

A Appendix

A.1 Proof: analytical form of spline derivatives

Theorem 1. . *The derivative of B-spline curve can be analytically evaluated as:*

$$\dot{y}(t) = \sum_{s=0}^{r+k-1} \dot{N}_{s,k}(t) \theta_s, \quad (19)$$

where

$$\dot{N}_{s,k}(t) = \frac{k}{\tau_{s+k} - \tau_s} N_{s,k-1}(t) - \frac{k}{\tau_{s+k+1} - \tau_{s+1}} N_{s+1,k-1}(t). \quad (20)$$

Proof. We will prove by the induction. For the base case $k = 1$, we have

$$\dot{N}_{s,1}(t) = \begin{cases} \frac{1}{\tau_{s+1} - \tau_s} & t \in [\tau_s, \tau_{s+1}] \\ -\frac{1}{\tau_{s+2} - \tau_{s+1}} & t \in [\tau_{s+1}, \tau_{s+2}] \end{cases} = \frac{1}{\tau_{s+1} - \tau_s} N_{s,0}(t) - \frac{1}{\tau_{s+2} - \tau_{s+1}} N_{s+1,0}(t). \quad (21)$$

Let's suppose that the formula holds for k up to n . We will prove that this formula also holds for $k = n + 1$. By the definition in Eq. 4 and the chain rule, we can get that:

$$\begin{aligned} \dot{N}_{s,n+1}(t) &= \frac{t - \tau_s}{\tau_{s+n+1} - \tau_s} \dot{N}_{s,n}(t) + \frac{N_{s,n}(t)}{\tau_{s+n+1} - \tau_s} + \frac{\tau_{s+n+2} - t}{\tau_{s+n+2} - \tau_{s+1}} \dot{N}_{s+1,n}(t) - \frac{N_{s+1,n}(t)}{\tau_{s+n+2} - \tau_{s+1}} \\ &= \frac{t - \tau_s}{\tau_{s+n+1} - \tau_s} \left(\frac{n}{\tau_{s+n} - \tau_s} N_{s,n-1}(t) - \frac{n}{\tau_{s+n+1} - \tau_{s+1}} N_{s+1,n-1}(t) \right) \\ &\quad + \frac{\tau_{s+n+2} - t}{\tau_{s+n+2} - \tau_{s+1}} \left(\frac{n}{\tau_{s+n+1} - \tau_{s+1}} N_{s+1,n-1}(t) - \frac{n}{\tau_{s+n+2} - \tau_{s+2}} N_{s+2,n-1}(t) \right) \\ &\quad + \frac{1}{\tau_{s+n+1} - \tau_s} N_{s,n}(t) - \frac{1}{\tau_{s+n+2} - \tau_{s+1}} N_{s+1,n}(t) \\ &= \frac{n+1}{\tau_{s+n+1} - \tau_s} N_{s,n}(t) - \frac{n+1}{\tau_{s+n+2} - \tau_{s+1}} N_{s+1,n}(t). \end{aligned} \quad (22)$$

□

A.2 Spline representation

In this section, we give error bounds for spline representation. For simplicity, we consider 1D scenario and assume the target function $u : [0, 1] \rightarrow R$ is periodic and defined on the unit interval $\Omega = [0, 1]$. Consider a set of uniform knots $\Gamma : 0 = \tau_0 \leq \tau_1 \leq \dots \leq \tau_{r+k} = 1$ with . The space of k th degree $\{N_{s,k}\}_{s=0}^{r+k-1}$ splines is

$$S^k(\Omega, \Gamma) = \{p|p(t) \text{ is a polynomial of degree } k \text{ in each } (\tau_i, \tau_{i+1})\} \cap \mathcal{C}^{k-1}(\Omega).$$

Spline interpolation seeks $\hat{u} \in S^k(\Omega, \Gamma)$ that satisfies $u(\tau_i) = \hat{u}(\tau_i) \quad \forall \quad 0 \leq r + k$.

Theorem 2 (Spline interpolation error bounds [49, 50]). *Assume that u is periodic, for odd degree spline interpolation k , we have*

$$\begin{aligned} \|u - \hat{u}\|_\infty &= \Delta\tau^{k+1} \left(C_{k+1} \|u^{(k+1)}\|_\infty + \mathcal{O}(\omega(u^{(k+1)}, \Delta\tau)) \right), \\ \|u^{(l)} - \hat{u}^{(l)}\|_\infty &= \Delta\tau^{k+1-l} \left(D_{k+1-l} \|u^{(k+1)}\|_\infty + \mathcal{O}(\omega(u^{(k+1)}, \Delta\tau)) \right) \quad \forall l \leq k - 1. \end{aligned} \quad (23)$$

Here C_{k+1} and D_{k+1-l} are constant parameters, which are independent of $\Delta\tau$ and u , and $\omega(u^{(k+1)}, \Delta\tau) = \sup_{|x-y| \leq \Delta\tau} |u^{(k+1)}(x) - u^{(k+1)}(y)|$.

In the present work, we focus on using spline for smoothing noisy data. It is essentially a nonparametric estimation of function u from noisy data $\{t_i, \tilde{u}_i\}_{i=1}^n$,

$$\tilde{u}_i = u(t_i) + \eta_i \quad \text{with} \quad \eta_i \sim \mathcal{N}(0, \delta_\eta^2).$$

We further assume that $\{t_i\}$ are uniformly sampled from Ω . The unregularized smoothing process estimates spline basis coefficients

$$\hat{\boldsymbol{\theta}} = (\mathbf{N}_m^T \mathbf{N}_m)^{-1} \mathbf{N}_m^T \cdot \tilde{\mathbf{U}}$$

through minimizing $\|\tilde{\mathbf{U}} - \mathbf{N}_m \cdot \boldsymbol{\theta}\|$. Here $\tilde{\mathbf{U}} = [\tilde{u}_1, \tilde{u}_2, \dots, \tilde{u}_n]^T$ and \mathbf{N}_m is the spline basis matrix evaluated at these measurement locations. The optimal $\boldsymbol{\theta}^{\text{opt}}$ satisfies $\hat{u}(t) = \mathbf{N}(t) \cdot \boldsymbol{\theta}^{\text{opt}}$, where \hat{u} is the spline interpolation of u , and $\mathbf{N}(t) = [N_{0,k}(t), N_{1,k}(t), \dots, N_{r+k-1,k}(t)]^T$ denotes spline basis function vector. Following [51], we have spline fitting error bounds, as following.

Theorem 3 (Spline fitting error bounds). *Assume that u is periodic and the number of data n is sufficient large, for odd degree spline interpolation k , we have*

$$\|\mathbb{E}\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^{\text{opt}}\|_2 \leq C_1 \Delta \tau^{k+1} \quad \|\text{Cov}\hat{\boldsymbol{\theta}}\|_2 \leq C_2 \frac{\delta_\eta^2}{n},$$

where C_1 and C_2 are constant and independent of n .

