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PyGpPHs: A Python Package for Bayesian Modeling of Port-Hamiltonian Systems

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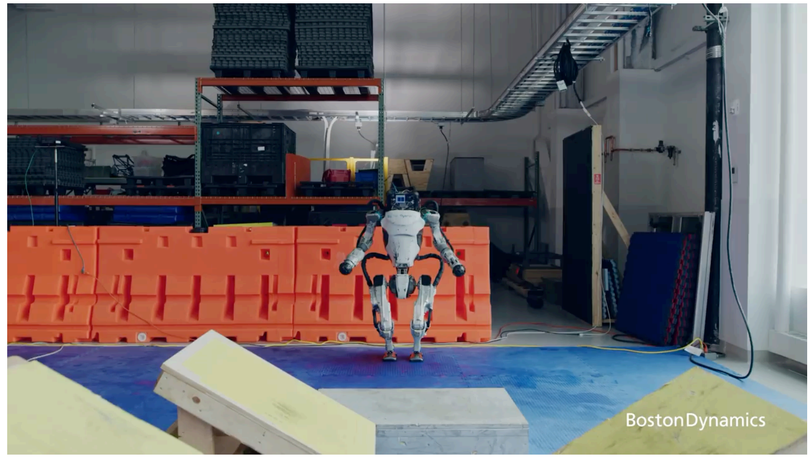
Motivation



[Boston Dynamics]

[Festo]

Modeling and control of electromechanical systems become more challenging

Need for expressive, reliable and well-generalizing modeling tools

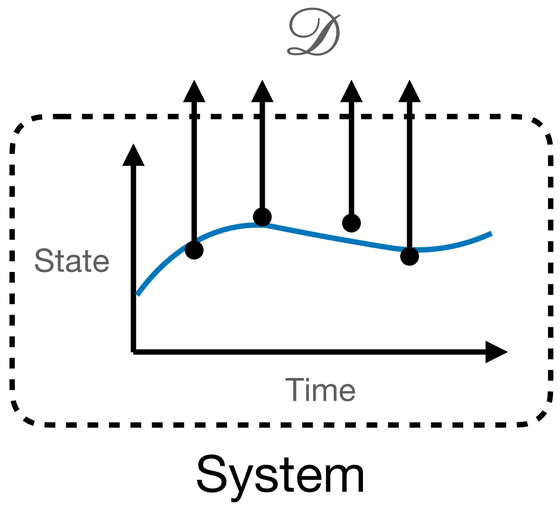
Problem statement

unknown

(Electro-)mechanical system $\dot{x}(t) = f(x) + G(x)u(t)$

Noisy measurements $\tilde{x}_i = x_i + \nu, \quad \nu \sim \mathcal{N}(0, \sigma^2 I)$

Dataset $\mathscr{D} = \{(t_1, \tilde{x}_1, u_1), \ldots, (t_N, \tilde{x}_N, u_N)\}$



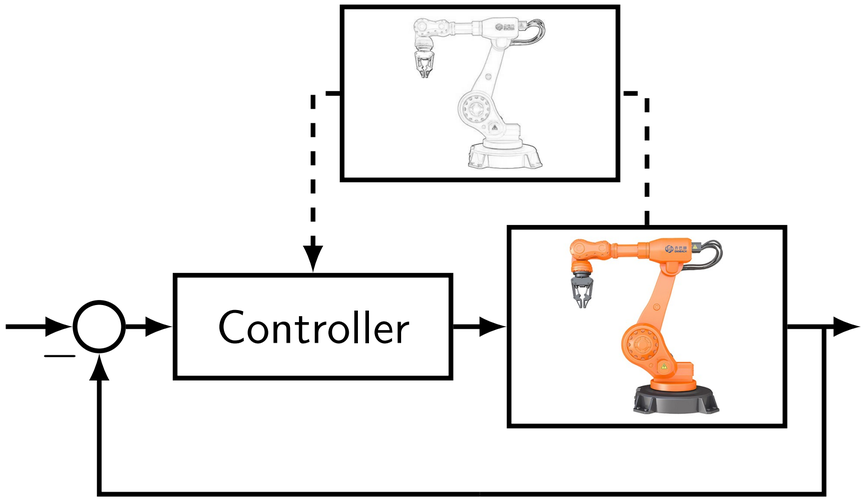
Goal

Given the dataset $\mathscr{D}$, we aim to find a model toolbox that

- represents a large class of systems -> Expressive
- allows uncertainty quantification -> Reliable
- consistent with physics -> Generalizes well

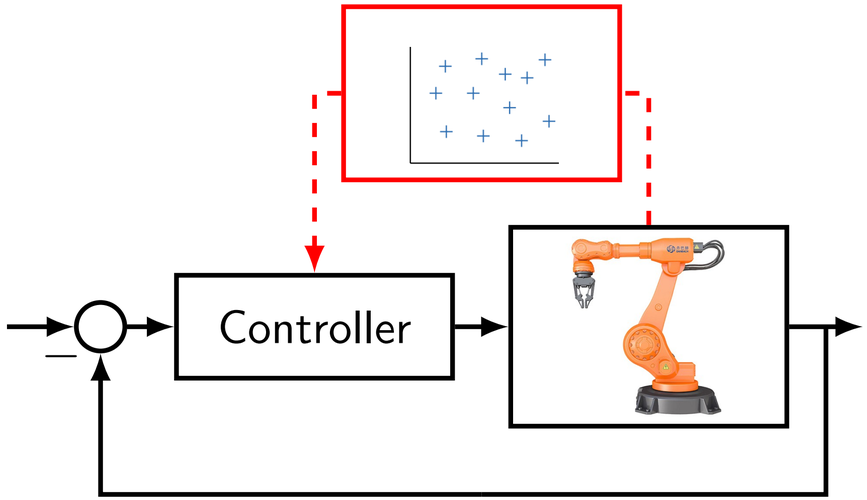
Modeling and control of physical systems

Physics-based



- ✓ Generalization
- ✓ Physical correctness
- ✗ Model selection
- ✗ Time-consuming

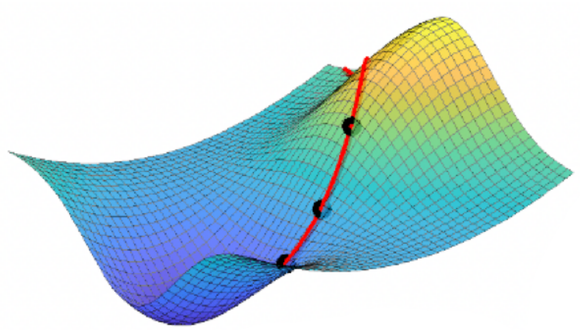
Learning-based



- ✓ Highly flexible
- ✓ Minimal expert knowledge
- ✗ Generalization
- ✗ Physical correctness

