$\Rightarrow \quad D(x,v,t)\partial_v \ln P(x,v,t) = \frac{3}{4}\left[\left\langle\frac{\Delta\hat{v}(t)}{\Delta t}\right\rangle_{x(t),\hat{v}(t)} - \left\langle\frac{\Delta\hat{v}(t-\Delta t)}{\Delta t}\right\rangle_{x(t),\hat{v}(t)}\right]$$

Method

| Derivation of Estimators for *Underdamped Systems*

Drift estimator

Correction

$$\boldsymbol{\Phi}(x,v,t) = \boldsymbol{\Psi}_f(x,v,t) + \frac{1}{4}[\boldsymbol{\Psi}_f(x,v,t) - \boldsymbol{\Psi}_b(x,v,t)]$$

and

Diffusion estimator

$$\boldsymbol{D}(x,v,t) = \frac{3}{2}\left\langle \frac{\Delta\hat{v}(t)\Delta\hat{v}(t)^{\mathrm{T}}}{2\Delta t} \right\rangle_{x(t),\hat{v}(t)}$$

$$\Psi_f(x,v,t) = \left\langle \frac{\Delta\hat{v}(t)}{\Delta t} \right\rangle_{x(t),\hat{v}(t)} \qquad \Psi_b(x,v,t) = \left\langle \frac{\Delta\hat{v}(t-\Delta t)}{\Delta t} \right\rangle_{x(t),\hat{v}(t)}$$

Dataset $\mathcal{D}$

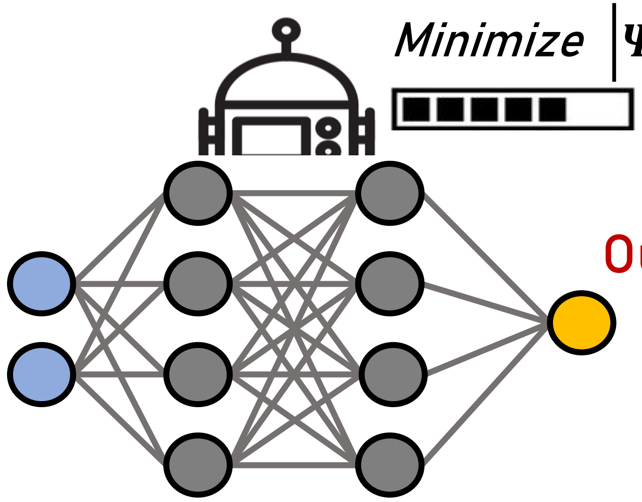
$\boldsymbol{\Psi}_{b,\theta}(\boldsymbol{x},\hat{\boldsymbol{v}},\boldsymbol{t})$

Input	$\boldsymbol{x}(\boldsymbol{t})$	-2.09	-2.13	$\cdots$	1.19	1.63
	$\hat{\boldsymbol{v}}(\boldsymbol{t})$	-0.46	0.074	$\cdots$	5.12	4.31
Label	$\frac{\Delta\hat{v}(t)}{\Delta t}$	0.54	0.11	$\ldots$	2.83	-0.81
Time t		0	Δt		$(L-3)\Delta t$	$(L-2)\Delta t$

Sampling

Minimize $\left|\boldsymbol{\Psi}_{f,\theta}(\boldsymbol{x},\boldsymbol{v},\boldsymbol{t}) - \frac{\Delta\hat{v}(t)}{\Delta t}\right|$

Input $\boldsymbol{x}(\boldsymbol{t}),\hat{\boldsymbol{v}}(\boldsymbol{t})$

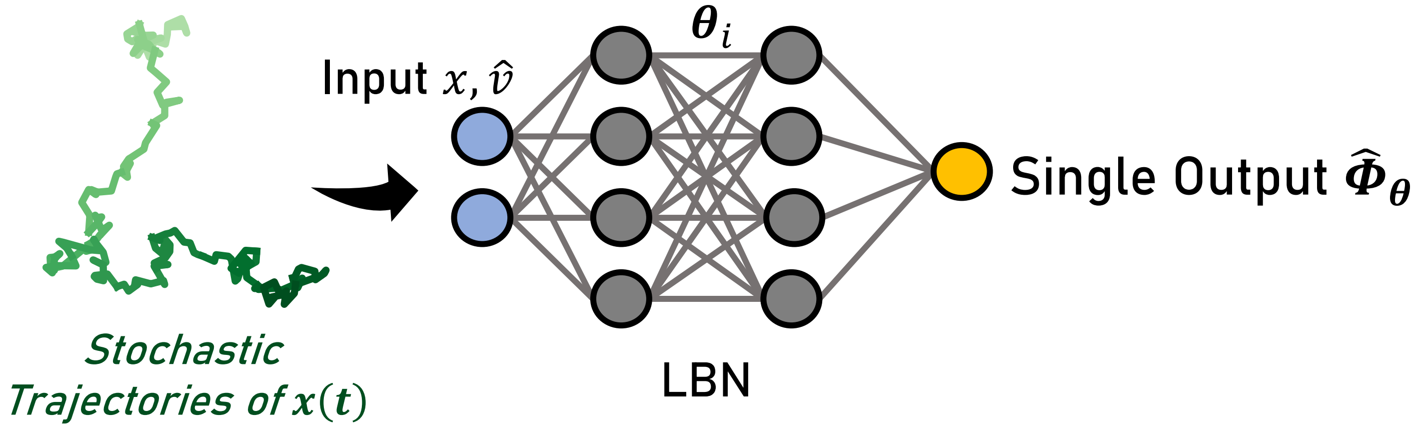


Output $\boldsymbol{\Psi}_{f,\theta}(\boldsymbol{x},\hat{\boldsymbol{v}},\boldsymbol{t})$

$\boldsymbol{\theta}$: network parameter

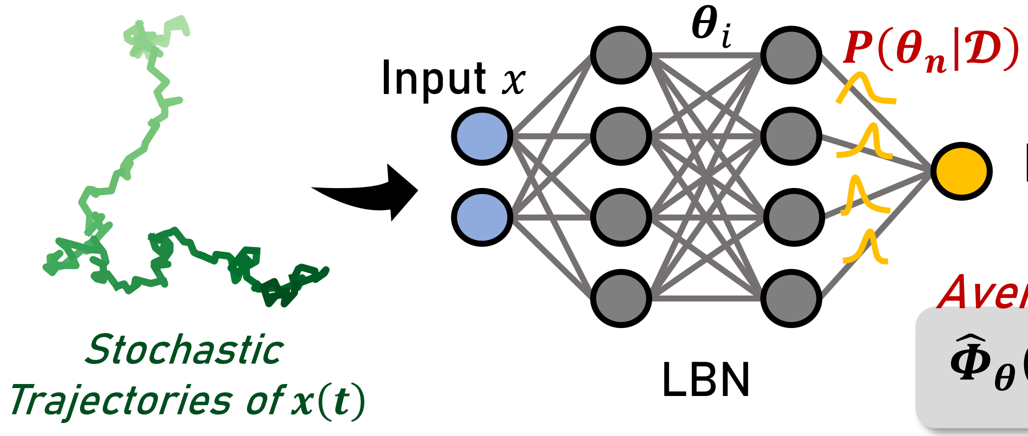
Method

| Network architecture & *Uncertainty*



Method

| Network architecture & *Uncertainty*



Ensemble of Outputs $\{\boldsymbol{\Phi}_{\theta^1}(\boldsymbol{x},\boldsymbol{t}), \boldsymbol{\Phi}_{\theta^2}(\boldsymbol{x},\boldsymbol{t}), \dots, \boldsymbol{\Phi}_{\theta^{N_\theta}}(\boldsymbol{x},\boldsymbol{t})\}$