Proof. Let us denote

$$\begin{aligned} \mathbf{U} &= [u(t_1), u(t_2), \dots, u(t_n)]^T & \hat{\mathbf{U}} &= [\hat{u}(t_1), \hat{u}(t_2), \dots, \hat{u}(t_n)]^T \\ \boldsymbol{\eta} &= [\eta_1, \eta_2, \dots, \eta_n]^T & \mathbf{e} &= \mathbf{U} - \hat{\mathbf{U}}. \end{aligned}$$

We have

$$\begin{aligned} \hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^{\text{opt}} &= (\mathbf{N}_m^T \mathbf{N}_m)^{-1} \mathbf{N}_m^T \cdot \tilde{\mathbf{U}} - (\mathbf{N}_m^T \mathbf{N}_m)^{-1} \mathbf{N}_m^T \mathbf{N}_m \boldsymbol{\theta}^{\text{opt}} \\ &= (\mathbf{N}_m^T \mathbf{N}_m)^{-1} \mathbf{N}_m^T \cdot (\mathbf{U} + \boldsymbol{\eta} - \hat{\mathbf{U}}) \\ &= (\mathbf{N}_m^T \mathbf{N}_m)^{-1} \mathbf{N}_m^T \cdot (\mathbf{e} + \boldsymbol{\eta}). \end{aligned} \quad (24)$$

We will first prove that

$$\|\mathbf{N}_m^T \mathbf{N}_m\|_2 = \mathcal{O}(n) \quad \|(\mathbf{N}_m^T \mathbf{N}_m)^{-1}\|_2 = \mathcal{O}\left(\frac{1}{n}\right). \quad (25)$$

For any $\boldsymbol{\theta}$, $\frac{1}{n} \boldsymbol{\theta}^T \mathbf{N}_m^T \mathbf{N}_m \boldsymbol{\theta}$ is the Monte Carlo approximation of $\int (\mathbf{N}(t)^T \cdot \boldsymbol{\theta})^2 dt$, and hence

$$\frac{1}{n} \boldsymbol{\theta}^T \mathbf{N}_m^T \mathbf{N}_m \boldsymbol{\theta} = \int (\mathbf{N}(t)^T \boldsymbol{\theta})^2 dt + \mathcal{O}\left(\frac{1}{\sqrt{n}}\right). \quad (26)$$

Bringing the following property of B-splines [52]

$$M_1 \boldsymbol{\theta}^T \boldsymbol{\theta} \leq \int (\mathbf{N}(t)^T \boldsymbol{\theta})^2 dt \leq M_2 \boldsymbol{\theta}^T \boldsymbol{\theta} \quad \exists M_1, M_2 > 0$$

into Eq. (26) leads to Eq. (25). Then we prove that

$$\|\mathbf{N}_m^T \mathbf{e}\|_2 = \mathcal{O}(n \Delta \tau^{k+1}). \quad (27)$$

Since $\sum_s N_{s,k}(t) = 1$ and $\|\mathbf{e}\|_\infty = \mathcal{O}(\Delta \tau^{k+1})$, we have

$$\|\mathbf{N}_m^T \mathbf{e}\|_2 \leq \|\mathbf{N}_m^T \mathbf{e}\|_1 = \mathcal{O}(n \Delta \tau^{k+1}).$$

Finally, combining Eq. (24), Eq. (25) and Eq. (27) leads to

$$\begin{aligned} \|\mathbb{E}\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^{\text{opt}}\|_2 &= \|(\mathbf{N}_m^T \mathbf{N}_m)^{-1} \mathbf{N}_m^T \cdot \mathbf{e}\|_2 \leq \|(\mathbf{N}_m^T \mathbf{N}_m)^{-1}\|_2 \|\mathbf{N}_m^T \cdot \mathbf{e}\|_2 \leq C_1 \Delta \tau^{k+1} \\ \|\text{Cov}\hat{\boldsymbol{\theta}}\|_2 &= \sigma_\eta^2 \|(\mathbf{N}_m^T \mathbf{N}_m)^{-1}\|_2 \leq C_2 \frac{\delta_\eta^2}{n} \end{aligned}$$

□

In our sparse Bayesian regression, in stead of solving the aforementioned minimization problem, we have additional regularization terms.

A.3 Algorithms

In this section, we present detailed algorithms used in the present work, which include Bayesian Alternative Direction Optimization (ADO) Learning 1, Sequential Threshold Sparse Bayesian Learning 2, and Ensemble Kalman Filter 3.

Algorithm 1: Bayesian Alternative Direction Optimization (ADO) Learning

Input : Library Φ , spline basis \mathbf{N} , time derivative of spline basis matrix $\dot{\mathbf{N}}_c$, negative log form of equation Eq. 11 \mathcal{L}

Output : Mean estimation: $\theta_{\text{SWA}}, \mathbf{W}_{\text{SWA}}, \mathbf{B}_{\text{SWA}}, \mathbf{P}_{\text{SWA}}$
Samples from posterior distributions: $\hat{\theta}, \hat{\mathbf{W}}, \hat{\mathbf{B}}, \hat{\mathbf{P}}$

Pretrain:

for $i = 1 : T_{\text{Pretrain}}$ **do**

SDG optimization with the fixed library

$\{\theta_{i+1}, \mathbf{W}'_{i+1}, \mathbf{B}_{i+1}, \mathbf{P}'_{i+1}\} = \arg \min \mathcal{L}$

Update library

$\mathbf{W}_{i+1}, \mathbf{P}_{i+1} = \text{STSparseBayesian}(\Phi, \dot{\mathbf{U}}_{i+1} = \dot{\mathbf{N}}_c \theta_{i+1}, \mathbf{W}'_{i+1}, \mathbf{P}'_{i+1})$

if $\mathcal{L}(\theta_{i+1}, \mathbf{W}_{i+1}, \mathbf{B}_{i+1}, \mathbf{P}_{i+1}) < \mathcal{L}^*$ **then**

$\mathcal{L}^* = \mathcal{L}(\theta_{i+1}, \mathbf{W}_{i+1}, \mathbf{B}_{i+1}, \mathbf{P}_{i+1})$

$\theta^*, \mathbf{W}^*, \mathbf{B}^*, \mathbf{P}^* = \theta_{i+1}, \mathbf{W}_{i+1}, \mathbf{B}_{i+1}, \mathbf{P}_{i+1}$

else

break

end

Stochastic Weight Averaging-Gaussian (SWAG) for posterior approximation:

$\theta_{\text{SWA}}, \mathbf{W}_{\text{SWA}}, \mathbf{B}_{\text{SWA}}, \mathbf{P}_{\text{SWA}} = \theta^*, \mathbf{W}^*, \mathbf{B}^*, \mathbf{P}^*$

With a constant learning rate **for** $i = 1 : T_{\text{SWAG}}$ **do**

 SGD update $\theta_i, \mathbf{W}_i, \mathbf{B}_i, \mathbf{P}_i$

$\theta_{\text{SWA}}, \mathbf{W}_{\text{SWA}}, \mathbf{B}_{\text{SWA}}, \mathbf{P}_{\text{SWA}} = \frac{i\theta_{\text{SWA}} + \theta_i}{i+1}, \frac{i\mathbf{W}_{\text{SWA}} + \mathbf{W}_i}{i+1}, \frac{i\mathbf{B}_{\text{SWA}} + \mathbf{B}_i}{i+1}, \frac{i\mathbf{P}_{\text{SWA}} + \mathbf{P}_i}{i+1}$

end

Compute low-rank square root of empirical covariance matrices $\Lambda_\theta, \Lambda_W, \Lambda_B, \Lambda_P$ from