Port-Hamiltonian systems + Gaussian Processes

Physics model



Port-Hamiltonian systems

Interconnection Dissipation Hamiltonian

$$\dot{x} = [J(x) - R(x)]\frac{\partial H}{\partial x} + G(x)u$$

$$y = G(x)^\top \frac{\partial H}{\partial x}$$

Input

Output

- Skew-symmetric J ensures energy conservation
- Input and output defines a passive systems
- Connection with another PHS preserves the structure
- Suitable for multi-domain applications via energy flows

Gaussian process

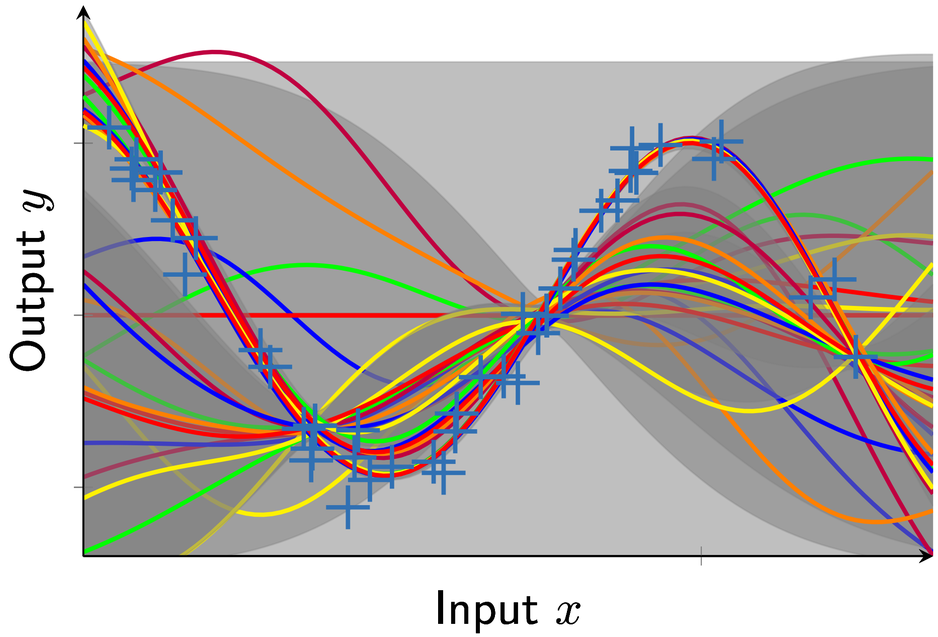
Prior: Gaussian distribution over function space

$$f(x) \sim GP(m(x), k(x, x'))$$

Mean function

Covariance

$$\text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{marginal likelihood}}$$



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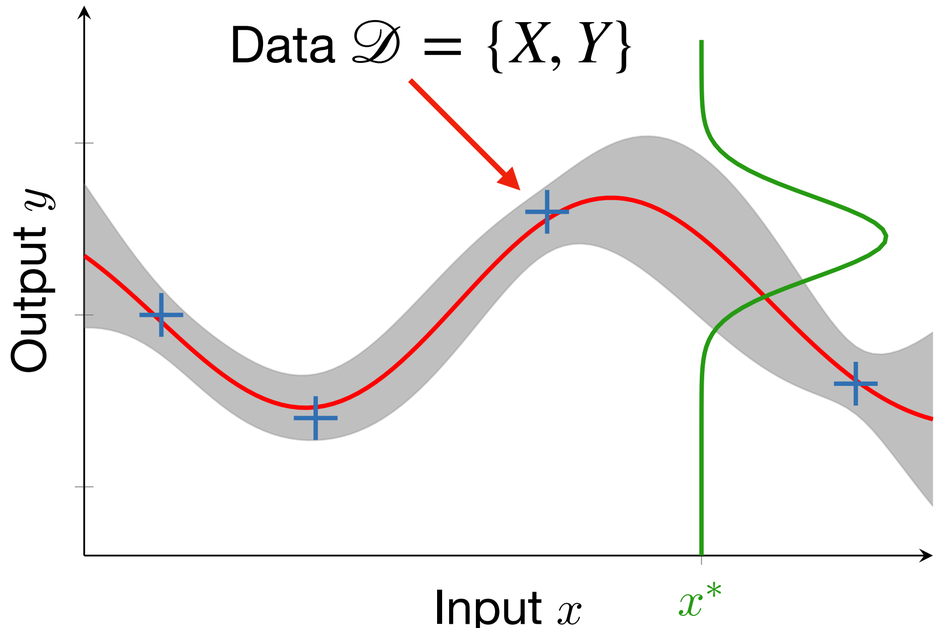

Posterior

$$\mu(y^* \,|\, x^*, \mathscr{D}) = k(x^*, X)[K(X, X) + \sigma^2 I]^{-1} Y$$

$$\Sigma(y^* \,|\, x^*, \mathscr{D}) = k(x^*, x^*) - k(x^*, X)[K(X, X) + \sigma^2 I]^{-1} k(x^*, X)^\top$$

C.E. Rasmussen. Gaussian Processes for Machine Learning. 2006

Gaussian process

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Mean function

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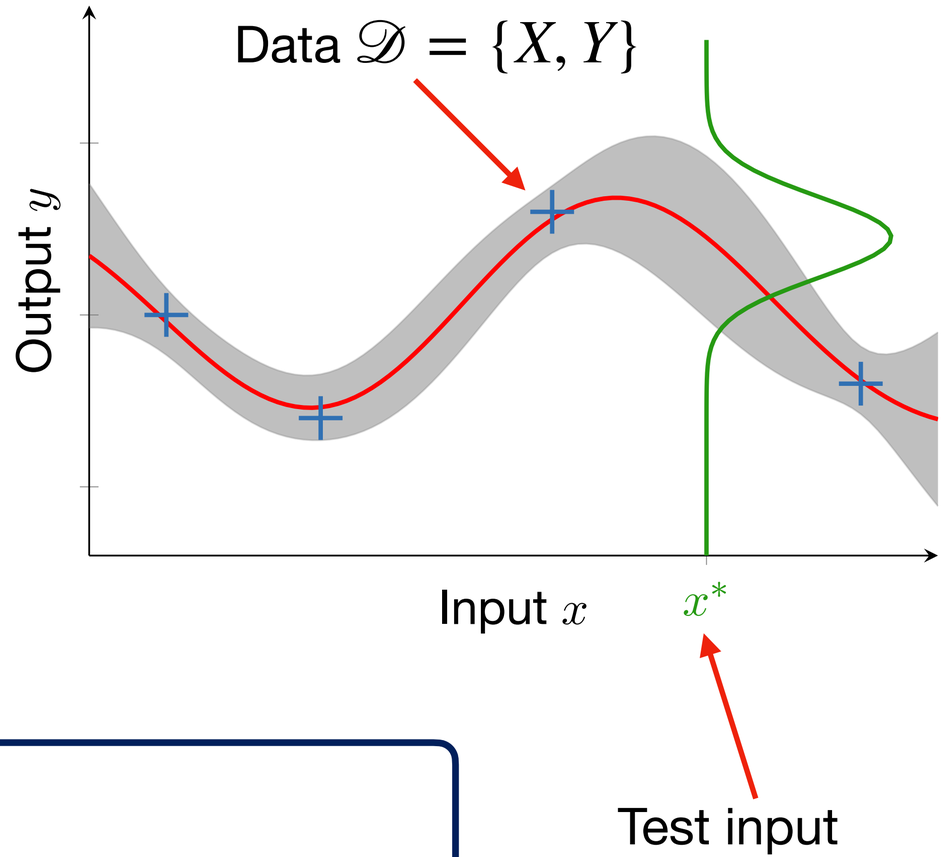