Average prediction *Relative uncertainty*

$\widehat{\boldsymbol{\Phi}}_{\theta}(\boldsymbol{x},\boldsymbol{t}) \equiv \langle \boldsymbol{\Phi}_{\theta}(\boldsymbol{x},\boldsymbol{t}) \rangle_{\theta}$ and $\widehat{\boldsymbol{\Sigma}}_{\boldsymbol{\Phi}} \equiv \mathrm{Var}\big(\boldsymbol{\Phi}_{\theta}(\boldsymbol{x},\boldsymbol{t})\big) / \big\langle \boldsymbol{\Phi}_{\theta}(\boldsymbol{x},\boldsymbol{t})^2 \big\rangle_{\theta}$

Pointwise error

$$e_{\boldsymbol{\Phi}}^2(\boldsymbol{x},t) \equiv \frac{\langle [\boldsymbol{\Phi}(\boldsymbol{x},t) - \boldsymbol{\Phi}_{\theta}(\boldsymbol{x},t)]^2 \rangle_{\theta}}{\langle \boldsymbol{\Phi}_{\theta}^2(\boldsymbol{x},t) \rangle_{\theta}}$$

$$e_{\boldsymbol{\Phi}}^2(\boldsymbol{x},\boldsymbol{t}) = \widehat{\boldsymbol{\Sigma}}_{\boldsymbol{\Phi}}(\boldsymbol{x},\boldsymbol{t}) + \frac{\mathrm{Bias}^2\big(\Phi_{\theta}(x,t)\big)}{\langle \Phi_{\theta}^2(x,t) \rangle_{\theta}}$$

where $\mathrm{Bias}^2\big(\Phi_{\theta}(x,t)\big) \equiv \big[\Phi_{\theta}(x,t) - \widehat{\Phi}(x,t)\big]^2$

➡ $e_{\boldsymbol{\Phi}}^2(\boldsymbol{x},\boldsymbol{t}) \geq \widehat{\boldsymbol{\Sigma}}_{\boldsymbol{\Phi}}(\boldsymbol{x},\boldsymbol{t})$ *& Positive relation*

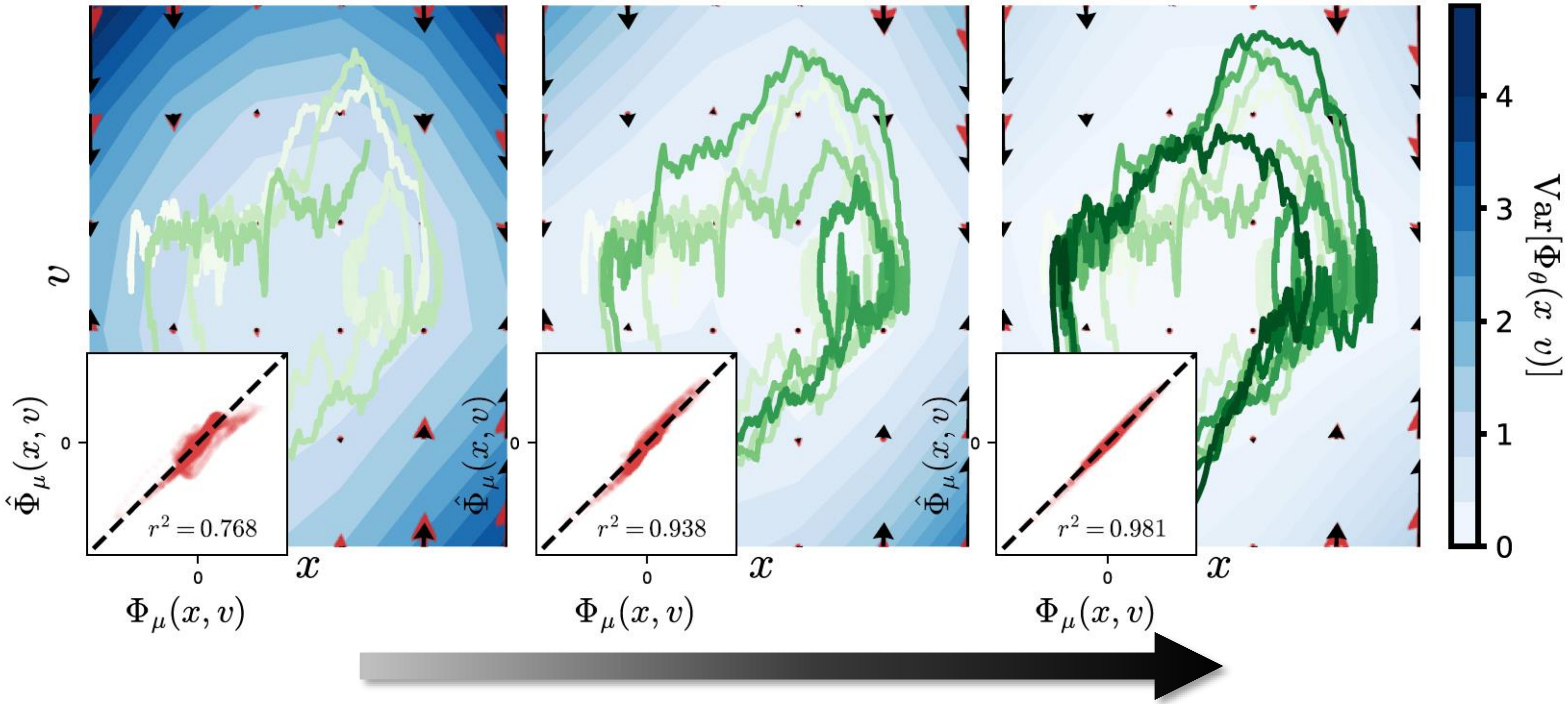
Uncertainty can serve as a proxy for errors

Result

| #1. (ULE) Nonlinear force field

- A stochastic Van der Pol oscillator : $\Phi_\mu(x, v) = k(1 - x_\mu^2)v_\mu - x_\mu$