$\{\theta_i - \theta_{\text{SWA}}\}, \{\mathbf{W}_i - \mathbf{W}_{\text{SWA}}\}, \{\mathbf{B}_i - \mathbf{B}_{\text{SWA}}\}, \{\mathbf{P}_i - \mathbf{P}_{\text{SWA}}\}$

Sampling:

$\hat{\theta} = \theta_{\text{SWA}} + \Lambda_\theta \hat{z}_\theta$ $\hat{\mathbf{W}} = \mathbf{W}_{\text{SWA}} + \Lambda_W \hat{z}_W$ $\hat{\mathbf{B}} = \mathbf{B}_{\text{SWA}} + \Lambda_B \hat{z}_B$ $\hat{\mathbf{P}} = \mathbf{P}_{\text{SWA}} + \Lambda_P \hat{z}_P$
where \hat{z}_* are the random samples from $\mathcal{N}(0, I)$.

Algorithm 2: Sequential Threshold Sparse Bayesian Learning

Input : Spline trainable parameter θ , library $\Phi(\theta)$, approximated derivative $\dot{\mathbf{U}}$, library weight \mathbf{W} , and process error matrix \mathbf{P}

Output : Best solution library $\Phi^*, \mathbf{W}^*, \mathbf{P}^*$

Initialize : Threshold ϵ , number of library terms p_{old} , and **Flag** = **True**

while *Flag is True* **do**

while not converged do

 1. Compute the relevance variable $\eta_i = q_i^2 - s_i$ as defined in [19]

 2. Update library Φ^* , weight \mathbf{W}^* , and process error matrix \mathbf{P}^* , as shown in [19]

end

for $j = 1 : p_{\text{old}}$ **do**

$\mathbf{W}^*(j) = 0$ **if** $|\mathbf{W}^*(j)| \leq \epsilon$

end

 Find the nonzero entries in \mathbf{W}^* , record the index as \mathbf{I} , update $\Phi = \Phi(:, \mathbf{I})$ and $p_{\text{new}} = \text{length of } \mathbf{I}$;

if $p_{\text{new}} = p_{\text{old}}$ **then**

Flag = **False**

end

Algorithm 3: Ensemble Kalman Filter

Input : ensemble number J , sampled weights $\{\mathbf{W}^j\}_{j=1}^J$, discovered dynamical model $\mathbf{M}(\cdot; \mathbf{W})$, process noise covariance \mathbf{P} , observation model \mathbf{h} , observation $\tilde{\mathbf{U}}$, observation noise covariance \mathbf{B}

Output : Analysis ensemble trajectories $\mathbf{U}_a^j(t)$

Forecast : $\mathbf{U}_f^j(t_{i+1}) = \mathbf{M}(\mathbf{U}_a^j(t_i); \mathbf{W}^j) + \boldsymbol{\epsilon}_2^j$, $\boldsymbol{\epsilon}_2^j \sim (\mathbf{0}, \mathbf{P})$

$$\bar{\mathbf{U}}_f(t_{i+1}) = \frac{1}{J} \sum_{j=1}^J \mathbf{U}_f^j(t_{i+1})$$

Analysis : $\mathbf{U}_h^j(t_{i+1}) = \mathbf{h}(\mathbf{U}_f^j(t_{i+1}))$ $\bar{\mathbf{U}}_h(t_{i+1}) = \frac{1}{J} \sum_{j=1}^J \mathbf{U}_h^j(t_{i+1})$

$$\mathbf{C}^{fh}(t_{i+1}) = \frac{1}{J-1} \sum_{j=1}^J (\mathbf{U}_f^j(t_{i+1}) - \bar{\mathbf{U}}_f(t_{i+1})) (\mathbf{U}_h^j(t_{i+1}) - \bar{\mathbf{U}}_h(t_{i+1}))^T$$

$$\mathbf{C}^{hh}(t_{i+1}) = \frac{1}{J-1} \sum_{j=1}^J (\mathbf{U}_h^j(t_{i+1}) - \bar{\mathbf{U}}_h(t_{i+1})) (\mathbf{U}_h^j(t_{i+1}) - \bar{\mathbf{U}}_h(t_{i+1}))^T + \mathbf{B}$$

$$\mathbf{K}(t_{i+1}) = \mathbf{C}^{fh} (\mathbf{C}^{hh})^{-1}$$

$$\mathbf{U}_a^j(t_{i+1}) = \mathbf{U}_f^j(t_{i+1}) + \mathbf{K}(t_{i+1}) \left(\tilde{\mathbf{U}}(t_{i+1}) - \mathbf{U}_h^j(t_{i+1}) - \boldsymbol{\epsilon}_1^j \right), \quad \boldsymbol{\epsilon}_1^j \sim (\mathbf{0}, \mathbf{B})$$

A.4 Training Details

Additional training hyper parameters used in Sec. 4 is shown in the Tab. 2.

Table 2: Training Details

Case	Van der Pol	Lorenz 96	Advection	Burgers'
ADO Iter	5	5	1	5
ADO Epoch	20K	50K	20K	20K
Post Epoch	1K	65K	2K	0.5K
SWAG Epoch	1.5K	80K	0.5K	0.5K
LR	1×10^{-2}	1×10^{-2}	1×10^{-2}	1×10^{-2}
SWAG LR	1×10^{-3}	1×10^{-3}	1×10^{-3}	1×10^{-3}

A.5 Additional Result: ODE

We list additional discovery and UQ results in this section. Fig. 5 shows 4 distributions of the coefficients for Van der Pol system in red box and Lorenz 96 system in blue box. Fig. 4 shows additional UQ result from the identified L96 systems without incorporating the data assimilation process. The truth trajectory is marked by red. The measurement is marked by green dots and the ensemble trajectories are marked by blue. Although the system has been identified with high accuracy, as shown in Tab. 3, the predicted ensembles of the state variables still become chaotic after several seconds. It is inevitable since the chaotic nature of the underlying system, which means any small perturbation in any parameters would significantly influence the future trajectories. Fortunately, the predicted covariance matrix of the Bayesian framework makes it easy to incorporate the data assimilation with the identified systems. With the identified distribution of system coefficients, the data assimilation can be used to predict the future states with reduced uncertainty, given noisy measurement data in the past. Fig. 6 shows additional UQ result for all the 6 state variables for Lorenz 96 system, incorporating EnKF algorithms.