Closed under linear operators

$$f(x) = \mathscr{G}_x g(x) \sim GP(\mathscr{G}_x \mu_g, \mathscr{G}_x k_g \mathscr{G}_x^\top)$$

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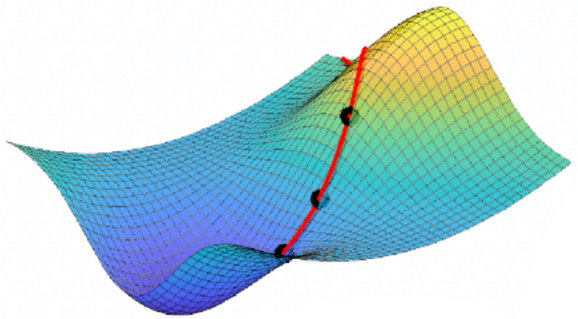
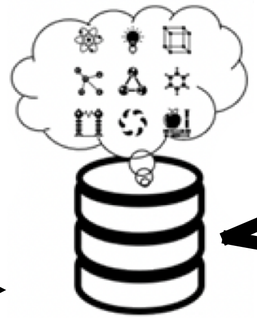
GP-PHS

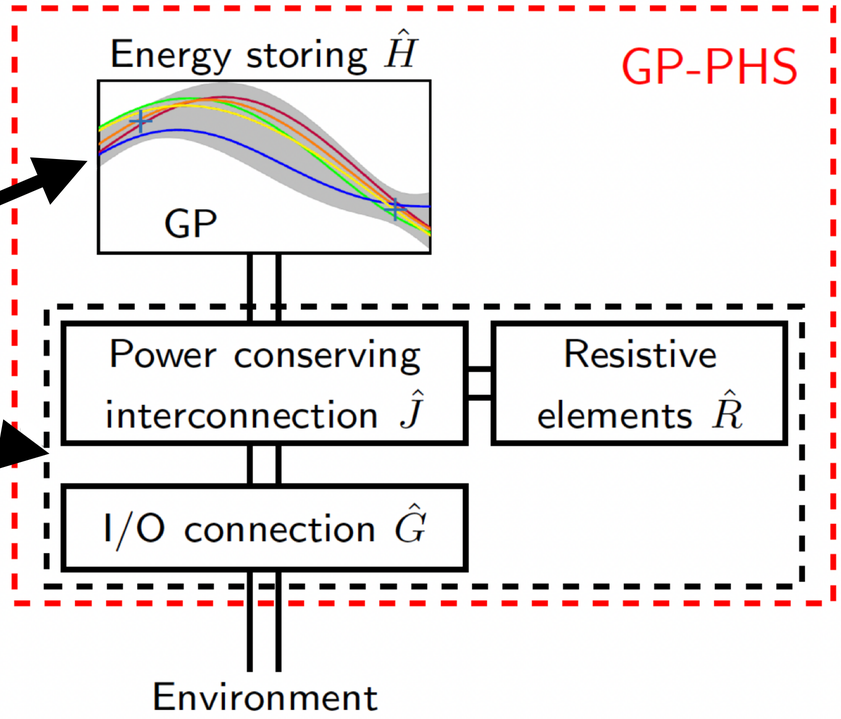




Data of physical System

Nonparametric modeling

Parameter estimation



- Gaussian Process model to learn the Hamiltonian
- GP-PHS includes all possible PHS under the GP prior on the Hamiltonian