Colormap = Uncertainties



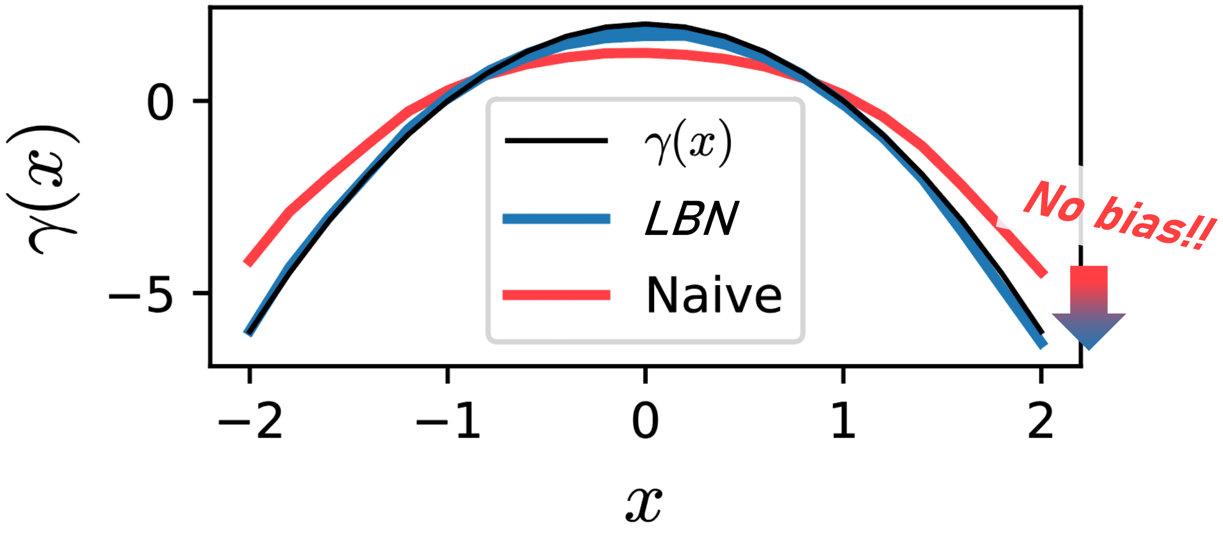
Increasing data points

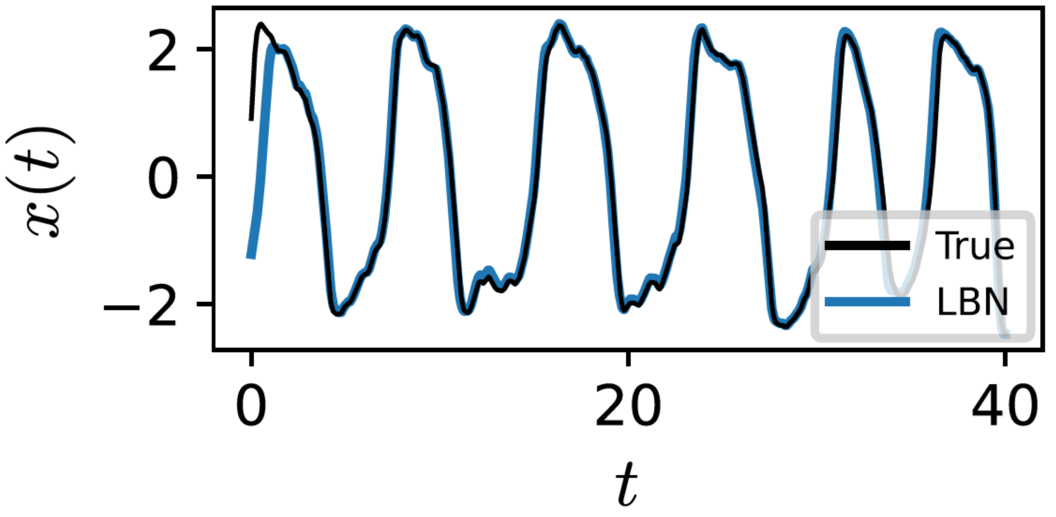
More accurate & Less uncertain

Result

| #1. (ULE) Nonlinear force field

- A stochastic Van der Pol oscillator : $\Phi_\mu(\boldsymbol{x}, \boldsymbol{v}) = \underbrace{\boldsymbol{k}(\boldsymbol{1} - \boldsymbol{x}_\mu^2)}_{= \boldsymbol{\gamma}(\boldsymbol{x})} v_\mu - x_\mu$





✓ *Inferring drift fields with no bias*

✓ *Predicting system evolution over time*

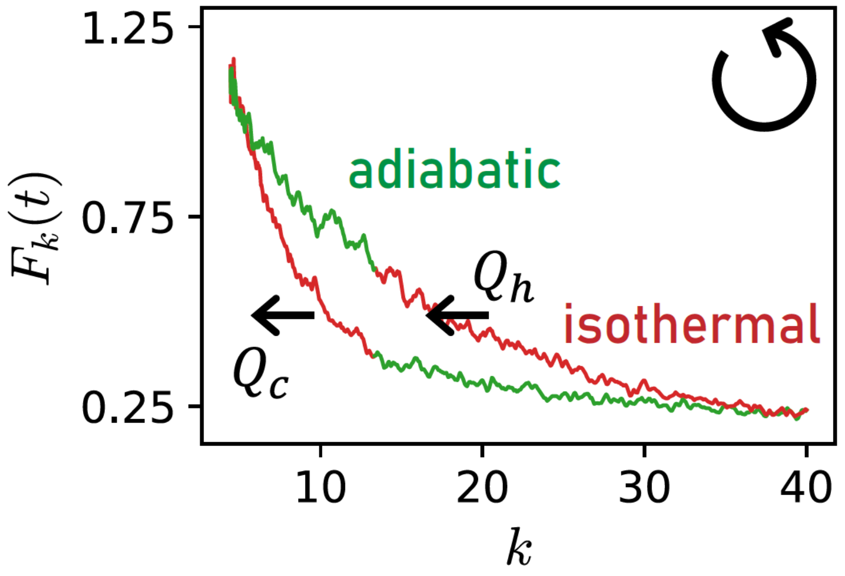
(with same random seed)

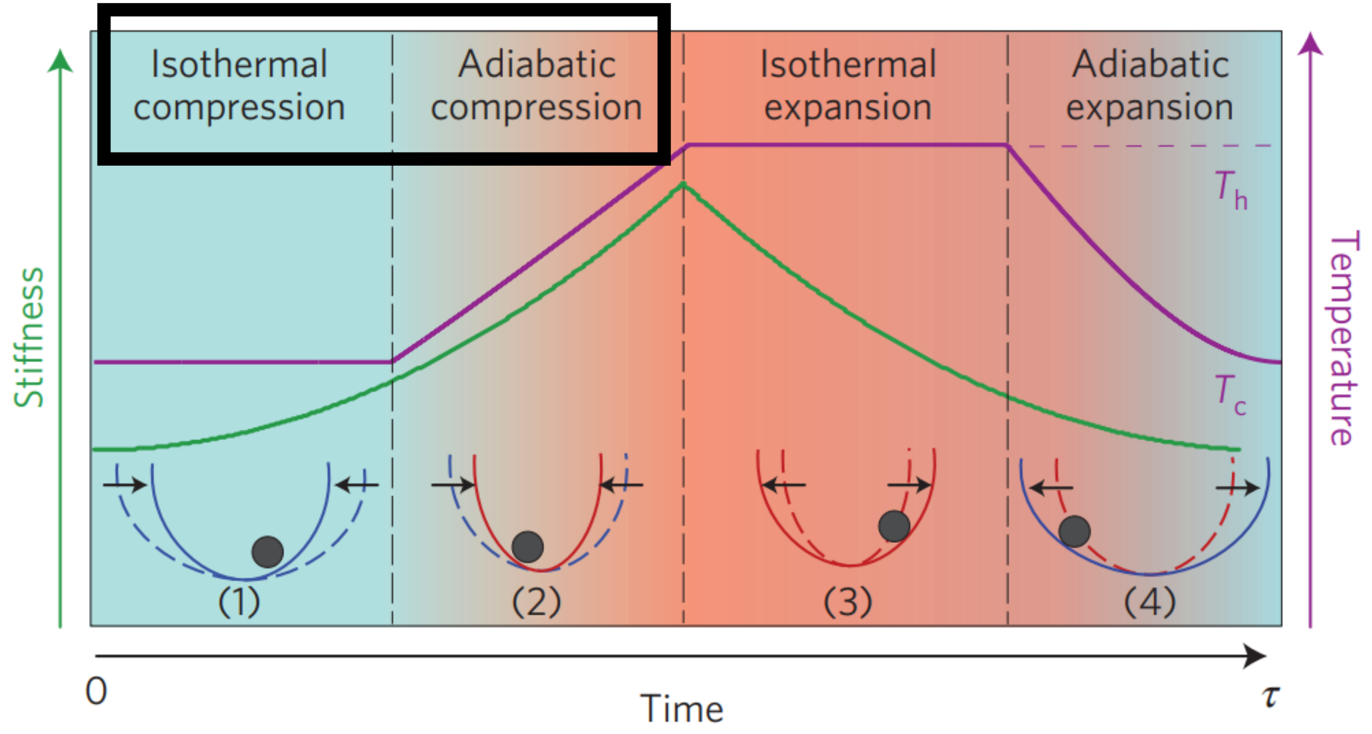
Result

| #2. (ULE) Brownian Carnot engine

I. A. Martinez et al., *Nat. Phys.* 12, 595 (2016)

- *The Brownian Carnot engine* is the experimental realization of a microscopic heat engine using optical tweezers, consisting of isothermal and adiabatic processes.