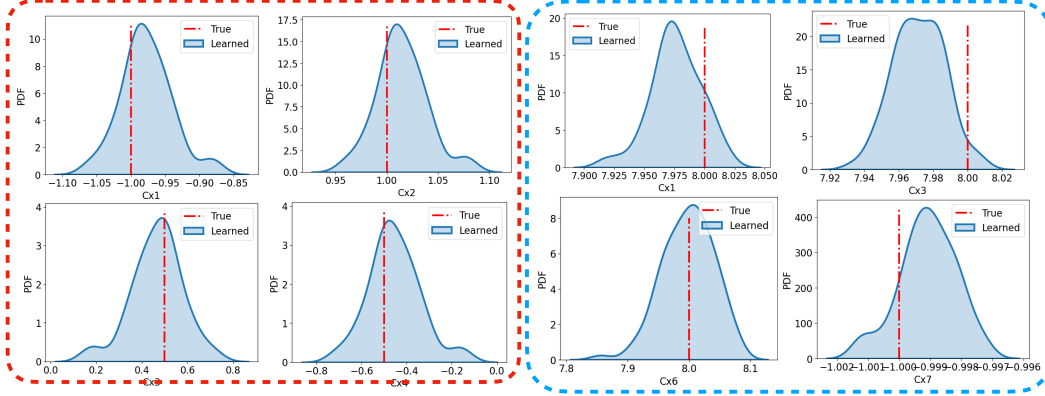


Figure 4: Additional discovery results for ODE systems; the red box shows results coefficients distribution for the Van der Pol system, and the blue box shows the result for Lorenz 96 system.

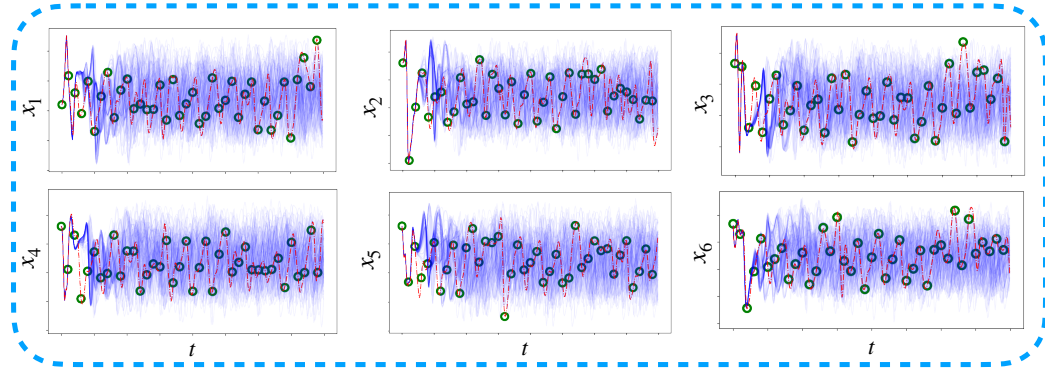


Figure 5: Additional UQ results for ODE systems; the blue box shows the all the states prediction for Lorenz 96 system without ensemble Kalman filter.

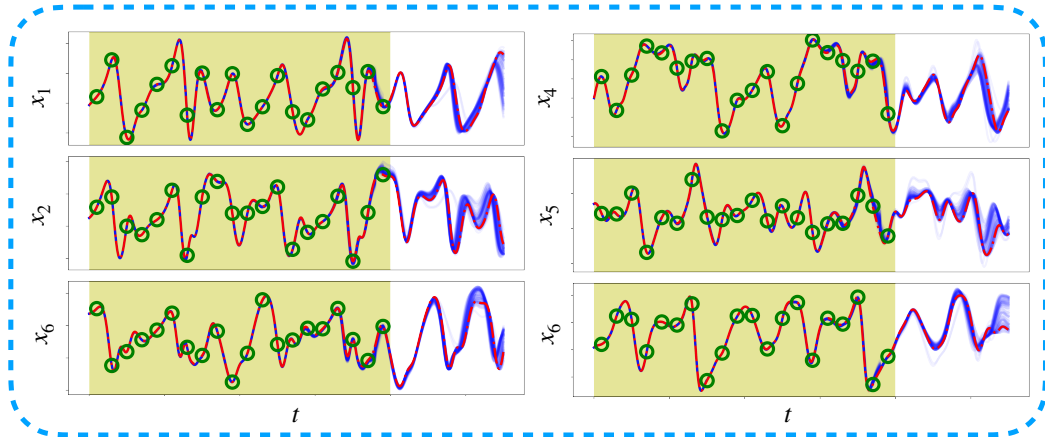


Figure 6: Additional UQ results for ODE systems; the blue box shows the all the states prediction for Lorenz 96 system with ensemble Kalman filter.

A.6 Additional Result: PDE

In this section, we attached the qualitative result for PDE discovery and the uncertainty quantification. The contour plot and the cross section result are shown in Fig 7 (for advection equation and Burgers

equation) and Fig. 8 (for Burgers equation with source). The analytical form of the mentioned PDEs are listed in Tab. 5. Probability distribution for the PDE coefficient are shown in Fig. 9. Additional UQ prediction result for advection and Burgers' equation are shown in and Fig. 10.

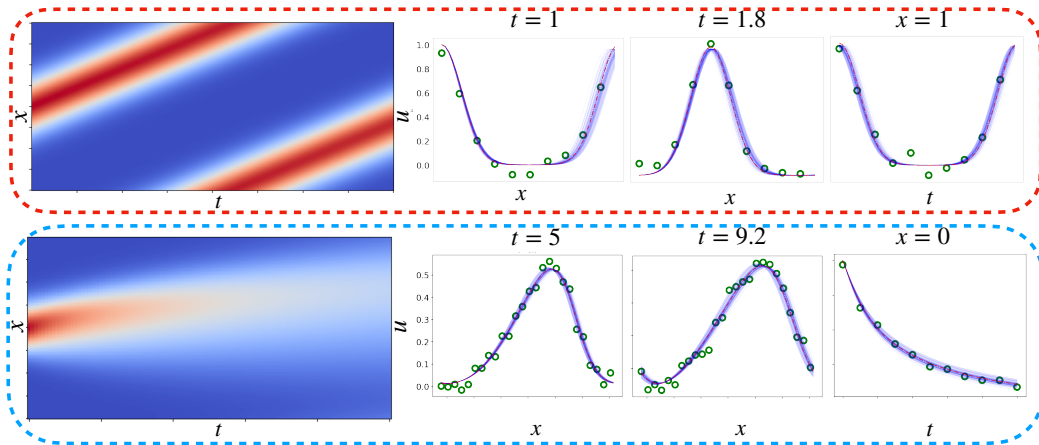


Figure 7: The discovery results for PDE systems; the red box shows results for the advection system, and the blue box shows the result for the Burgers' system. The layout inside each box follows the rules below. Leftmost sub-fig: true contour plot; Middle two sub-figs: the spatial results at different time t ; Rightmost sub-figs: the temporal result at a fixed point x .