PyGpPHs Toolbox

Python Gaussian Process port-Hamiltonian System

User-friendly interface

Object-oriented programming

Analogous to popular ML toolboxes

Fast & accurate computation

Acceleration of expensive operations

C++ Eigen library

Efficient GP algorithm

GPyTorch

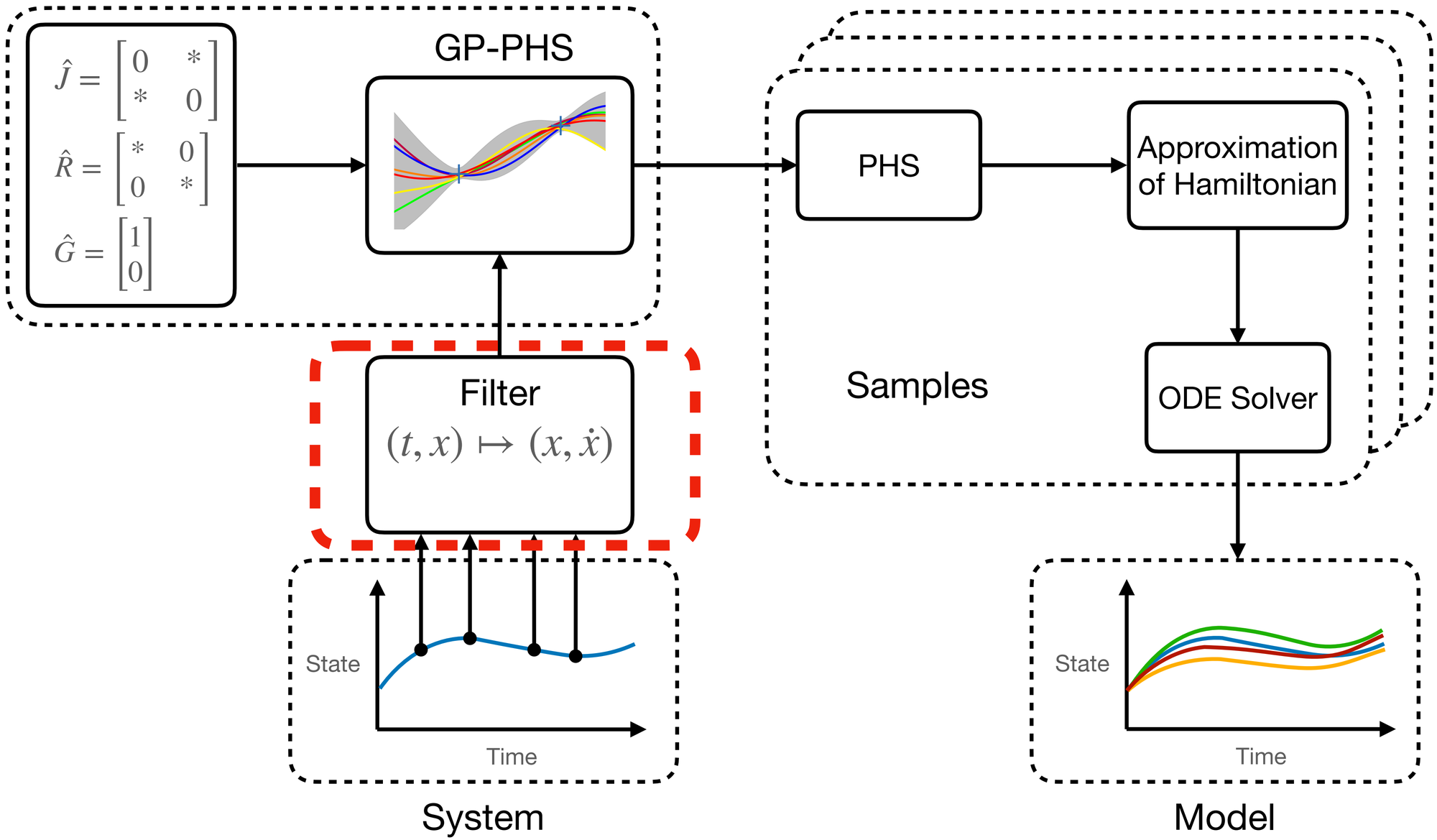
CPU & GPU support

Support

Comprehensive documentation

maintenance, new features, …

GP-PHS


$\hat{J} = \begin{bmatrix} 0 & * \\ * & 0 \end{bmatrix}$
$\hat{R} = \begin{bmatrix} * & 0 \\ 0 & * \end{bmatrix}$
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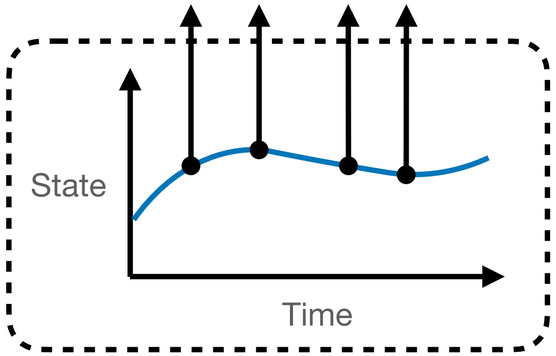
GP-PHS
Filter
$(t, x) \mapsto (x, \dot{x})$
State
Time
System
PHS
Approximation of Hamiltonian
ODE Solver
Samples
State
Time
Model

1. Initialization

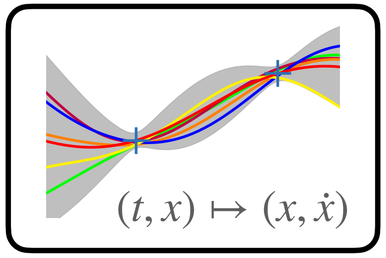


Time stamps $T = [t_1, \ldots, t_N]$

State observations $X = [\tilde{x}_1, \ldots, \tilde{x}_N]$

```
model = Model(T, X, dX=None, G=G, u=u)
```

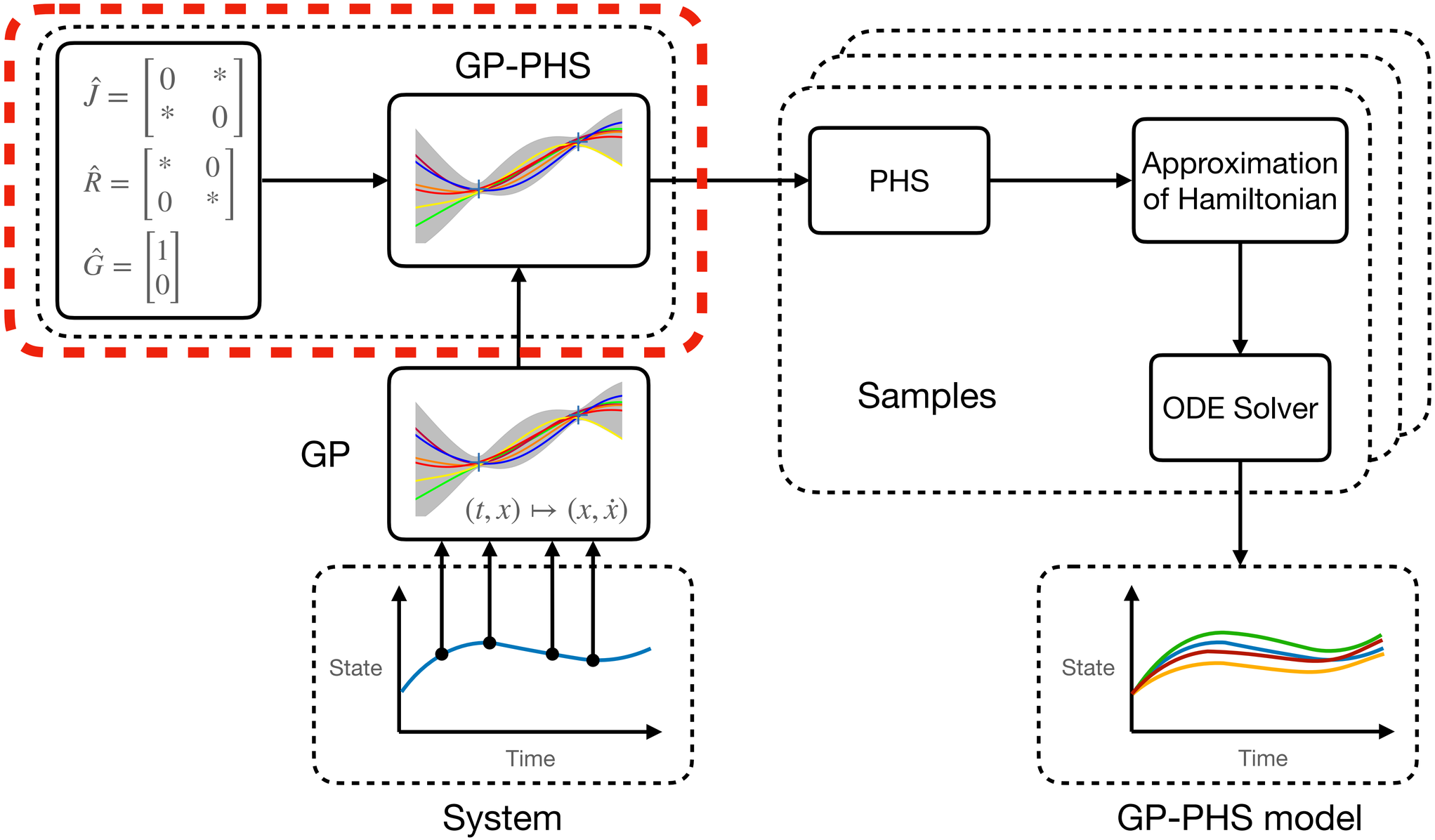
GP



$$\mu(x \mid t, \mathscr{D}) = k(t, T)K(T, T)^{-1}Y \qquad \mu(\dot{x} \mid t, \mathscr{D}) = \frac{\partial}{\partial t}k(t, T)K(T, T)^{-1}Y$$