Result

| #2. (ULE) Brownian Carnot engine

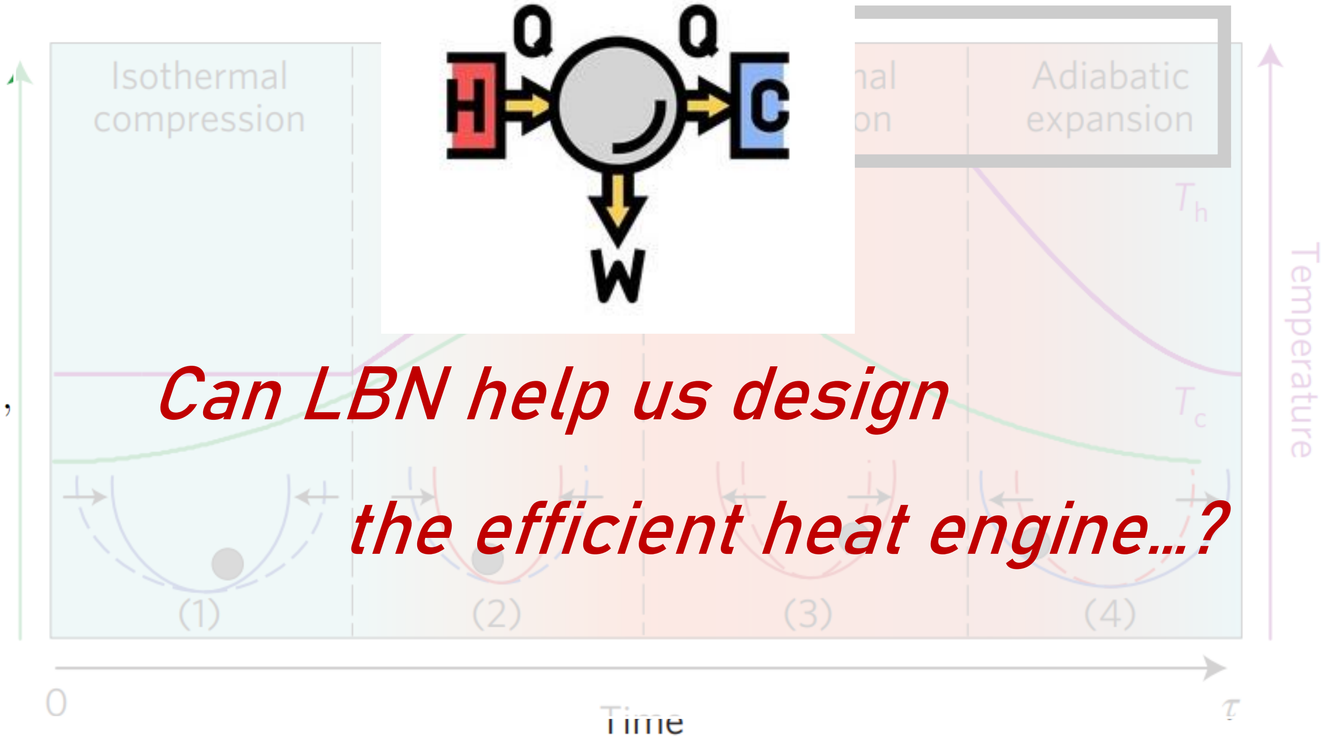
I. A. Martinez et al., *Nat. Phys.* 12, 595 (2016)

- *The Brownian Carnot engine* is the experimental realization of a microscopic heat engine using optical tweezers, consisting of isothermal and adiabatic processes.

$$\Phi(x, v, t) = -\gamma v(t) - k(t)x(t)$$

$$k(t) = k_m + k_s t^2 \qquad t \in [0, \tau/2],$$

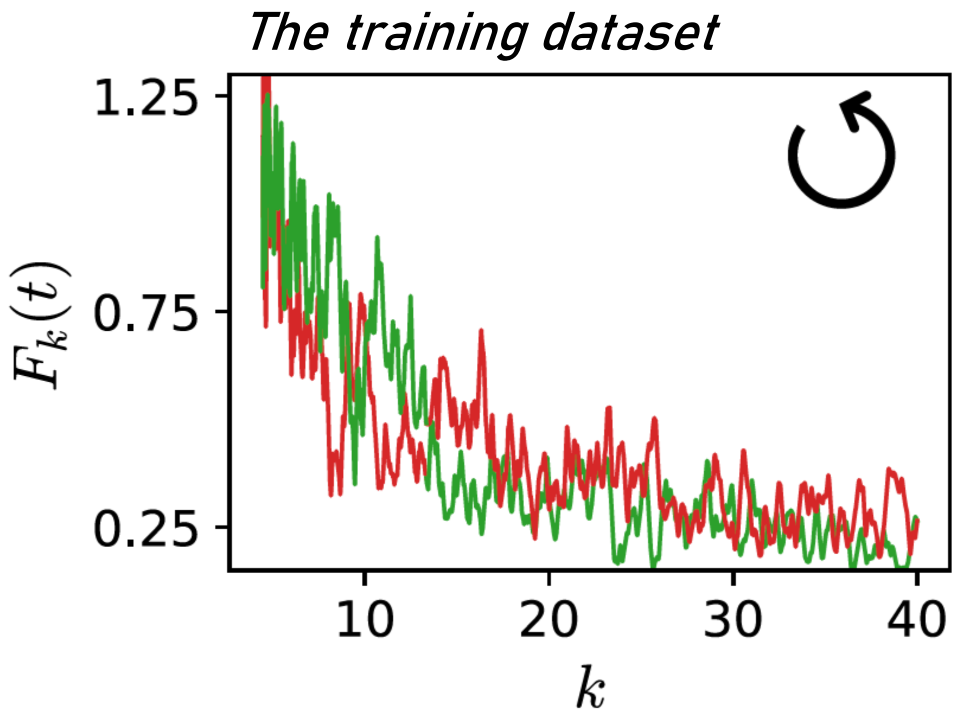
$$D(t) = \begin{cases} \gamma T_c & 0 \le t < \frac{1}{4}\tau_{cyc} \ \text{(isothermal)}, \\ \gamma T_c \left[k(t)/k_{qt}\right]^{1/2} & \frac{1}{4}\tau_{cyc} \le t < \frac{1}{2}\tau_{cyc} \ \text{(adiabatic)}, \\ \gamma T_h & \frac{1}{2}\tau_{cyc} \le t \le \frac{3}{4}\tau_{cyc} \ \text{(isothermal)}, \\ \gamma T_h \left[k(t)/k_{qt}\right]^{1/2} & \frac{3}{4}\tau_{cyc} \le t < \tau_{cyc} \ \text{(adiabatic)}, \end{cases}$$