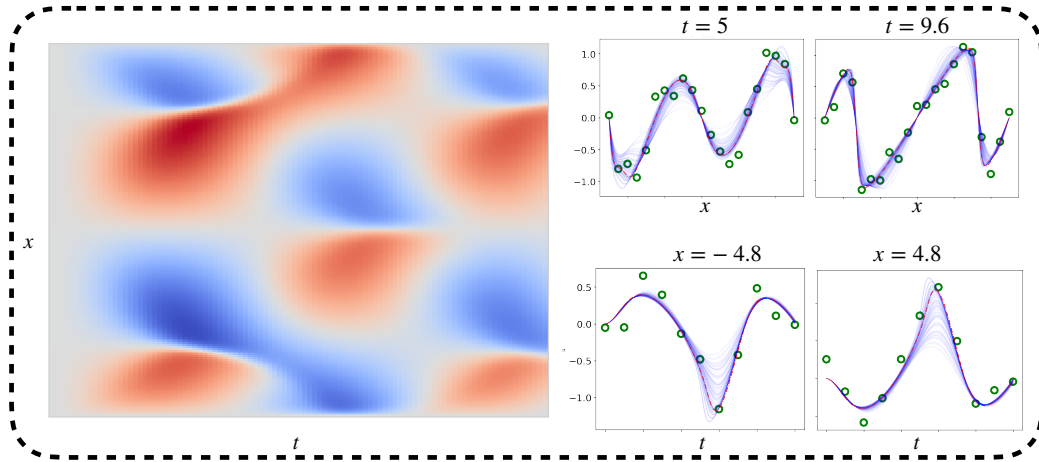


Figure 8: Additional UQ results for PDE; the black box shows the cross section UQ results for Burgers' equation with source.

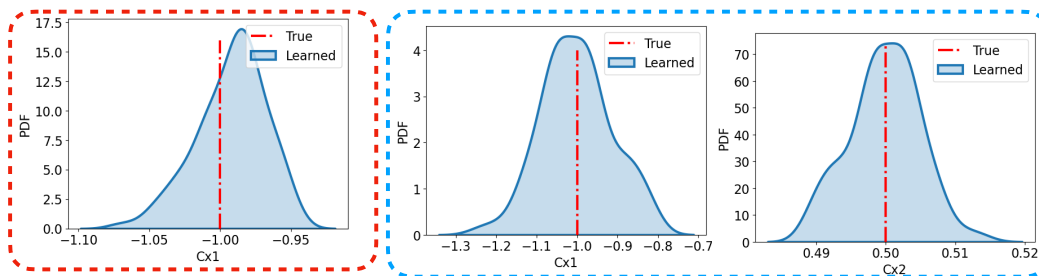


Figure 9: Additional discovery results for PDE systems; the red box shows results coefficients distribution for the advection equation, and the blue box shows the result for Burgers' equation.

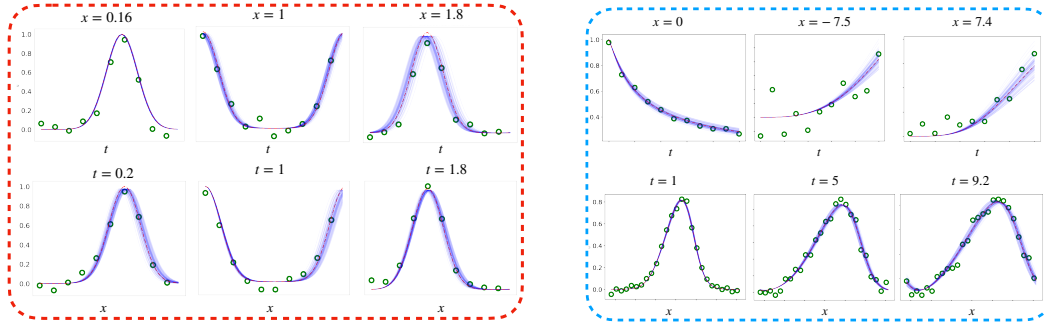


Figure 10: Additional UQ results PDE; the red box shows the cross section UQ results for Advection equation. The blue box shows the cross section UQ results for Burgers' equation.

A.7 Additional Discovery result

In this section, we list the full table that includes all the experiments made for current work, as attached in Tab. 3.

Table 3: ODE and PDE discovery comparison

Name	rmse(0%)	rmse(1%)	rmse (large ⁸)	M _P	M _R ⁹	Training Cost ¹⁰
Van der Pol Oscillator						
BSL(Ours)	0.2	2.82	18.04	1	1	~ 133(+3)s
PINN-SR	Fail ¹¹	Fail	Fail	0.214	0.75	~ 1213s
SINDy	1.0	1.93	Fail	0.267	1.0	~ 10s
RVM	1.0	2.54	27.46	1	1	~ 10s
Lorenz 96						
BSL(Ours)	0.269	1.47	13.0	1	1	~ 1654(+438)s
PINN-SR	Fail	Fail	Fail	0.5	0.22	~ 10788s
SINDy	0.4	0.64	Fail	0.75	1	~ 10s
RVM	0.4	0.6	49.7	1	1	~ 25s
Advection Equation						
BSL(Ours)	0.26	1	1.9	1	1	~ 946(+233)s
PINN-SR	5.9	4.5	30.4	1	1	~ 650s
SINDy	2.3	8.2	38.9	1	1	~ 10s
RVM	0.77	6.76	Fail	0.2	1	~ 4s
Burgers' Equation						
BSL(Ours)	3.62	4.13	6.38	1	1	~ 117(+74)s
PINN-SR	10.2	3.3	10.3	1	1	~ 512s
SINDy	0.826	Fail	Fail	1	0.5	~ 10s
RVM	0.754	Fail	Fail	0.1429	0.5	~ 4s
Name	rmse(0%)	rmse(0.1%)	rmse (large)	M _P	M _R	Training Cost
Burgers' with Source						
BSL(Ours)	11	12.4	13.4	1	1	~ 396(+340)s
PINN-SR	10.5	15	34.6	1	1	~ 600s
SINDy	26.2	Fail	Fail	1	0.33	~ 10s
RVM	27.6	Fail	Fail	0.5	0.67	~ 10s
Heat Equation						
BSL(Ours)	19	19	38.9	1	1	~ 71(+8)s
PINN-SR	Fail	Fail	Fail	0	0	~ 285s
SINDy	1.9	17	Fail	0.25	1	~ 10s
RVM	2.8	6	Fail	0	0	~ 6s
Poisson Equation						
BSL(Ours)	1.18×10^{-2}	0.133	16.7	1	1	~ 92(+9)s
PINN-SR	Fail	Fail	Fail	0	0	~ 3737s
SINDy	1.15	87	962	1	1	~ 10s
RVM	1.15	232	968	1	1	~ 10s

⁸Large noise for different cases: Van der Pol: 5%, Lorenz 96: 10%, Advection: 20%, Burgers: 10%, Burgers' with source: 20%, Heat: 15%, Poisson: 5%

⁹M_P, M_R are only reported for the largest noise cases

¹⁰All cases are running on a Nvidia 2070 Ti GPU card

¹¹Fail means failure in discovery of the parsimonious ODE/PDE forms.