$$\mathscr{D}_x = \{x(t_i), \dot{x}(t_i)\}_{i=1,\ldots,N}$$

GP-PHS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GP-PHS
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$(t, x) \mapsto (x, \dot{x})$
State
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Samples
ODE Solver
State
Time
GP-PHS model

2. Training

GP prior on Hamiltonian

$$\dot{x} = [J(x) - R(x)]\frac{\partial H}{\partial x} + G(x)u \quad \rightarrow \quad \dot{x} \sim GP(\hat{G}(x)u, k_{phs}(x, x'))$$

Linear operator

Port-Hamiltonian Kernel

Parametrized estimates

$$k_{phs}(x, x') = \sigma_f^2 [\hat{J}(x) - \hat{R}(x)] \left[\frac{\partial}{\partial x \partial x'} \underbrace{\exp(-\|x - x'\|_\Lambda^2)}_{\text{Squared exp. kernel}} \right] \overbrace{[\hat{J}(x') - \hat{R}(x')]^\top}$$

Optimizing parameters by means of likelihood function $p(\dot{x} \,|\, x, \sigma_f, \Lambda, \hat{J}, \hat{R}, \hat{G})$

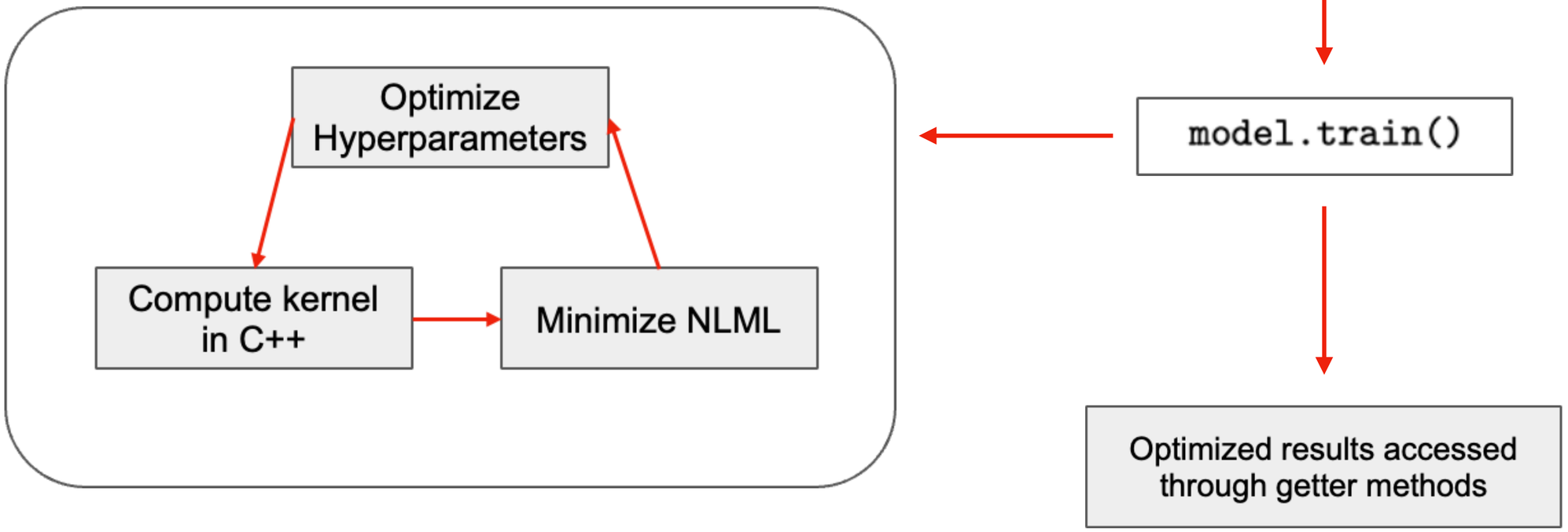
PHS kernel creates distribution over PHS

2. Training

Estimated parameters

$$\hat{J} - \hat{R} = \begin{bmatrix} jr_{11} & jr_{12} \\ -jr_{12} & jr_{22} \end{bmatrix}$$

```
hpr=Hyp(JR=[[jr11, jr12, jr22],to_optimize])
model.set_Hyp(hpr)
```