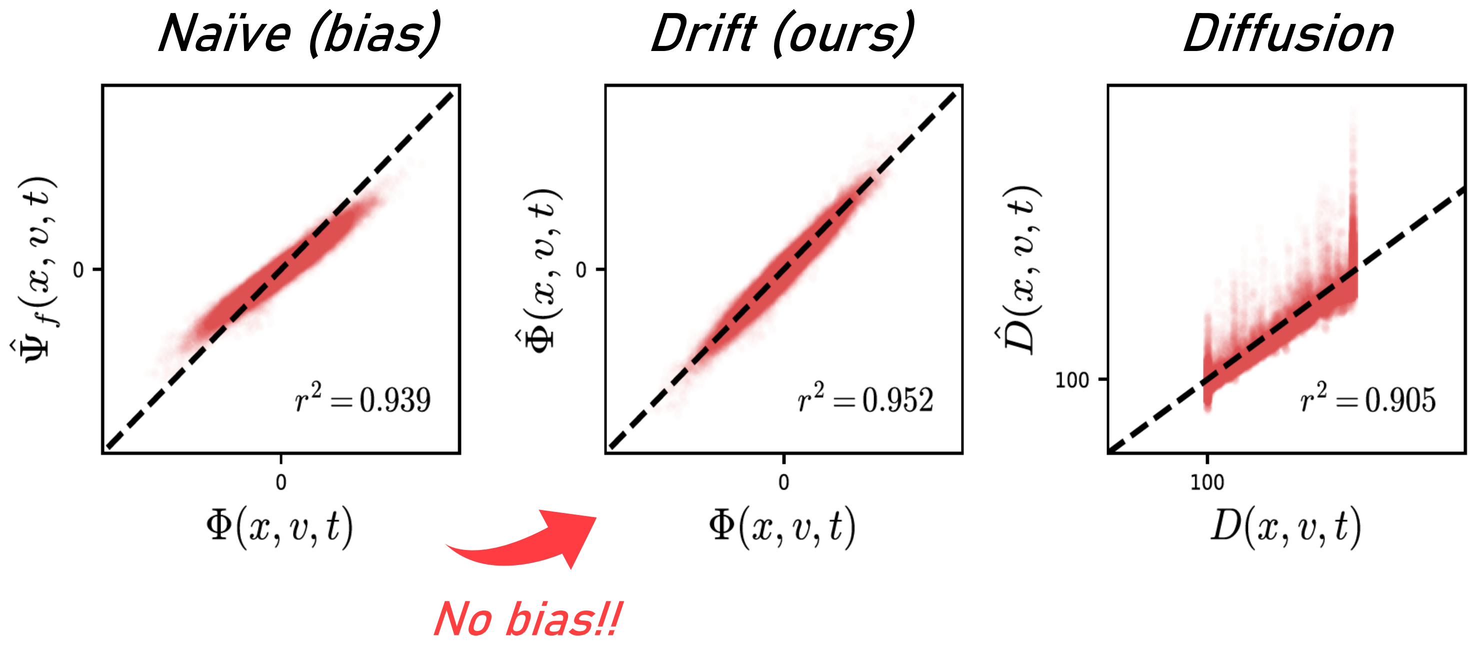


Result

| #2. (ULE) Brownian Carnot engine

I. A. Martinez et al., *Nat. Phys.* 12, 595 (2016)





Result

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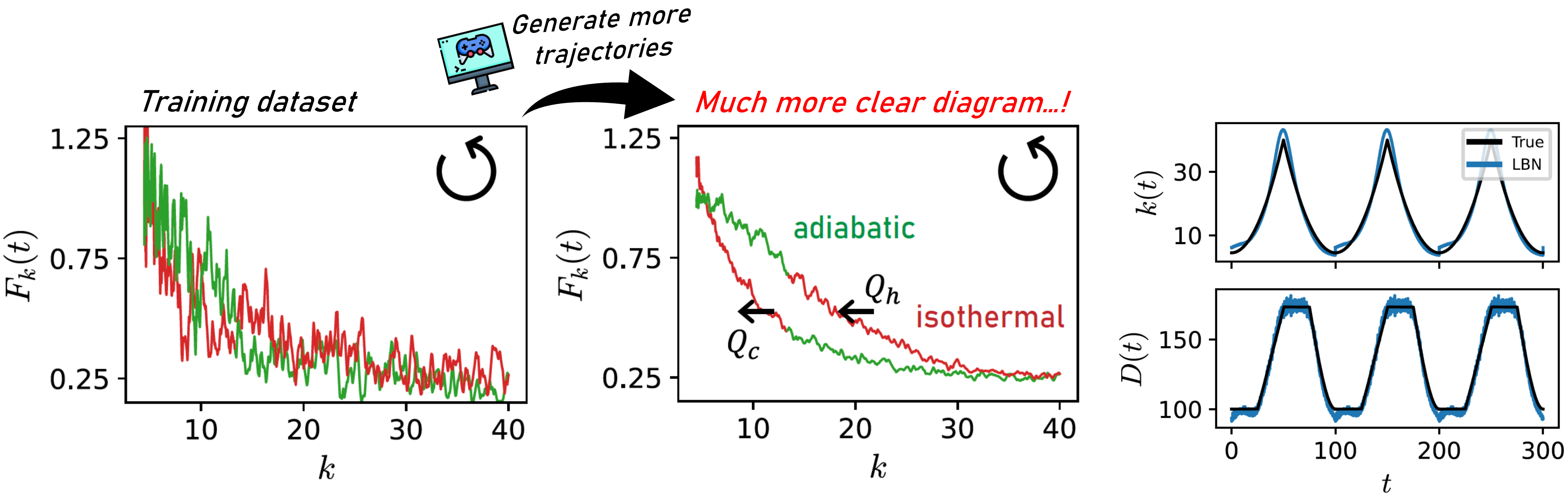
I. A. Martinez et al., *Nat. Phys.* 12, 595 (2016)