A.8 Analytical forms of the discovered system

Table 4: Analytical forms of ODE

Name	ϵ (large)
Vander Pol Oscillator	
True	$\frac{dx}{dt} = y, \frac{dy}{dt} = -x - 0.5x^2y + 0.5y$
BSL(Ours)	$\frac{dx}{dt} = 1.0096(\pm 0.024)y, \frac{dy}{dt} = -0.9858(\pm 0.037)x - 0.4801(\pm 0.114)x^2y + 0.4889(\pm 0.111)y$
PINN-SR	$\frac{dx}{dt} = 1.3079 - 0.1151x + 0.9982y + 0.1939x^2 - 0.4101xy + 0.8559y^2 - 0.3577x^3$ $+ 0.6764x^2y - 0.1207xy^2 + 0.6261y^3,$ $\frac{dy}{dt} = -0.6718x + 1.6035y + 1.6339y^2 + 0.4803y^3$
SINDy	$\frac{dx}{dt} = 0.1197 + 0.169x + 0.9975y - 0.0292x^2 + 0.0232xy - 0.0274y^2$ $- 0.0393x^3 + 0.0208x^2y - 0.0463xy^2,$ $\frac{dy}{dt} = -1.0909x + 0.149y + 0.0294x^3 - 0.4x^2y - 0.0356xy^2 + 0.0762y^3$
RVM	$\frac{dx}{dt} = 0.9957(\pm 0.073)y, \frac{dy}{dt} = -0.9943(\pm 0.0597)x - 0.4777(\pm 0.0809)x^2y + 0.4714(\pm 0.1204)y$
Lorenz 96	
True	$\frac{dX_1}{dt} = (X_2 - X_5)X_6 - X_1 + 8, \frac{dX_2}{dt} = (X_3 - X_6)X_1 - X_2 + 8,$ $\frac{dX_3}{dt} = (X_4 - X_1)X_2 - X_3 + 8, \frac{dX_4}{dt} = (X_5 - X_2)X_3 - X_4 + 8,$ $\frac{dX_5}{dt} = (X_6 - X_3)X_4 - X_5 + 8, \frac{dX_6}{dt} = (X_1 - X_4)X_5 - X_6 + 8$
BSL(Ours)	$\frac{dX_1}{dt} = 1.0033(\pm 2.37 \times 10^{-4})X_2X_6 - 0.9926(\pm 2.03 \times 10^{-4})X_5X_6,$ $- 0.9991(\pm 9.04 \times 10^{-4})X_1 + 7.9773(\pm 2.08 \times 10^{-2}),$ $\frac{dX_2}{dt} = 0.9963(\pm 5.54 \times 10^{-5})X_1X_3 - 0.9942(\pm 2.47 \times 10^{-4})X_1X_6$ $- 1.0054(\pm 2.31 \times 10^{-4})X_2 + 7.8719(\pm 7.05 \times 10^{-4}),$ $\frac{dX_3}{dt} = 1.0106(\pm 2.19 \times 10^{-4})X_2X_4 - 1.0029(\pm 2.03 \times 10^{-4})X_1X_2$ $- 0.9979(\pm 5.3 \times 10^{-4})X_3 + 7.9938(\pm 1.48 \times 10^{-2}),$ $\frac{dX_4}{dt} = 1.0067(\pm 1.01 \times 10^{-4})X_3X_5 - 1.0103(\pm 9.09 \times 10^{-5})X_2X_3$ $- 0.9926(\pm 2.36 \times 10^{-4})X_4 + 8.055(\pm 2.41 \times 10^{-3}),$ $\frac{dX_5}{dt} = 0.9953 \pm (4.39 \times 10^{-4})X_4X_6 - 0.9922 \pm (3.88 \times 10^{-4})X_3X_4$ $- 1.0072 \pm (4.1 \times 10^{-4})X_5 + 7.8538(\pm 2.1 \times 10^{-3}),$ $\frac{dX_6}{dt} = 1.0095(\pm 2.71 \times 10^{-4})X_1X_5 - 0.9967(\pm 2.83 \times 10^{-4})X_4X_5$ $- 0.9772(\pm 2.46 \times 10^{-4})X_6 + 7.9964(\pm 4.15 \times 10^{-2})$
PINN-SR	N/A
SINDy	$\frac{dX_1}{dt} = 8.0985 - 0.9423X_1 - 0.1007X_4 - 0.1659X_6 + 0.9582X_2X_6 - 0.944X_5X_6$ $\frac{dX_2}{dt} = 7.9372 - 0.1268X_1 - 0.9607X_2 + 0.9636X_1X_3 - 0.9558X_1X_6$ $\frac{dX_3}{dt} = 8.1523 - 0.0983X_1 - 0.1652X_2 - 0.9952X_3 - 0.9541X_1X_2 + 0.9651X_2X_4$ $\frac{dX_4}{dt} = 7.4958 - 0.9754X_4 + 0.1515X_5 - 0.973X_2X_3 + 0.9206X_3X_5,$ $\frac{dX_5}{dt} = 7.8556 - 0.1146X_4 - 0.9457X_5 - 0.9559X_3X_4 + 1.0023X_4X_6$ $\frac{dX_6}{dt} = 7.6026 + 0.0934X_2 - 0.927X_6 + 0.9711X_1X_5 - 0.9754X_4X_5$
RVM	$\frac{dX_1}{dt} = 0.9613(\pm 1.21)X_2X_6 - 0.962(\pm 1.27)X_5X_6,$ $- 0.8983(\pm 2.67)X_1 + 7.518(\pm 5.88),$ $\frac{dX_2}{dt} = 0.9578(\pm 1.31)X_1X_3 - 0.9693(\pm 1.24)X_1X_6$ $- 0.9217(\pm 2.8)X_2 + 7.6442(\pm 6.1575),$ $\frac{dX_3}{dt} = 0.9535(\pm 1.48)X_2X_4 - 0.9803(\pm 1.38)X_1X_2$ $- 0.9468(\pm 2.96)X_3 + 7.5323(\pm 6.56),$ $\frac{dX_4}{dt} = 0.9365(\pm 1.24)X_3X_5 - 0.9748(\pm 1.15)X_2X_3$ $- 0.9114(\pm 2.59)X_4 + 7.67(\pm 5.49),$ $\frac{dX_5}{dt} = 0.9981 \pm (1.26)X_4X_6 - 0.9667 \pm (1.2)X_3X_4$ $- 0.9216 \pm (2.75)X_5 + 7.6146(\pm 5.96),$ $\frac{dX_6}{dt} = 0.9677(\pm 1.42)X_1X_5 - 0.9757(\pm 1.38)X_4X_5$ $- 0.8986(\pm 2.86)X_6 + 7.6657(\pm 6.57)$