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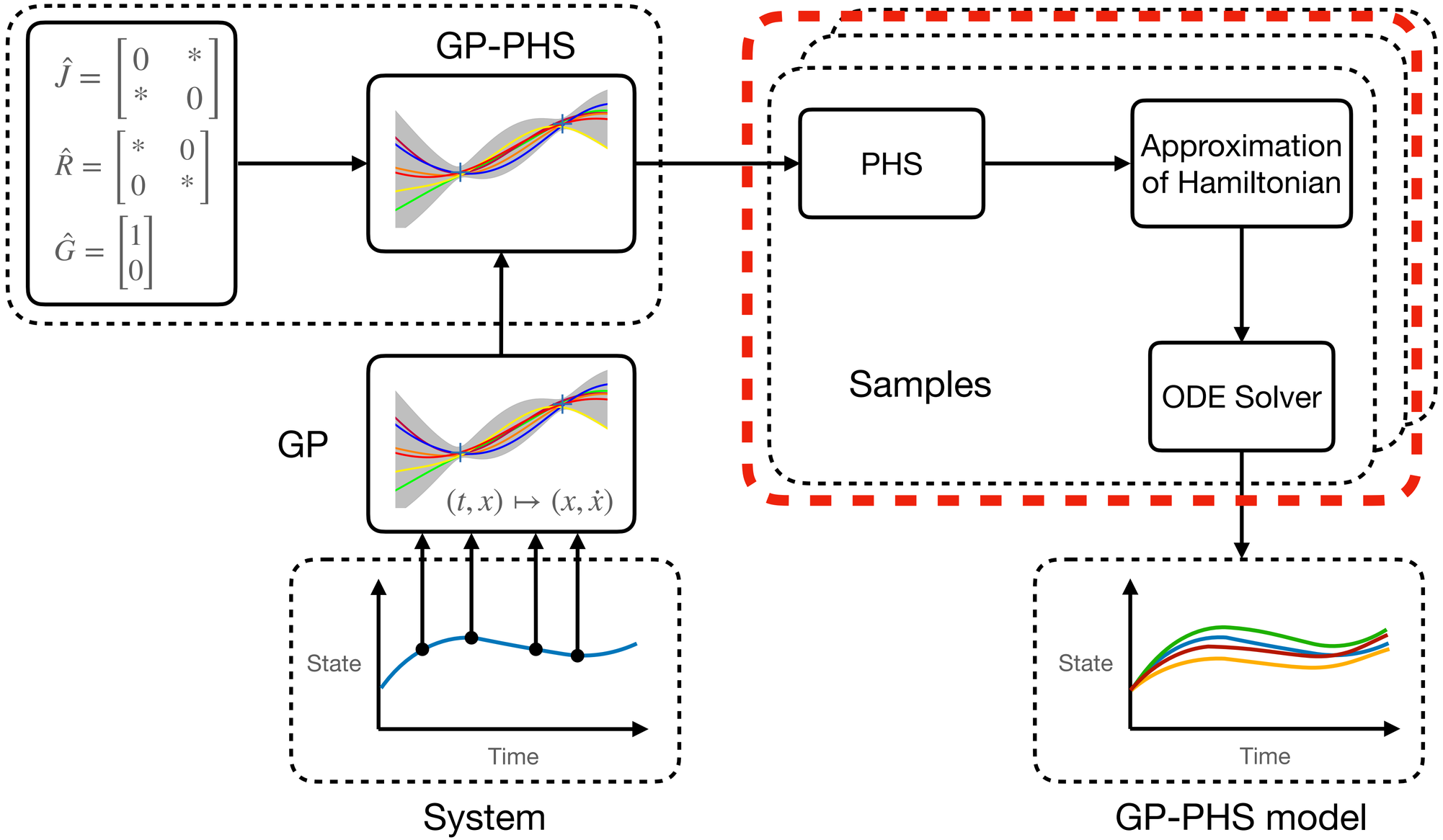
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GP-PHS model

3. Prediction

PHS

$$\begin{bmatrix} \dot{X} \\ \hat{f}(x^*) \end{bmatrix} = \mathcal{N}\left(0, \begin{bmatrix} K_{phs} & k_{phs}(X, x^*) \\ k_{phs}(X, x^*)^\top & k_{phs}(x^*, x^*) \end{bmatrix}\right)$$

$$\dot{x} = \hat{f}(x, \omega)$$

Not callable
(computational expensive)

Approximation of Hamiltonian

$$\begin{bmatrix} \dot{X} \\ \hat{H}(x^*) \end{bmatrix} = \mathcal{N}\left(0, \begin{bmatrix} K_{phs} & k_{\dot{x}H}(X, x^*) \\ k_{\dot{x}H}(X, x^*)^\top & k_{HH}(x^*, x^*) \end{bmatrix}\right)$$

$$\hat{H}(x^*, \omega) \xrightarrow{\text{Approx.}} \hat{H}^*(x^*)$$

ODE Solver

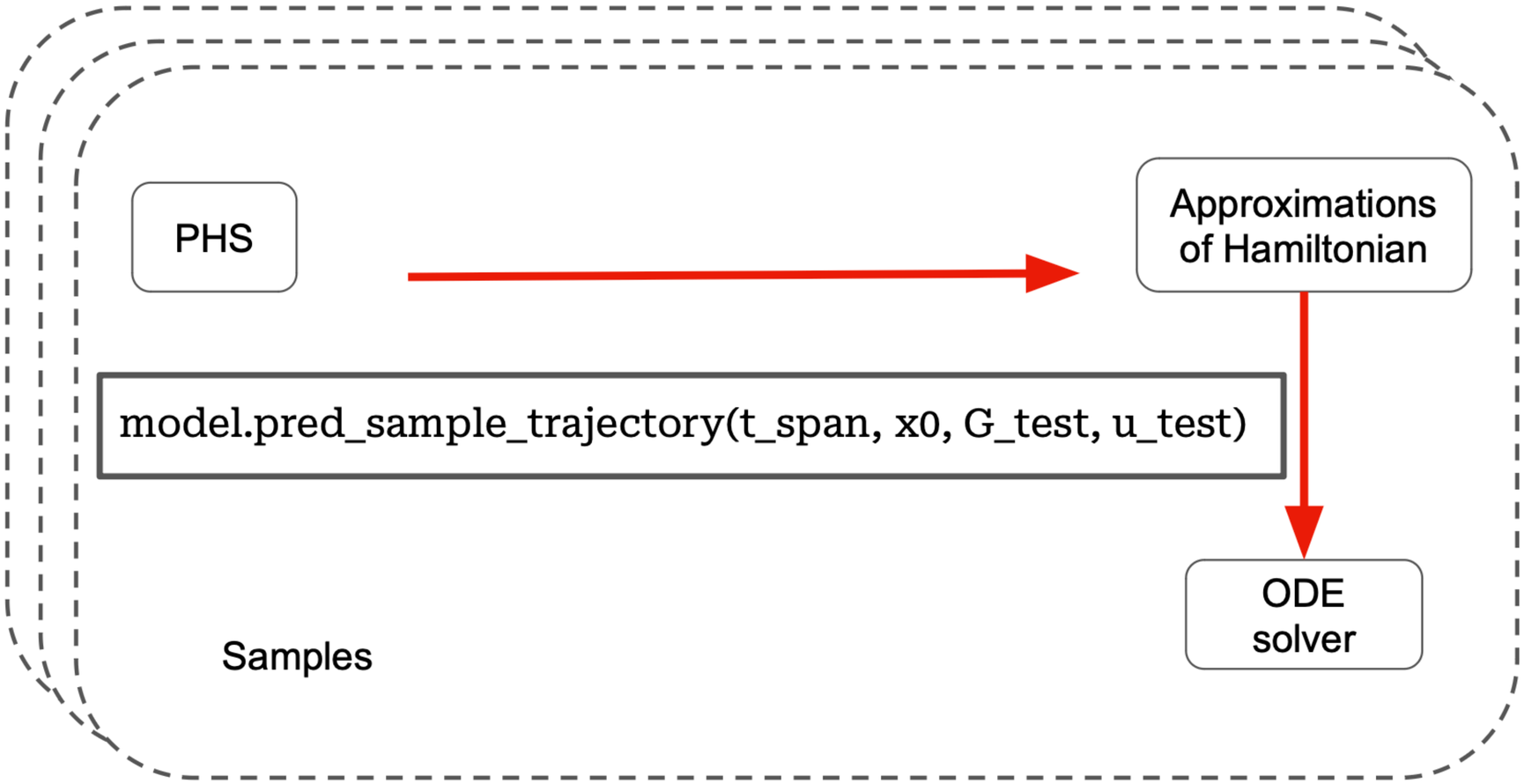
$$\dot{x} = [\hat{J}(x) - \hat{R}(x)]\frac{\partial \hat{H}^*}{\partial x} + \hat{G}(x)u \xrightarrow{\text{Solver}} x(t)$$