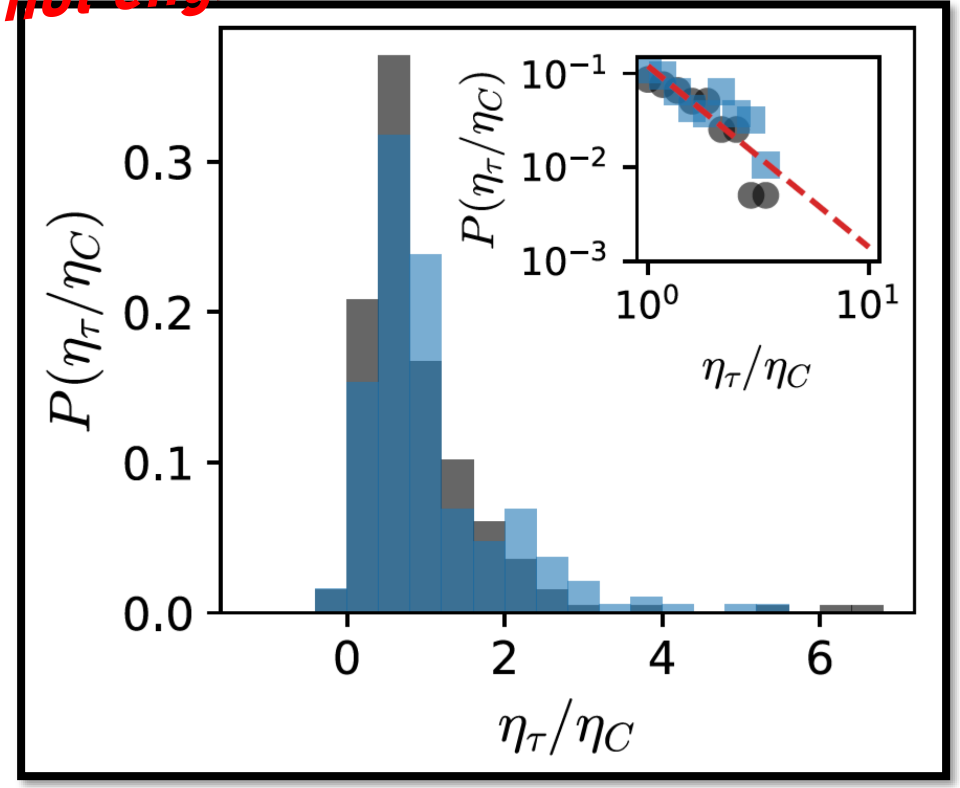


Result

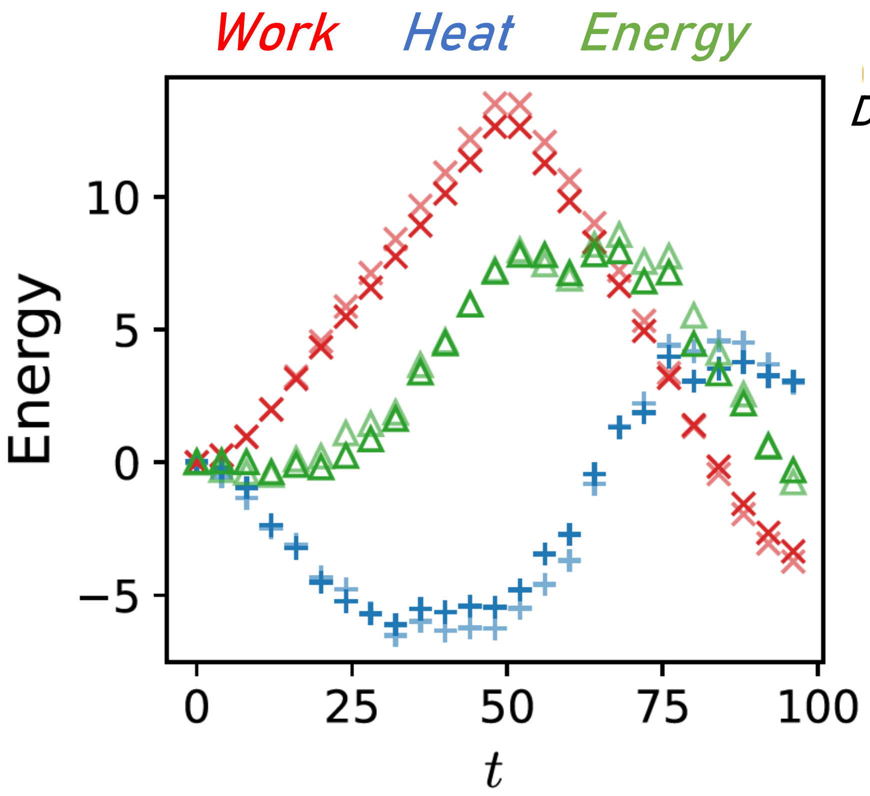
| #2. (ULE) Brownian Carnot engine

I. A. Martinez et al., *Nat. Phys.* 12, 595 (2016)

✓ ***Really works as the Carnot engine…!***



Engine efficiency η_τ, *Carnot efficiency* η_C

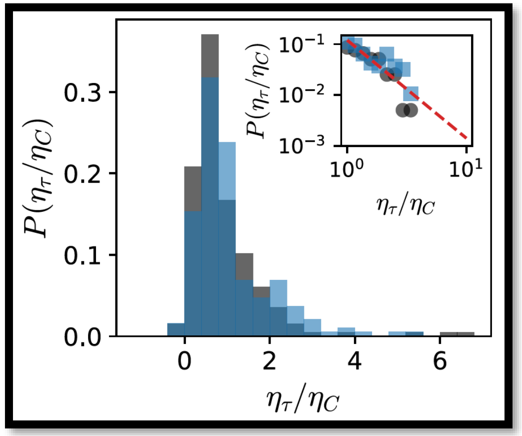


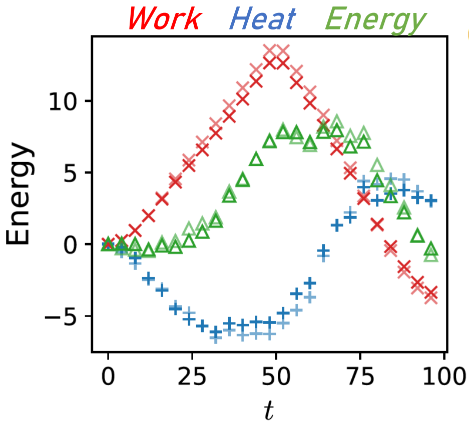
Darker - True

Result

| #2. (ULE) Brownian Carnot engine

I. A. Martinez et al., *Nat. Phys.* 12, 595 (2016)





✓ *Really works as the Carnot engine…!*

➡ *More powerful engine…?*