Table 5: Analytical forms of unsteady PDE

Name	ϵ (large)
Advection Equation	
True	$u_t = -u_x$
BSL(Ours)	$u_t = -0.9988(\pm 0.024)u_x$
PINN-SR	$u_t = -0.997u_x$
SINDy	$u_t = -0.9961u_x$
RVM	$u_t = -0.5148(\pm 0.106)u_x - 0.9797(\pm 0.384)uu_x$ $-0.018(\pm 0.208)u^2u_x - 0.075(\pm 0.148)u^2u_{xxx} + 0.049(\pm 0.111)u^3u_{xxx}$
Burgers' Equation	
True	$u_t = -uu_x + 0.5u_{xx}$
BSL(Ours)	$u_t = -0.9929(\pm 0.086)uu_x + 0.4993(\pm 0.005)u_{xx}$
PINN-SR	$u_t = -1.0103uu_x + 0.5051u_{xx}$
SINDy	$u_t = -0.8179uu_x$
RVM	$-0.0809(\pm 0.041)u_x - 1.6684(\pm 0.2618)uu_x + 4.1835(\pm 0.571)u^2u_x$ $-3.9068(\pm 0.391)u^3u_x + 0.1916(\pm 0.064)uu_{xx}$ $-1.0314(\pm 0.197)u^2u_{xx} + 1.5504(0.156)u^3u_{xx}$
Burgers' Equation with Source	
True	$u_t = -uu_x + 0.1u_{xx} + \sin(x)\sin(t)$
BSL(Ours)	$-0.9882(\pm 0.246)uu_x + 0.105(\pm 0.022)u_{xx} + 0.9859(\pm 0.005)\sin(x)\sin(t)$
PINN-SR	$u_t = -0.9576uu_x + 0.1168u_{xx} + 1.0179\sin(x)\sin(t)$
SINDy	$u_t = 0.8052\sin(x)\sin(t)$
RVM	$-0.0234(\pm 0.145)uu_x + 0.8318(\pm 0.142)\sin(x)\sin(t)$ $-0.0789(\pm 0.105)\sin(x) + 0.3558(\pm 0.156)\sin(x)\cos(t)$

Table 6: Analytical forms of steady PDE

Name	ϵ (large)
Heat Equation	
True	$u_{yy} = -u_{xx}$
BSL(Ours)	$u_{yy} = -0.9611(\pm 0.059)u_{xx}$
PINN-SR	$u_{yy} = 0.5544u_x$
SINDy	$u_{yy} = -0.069u_{xx} + 13.8988uu_x - 19.493u_x + 0.2468uu_{xx}$
RVM	$u_{yy} = -7.5861(\pm 202.6)u_x$
Poisson Equation	
True	$u_{yy} = -u_{xx} - \sin(x)\sin(y)$
BSL(Ours)	$u_{yy} = -0.9788(\pm 8.75 \times 10^{-4})u_{xx} - 0.9897(\pm 4.63 \times 10^{-4})\sin(x)\sin(y)$
PINN-SR	$u_{yy} = 0.13611752uu_x + 0.29748484uu_{xx}$
SINDy	$u_{yy} = 0.2316u_{xx} - 0.4221\sin(x)\sin(y)$
RVM	$u_{yy} = 0.2284(\pm 0.007)u_{xx} - 0.3954(\pm 0.01)\sin(x)\sin(y)$

A.9 Implementation detail for the spline

In the current work, we apply direct tensor product to extend spline for solving spatial-temporal field and the relevant statistics are attached in Tab. 7, where the number of control points (trainable weights) θ in 1-d is marked by red and the total number of control points for the 2-d scenario is listed in the last column. We only store the non-zero elements for two-dimensional basis to leverage the sparsity (local support) of the spline. However, we must claim that it is *not* an optimal way to extend spline for higher spatial dimensions. In that case, a spline kernel can be defined and the tensor-product is only processed in the subdomain, as shown in [43].

Table 7: Direct tensor-product spline for PDE

basis x	basis $t(y)$	basis $(x, t(y))$	sparsity	trainable params
Advection Equation				
50×54	50×54	62500	0.0086	2916
Burgers' Equation				
128×13	101×19	92872	0.058	247
Burgers' Equation with Source				
201×103	101×103	251415	0.0012	10609
Heat Equation				
51×11	51×11	41209	0.1309	121
Poisson				
101×53	101×53	162409	0.0057	2809

A.10 Relevant Terminologies

Table 8: Terminologies

Name	Symbol	Explanation
Control points	θ	Trainable weight θ for spline basis.
Knots	τ_s	Location of control points.
Measurement points		Sparse spatio-temporal points with labels.
Collocation points		Dense spatio-temporal points without labels.
	\mathbf{N}_m	Spline basis evaluated at measurement points.
	\mathbf{N}_c	Spline basis evaluated at collocation points.
Library candidates	Φ	A collection of polynomial terms that the system identification algorithm can choose parsimonious terms from it. e.g., $\{x, y, x^2y, \dots\}$ (for ODE) or $\{u, uu_x, u_{xx}\dots\}$ for (PDE).
ADO iteration		Alternating direction optimization to update the trainable parameters including control points θ , weight of library candidates \mathbf{W} and covariance matrices.
Aleatoric Uncertainty		Due to intrinsic randomness by nature, which is irreducible.
Epistemic Uncertainty		Because of a lack of knowledge, which can be reduced by adding more information.

A.11 Real world application: predator-prey system

In this section, we would test our proposed BSL model on one real-world case, predator-prey system. The real data set is obtained online and it depicts the population of hares and lynx from 1900 to 1920 from Hudson Bay Company. The data is presented in Tab. 11: The reference governing equation by mathematical analysis is:

$$\frac{dx}{dt} = 0.4807x - 0.0248xy \quad (28)$$

$$\frac{dy}{dt} = -0.9272y + 0.0276xy \quad (29)$$

We test the 4 methods on this data set and the result can be found in Tab 9. We have made assumptions about constructing the libraries. We assume the predator (lynx) only feeds on the prey (hares). Meantime, the prey (hares) only has one predator (lynx). Therefore, the change rate of these two species can only depend on themselves (x, y) and some higher order correlations between them (xy, x^2y, xy^2) . The discovered forms of the 4 methods are listed in Tab. 10. Finally, the UQ results are shown in Fig 11. In short, only the proposed method work on the real sparse and noisy dataset. And the UQ prediction covers more measurement points than the reference model Eq. 28, which helps to better explain the data set.

Table 9: ODE discovery comparison

Name	rmse (large)	M_P	M_R	Training Cost
Predator-prey				
BSL(Ours)	30.4	1	1	$\sim 2278(+6)s$
PINN-SR	Fail	0.5	0.25	$\sim 2988s$
SINDy	Fail	0.6	0.75	$\sim 10s$
RVM	Fail	0.8	1	$\sim 10s$

Table 10: Analytical forms of ODE

Name	ϵ (large)
Predator-prey (Lotka-Volterra)	
True	$\frac{dx}{dt} = 0.4807x - 0.0248xy, \frac{dy}{dt} = -0.9272y + 0.0276xy$
BSL(Ours)	$\frac{dx}{dt} = -0.5124(\pm 0.028)x - 0.0266(\pm 8.72 \times 10^{-4})xy$ $\frac{dy}{dt} = -0.9258(\pm 0.065)y + 0.0279(\pm 1.47 \times 10^{-3})xy$
PINN-SR	$\frac{dx}{dt} = -13.9238y$ $\frac{dy}{dt} = -0.1144y$
SINDy	$\frac{dx}{dt} = 0.5813x - 0.0261xy,$ $\frac{dy}{dt} = 0.2549x - 0.2702y$
RVM	$\frac{dx}{dt} = 0.5732(\pm 0.6488)x - 0.2386(\pm 0.4643)y - 0.0253(\pm 0.1432)xy,$ $\frac{dy}{dt} = -0.8018(\pm 0.9459)y + 0.0226(\pm 0.1481)xy$