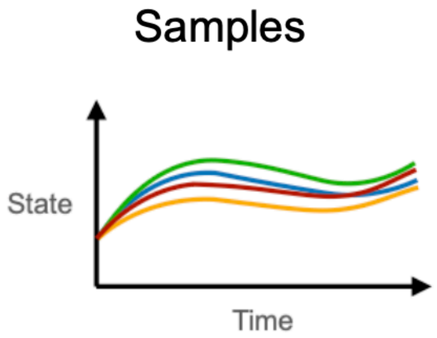
Approximation of H: Callable and structure preserving

3. Prediction

Time stamps $T_{span} = [t_1, \ldots, t_N]$

Initial value x_0, test input $u_{test}(t)$





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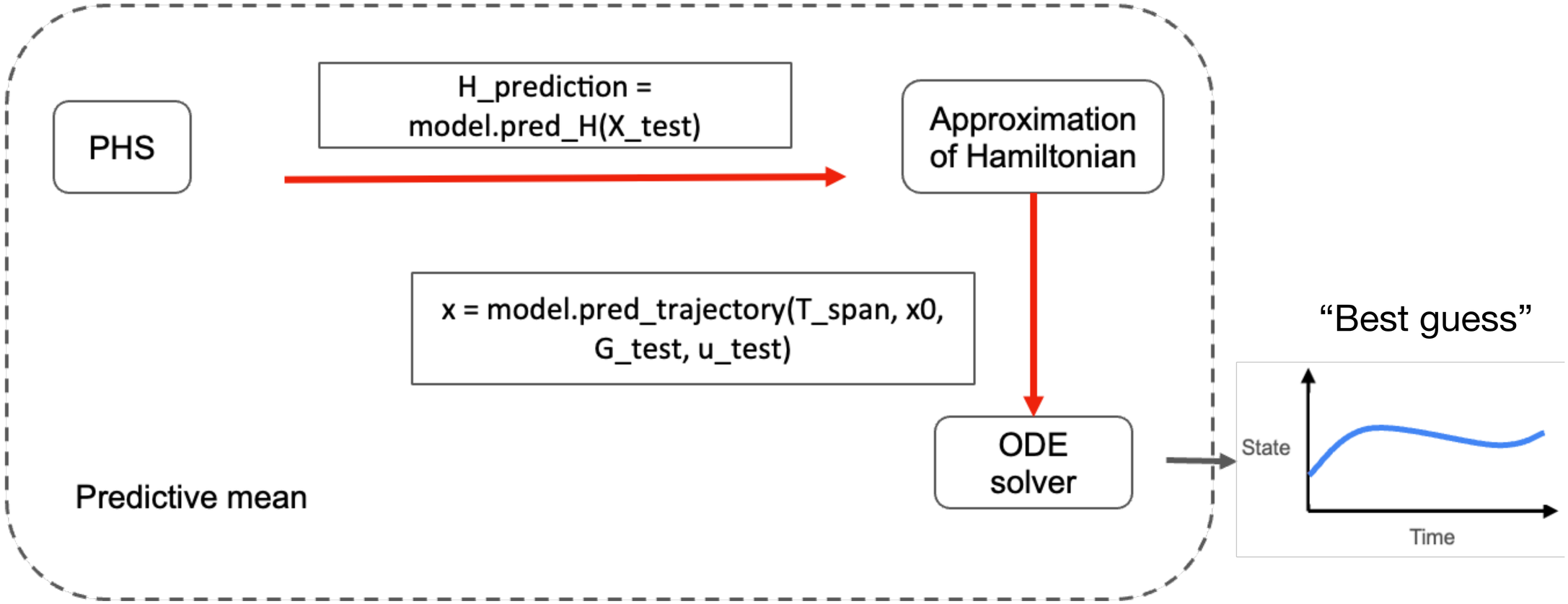
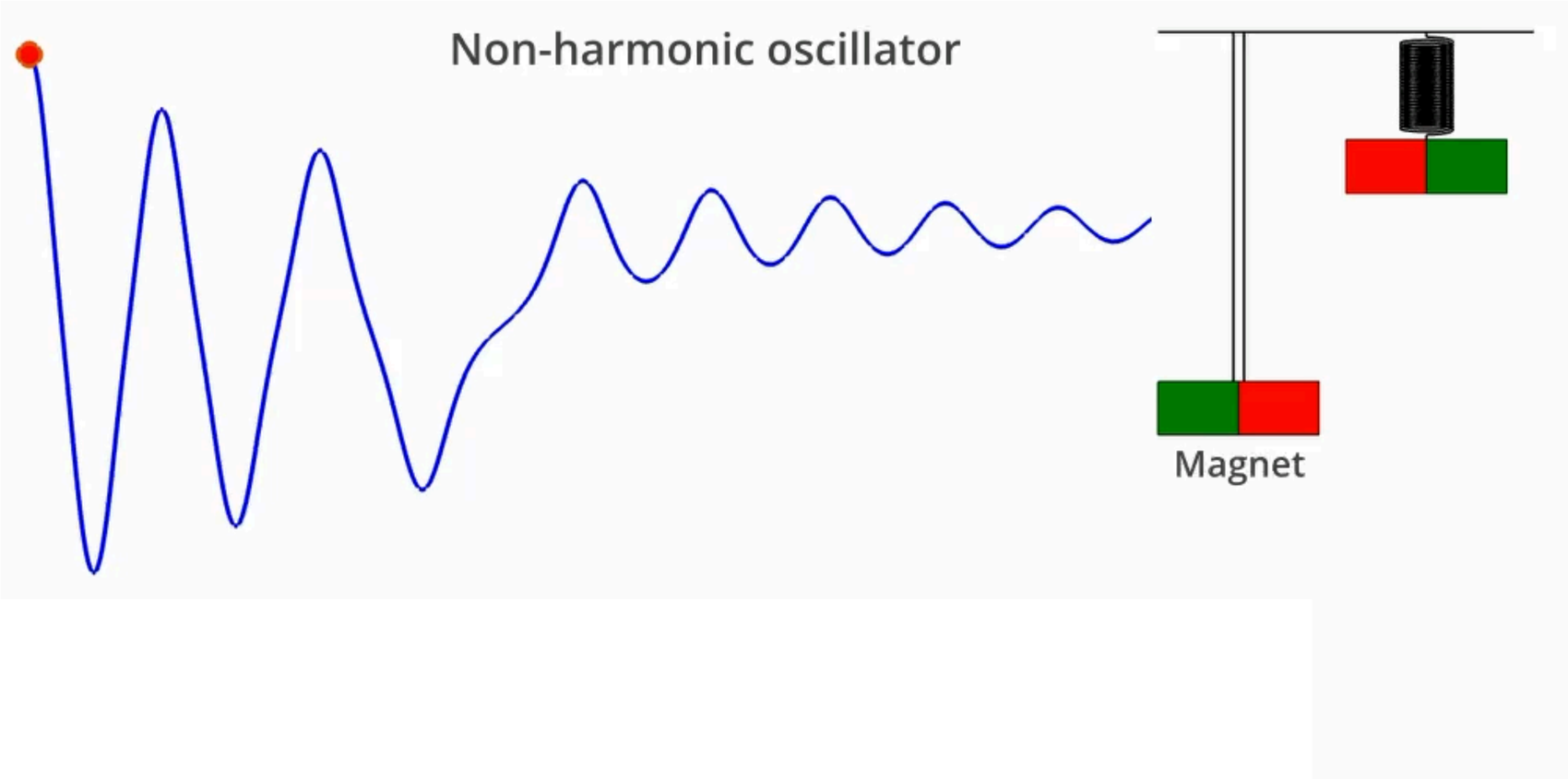