[Power $\mathcal{P} \equiv \langle -W/\tau_{cyc} \rangle$ *]*

Cycle duration

τ_{cyc}

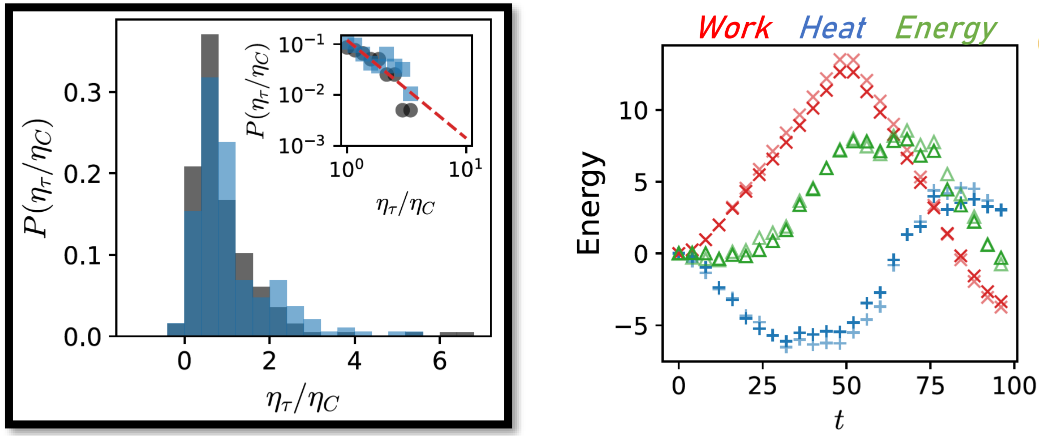
Efficiency

Power

Result

| #2. (ULE) Brownian Carnot engine

I. A. Martinez et al., *Nat. Phys.* 12, 595 (2016)

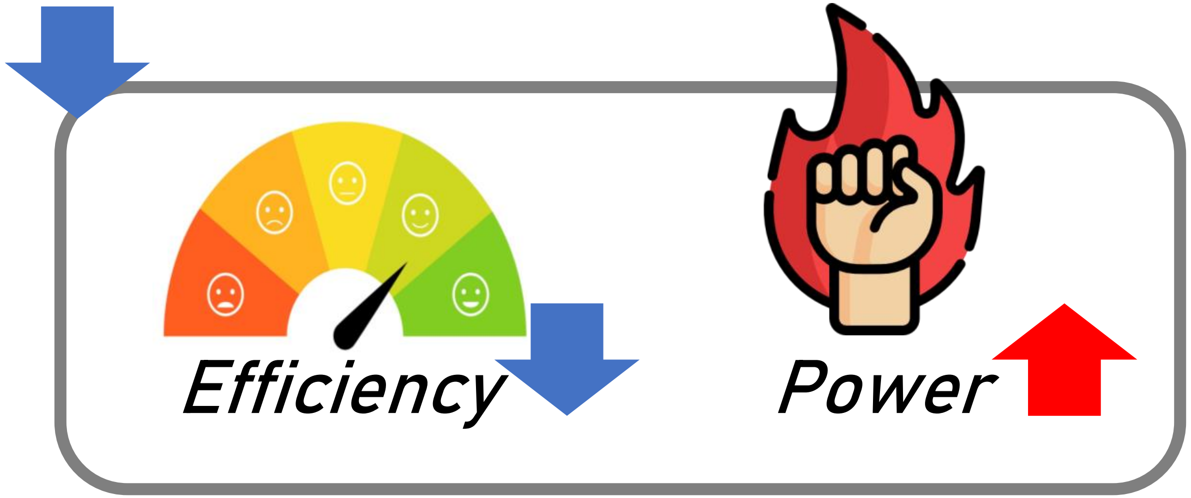


✓ *Really works as the Carnot engine…!*

➡ *More powerful engine…?*

$$[\text{Power } \mathcal{P} \equiv \langle -W/\tau_{cyc} \rangle]$$

Cycle duration τ_{cyc}



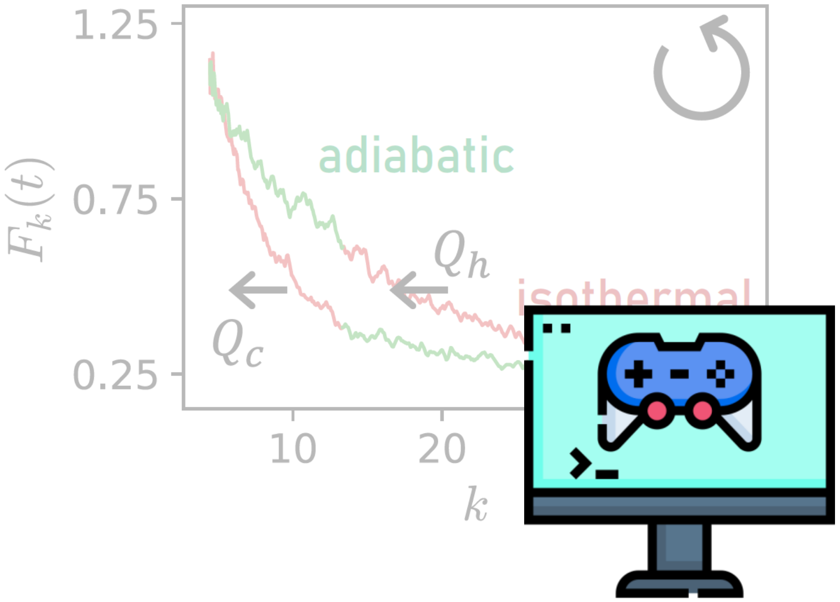
However, it takes too much time to experimentally find the optimal τ_{cyc}