Table 11: Lynx-Hares population

Year	Hares($\times 1000$)	Lynx($\times 1000$)
1900	30	4
1901	47.2	6.1
1902	70.2	9.8
1903	77.4	35.2
1904	36.3	59.4
1905	20.6	41.7
1906	18.1	19
1907	21.4	13
1908	22	8.3
1909	25.4	9.1
1910	27.1	7.4
1911	40.3	8
1912	57	12.3
1913	76.6	19.5
1914	52.3	45.7
1915	19.5	51.1
1916	11.2	29.7
1917	7.6	15.8
1918	14.6	9.7
1919	16.2	10.1
1920	24.7	8.6

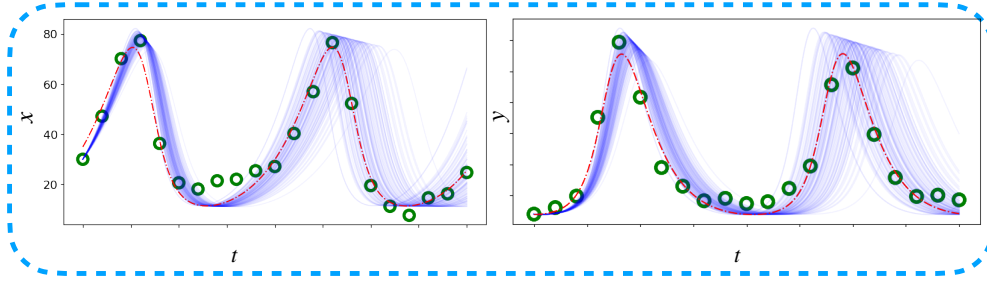


Figure 11: UQ results for predator-prey system; left sub-fig shows the result for state x , the hares population; the right sub-fig shows the result for state y , the lynx population. The green dot is the sparse and biased measurement data. The red line is the reference model and the blue curves are the ensemble predictions from our proposed model.

A.12 Experiment on different smoothing algorithms

This section we will test the effect of different smoothing algorithms and its impact to the SINDy result. These methods include smoothing based polynomial interpolation, convolutional smoother, smoothing with Tikhonov regularization and smoothing with spline fitting. We performed comparison of SINDy with these smoothing methods on a representative ODE system (Van der Pol system) and PDE system (Poisson equation) studied in this work. As shown in the Table 12 and Table 13 below, when the data noise is above 5%, although data is preprocessed using smoothing and uniform resampling, none of these method work. Basically, the SINDy still failed to discover the correct model forms with different smoothing schemes, and the identified systems are different from the true. In contrast, our proposed approach is very robust and superior to handling corrupted data, thanks to the spline learning in Bayesian settings.

Table 12: ODE and PDE discovery comparison

Name	rmse($\epsilon = 5\%$)	M_P	M_R	Training Cost
Van der Pol Oscillator				
BSL(Ours)	18.04	1	1	$\sim 133(+3)s$
SINDy(No smoother)	Fail	0.33	1	$\sim 10s$
SINDy(Poly)	Fail	0.6	0.75	$\sim 10s$
SINDy(Conv)	Fail	0.4	1	$\sim 10s$
SINDy(Tikhonov)	Fail	0.21	1	$\sim 10s$
SINDy(Spline)	Fail	0.25	1	$\sim 10s$
Poisson Equation				
BSL(Ours)	16.7	1	1	$\sim 92(+9)s$
SINDy(No smoother)	Fail	0.5	1	$\sim 10s$
SINDy(Poly)	962	1	1	$\sim 10s$
SINDy(Conv)	Fail	0.66	1	$\sim 10s$
SINDy(Tikhonov)	Fail	0.5	1	$\sim 10s$
SINDy(Spline)	Fail	0.5	1	$\sim 10s$

Table 13: Smoothing algorithm effects

Name	Analytical form
Van der Pol Oscillator	
True	$\frac{dx}{dt} = y$ $\frac{dy}{dt} = -x - 0.5x^2y + 0.5y$
SINDy(No smoother)	$\frac{dx}{dt} = 0.0277 - 0.217x + 1.4y - 0.025x^2$ $+0.0542x^3 - 0.1285x^2y + 0.1039xy^2 - 0.0896y^3,$ $\frac{dy}{dt} = -0.9835x + 0.3462y - 0.4675x^2y + 0.0325y^3$
SINDy(Poly)	$\frac{dx}{dt} = 0.1197 + 0.169x + 0.9975y - 0.0292x^2$ $+0.0232xy - 0.0274y^2 - 0.0393x^3 + 0.0208x^2y - 0.0463xy^2,$ $\frac{dy}{dt} = -1.0909x + 0.149y + 0.0294x^3 - 0.4x^2y - 0.0356xy^2 + 0.0762y^3$
SINDy(Conv)	$\frac{dx}{dt} = 0.1518 + 0.9978y - 0.0486x^2 + 0.0274xy - 0.0327y^2,$ $\frac{dy}{dt} = -1.1154x - 0.2143y + 0.0348x^3 - 0.4374x^2y + 0.0613y^3$
SINDy(Tikhonov)	$\frac{dx}{dt} = -0.2572 + 0.1486x + 1.1299y + 0.0982x^2 - 0.0721xy,$ $+0.0549y^2 - 0.0478x^2y - 0.0816xy^2 - 0.0542y^3$ $\frac{dy}{dt} = 0.2338 - 1.3282x + 0.1603y - 0.0718x^2$ $+0.058xy - 0.0564y^2 + 0.1069x^3 - 0.0842x^2y + 0.1373xy^2 - 0.0415y^3$
SINDy(Spline)	$\frac{dx}{dt} = 0.1916 + 1.5304y - 0.0614x^2 + 0.0215xy$ $-0.0325y^2 - 0.155x^2y + 0.0796xy^2 - 0.1168y^3$ $\frac{dy}{dt} = -0.35 - 1.0127x + 0.6756y + 0.0695x^2$ $+0.0741y^2 - 0.5493x^2y + 0.0523xy^2 - 0.0412y^3$
Poisson equation	
True	$u_{yy} = -u_{xx} - \sin(x)\sin(y)$
SINDy(No smoother)	$u_{yy} = 0.5635u_{xx} + 1.683uu_x + 0.088uu_{xx} - 0.17\sin(x)\sin(y)$
SINDy(Poly)	$u_{yy} = 0.2316u_{xx} - 0.4221\sin(x)\sin(y)$
SINDy(Conv)	$u_{yy} = 0.47u_{xx} - 0.2649\sin(x)\sin(y) + 0.073\sin(x)\cos(y)$
SINDy(Tikhonov)	$u_{yy} = -0.17u_{xx} - 0.087uu_x - 0.458\sin(x)\sin(y) + 0.02\sin(x)\cos(y)$
SINDy(Spline)	$u_{yy} = 0.1562u_{xx} + 0.1751uu_x - 0.3951\sin(x)\sin(y) - 0.0911\sin(x)\cos(y)$