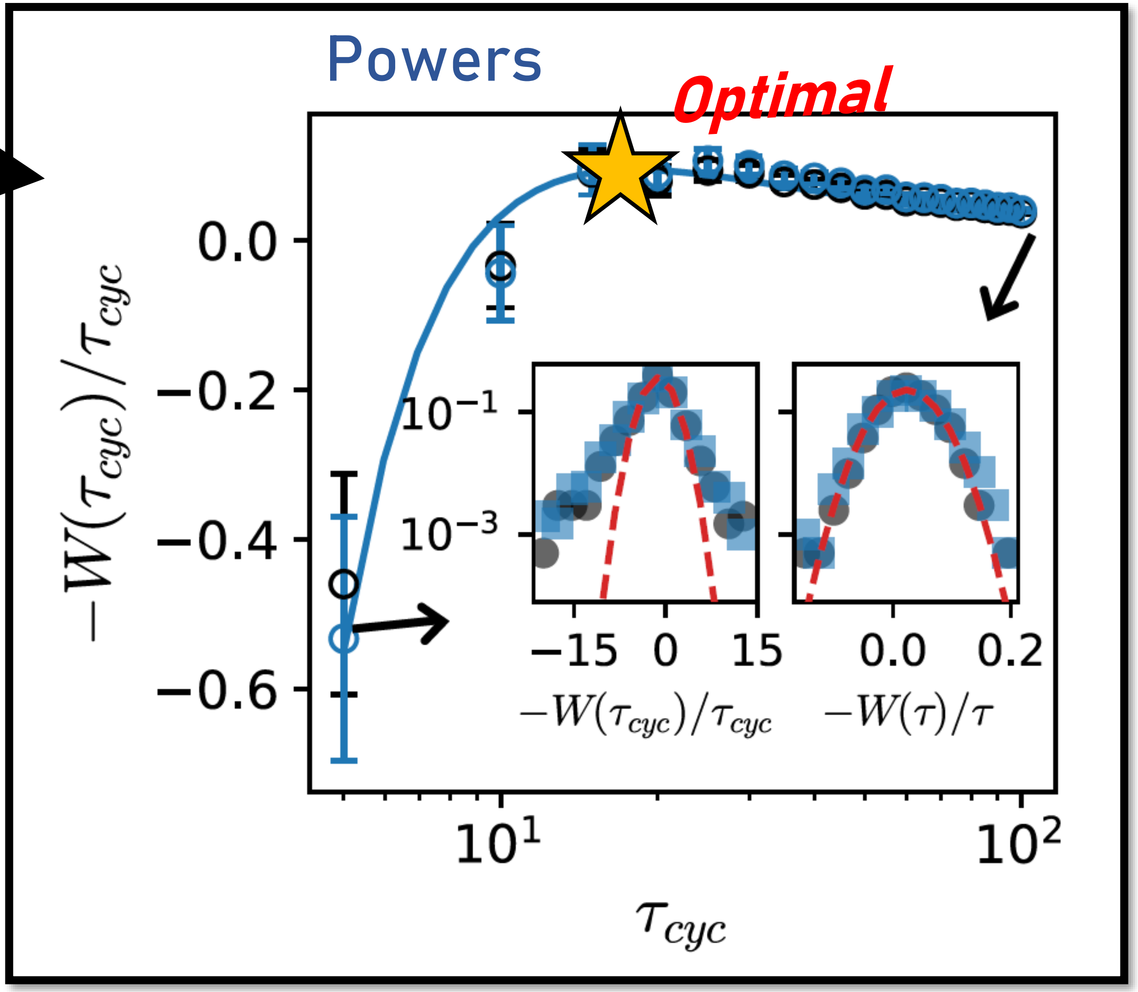
Optimal τ_{cyc}*…?*

Result

| #2. (ULE) Brownian Carnot engine

I. A. Martinez et al., *Nat. Phys.* 12, 595 (2016)





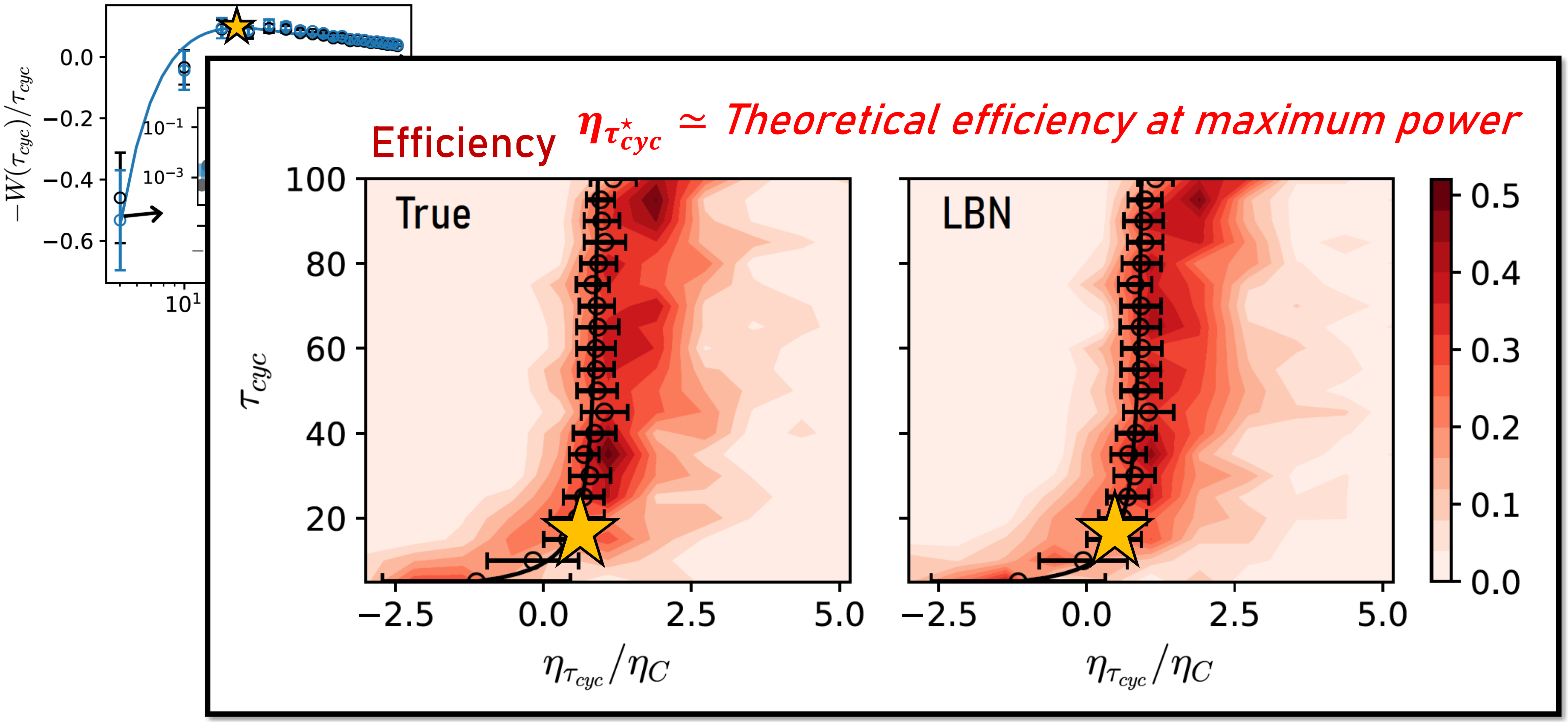
Emulate the Brownian Carnot engine

with different τ_{cyc}…!

Result

| #2. (ULE) Brownian Carnot engine

I. A. Martinez et al., *Nat. Phys.* 12, 595 (2016)



Conclusion

| Summary

- *Our general framework successfully learns Langevin dynamics from observed trajectories as well as provides the uncertainty of predictions.*

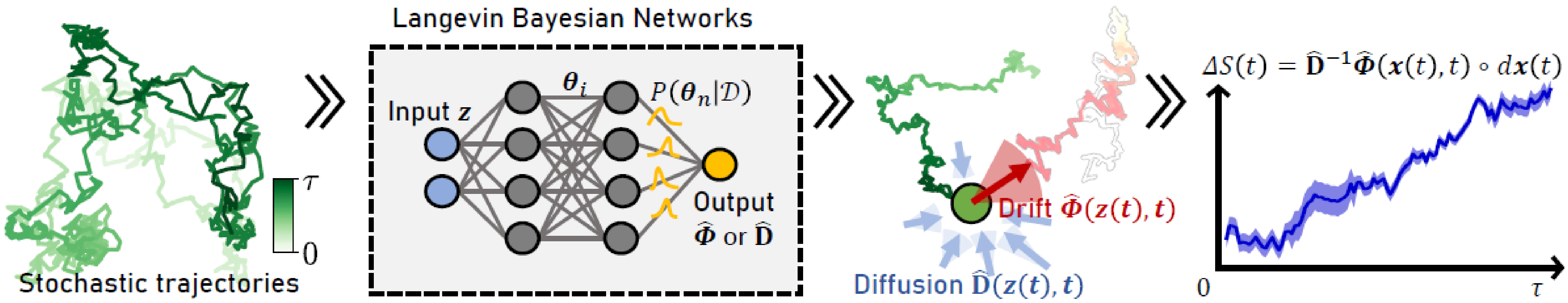
✓ (OLE) Nonlinear force field, ✓ (OLE) Inhomogeneous diffusion matrix,

✓ (OLE) Stochastic Hodgkin-Huxley model (*challenging*)

✓ (ULE) Nonlinear force field & Inhomogeneous diffusion matrix ✓ (ULE) Brownian Carnot engine (*challenging*)

- We show that the provided uncertainty is highly correlated to the error of predictions

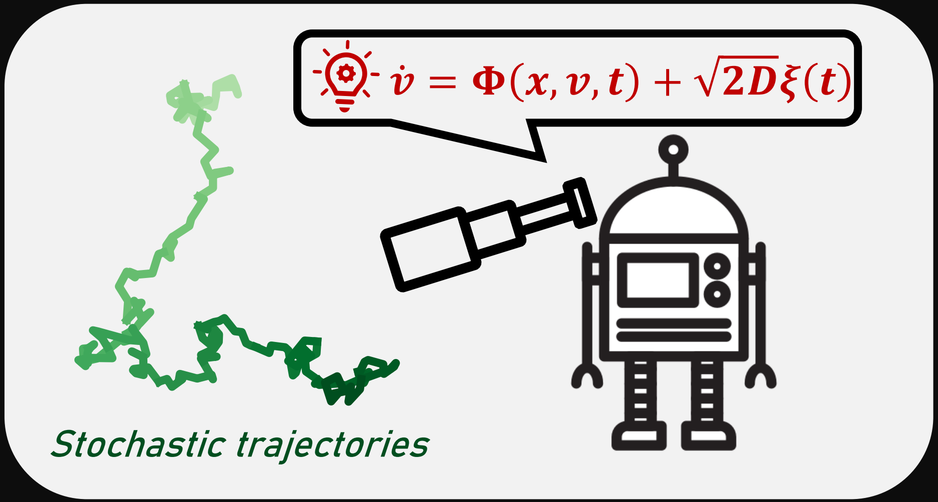
→ It can help us anticipate errors of predicted dynamics and avoid erroneous decision-making.



arXiv QR

Thank you for listening!

Presenter - Youngkyoung Bae ✉ *dudrud3085@gmail.com*



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