Example



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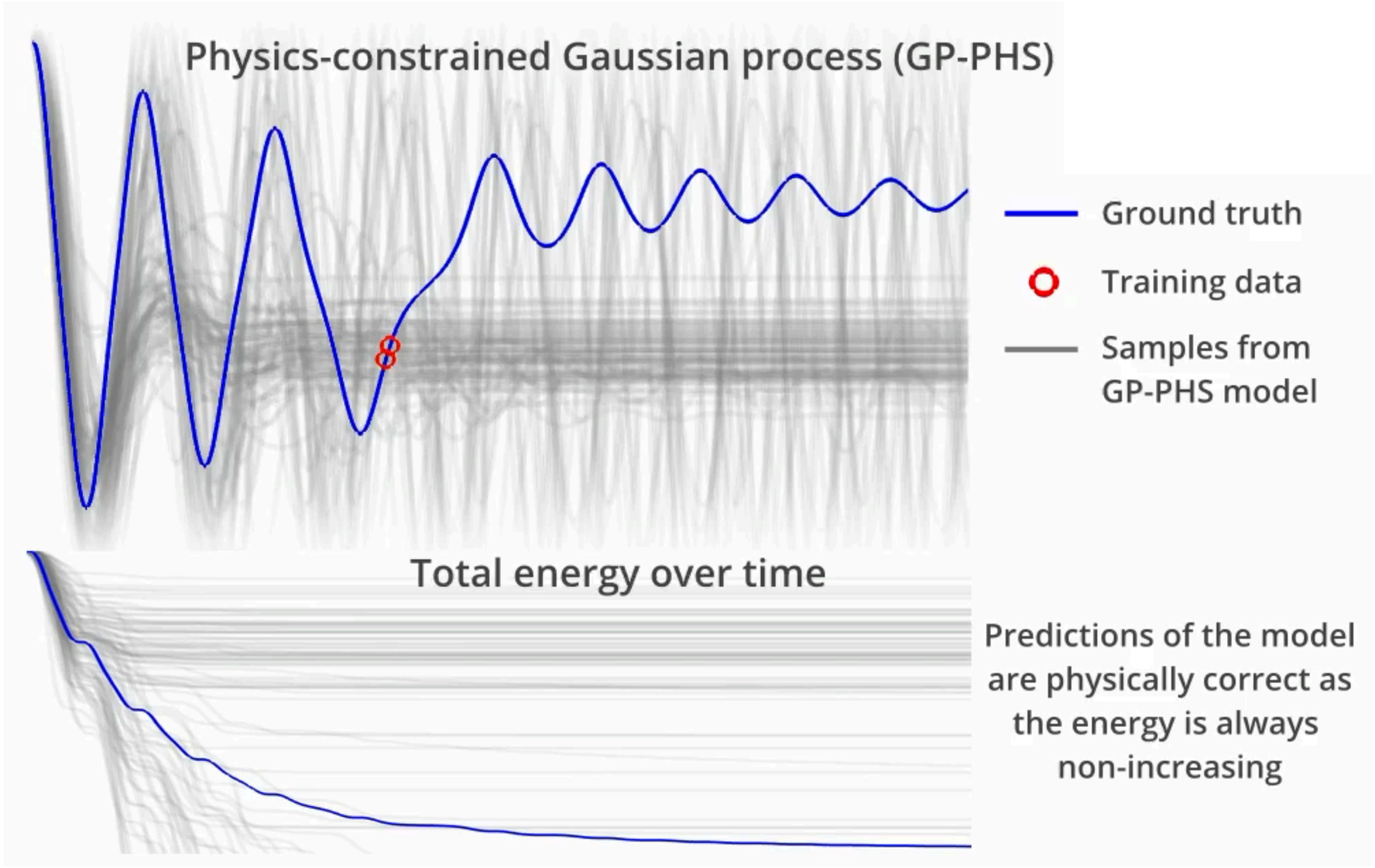
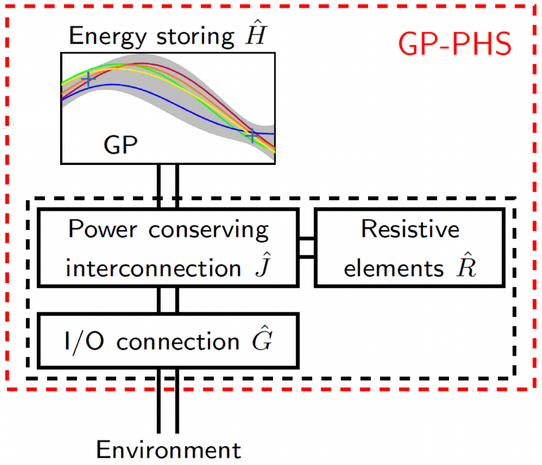

Physics-constrained Gaussian process (GP-PHS)
Ground truth
Training data
Samples from GP-PHS model
Total energy over time
Predictions of the model are physically correct as the energy is always non-increasing

Conclusion

Python Gaussian Process port-Hamiltonian System Toolbox



- User-friendly toolbox for learning of PHS based on observed data
- Physically correct data-driven model with uncertainty quantification
- Preserve the interconnection property and passivity characteristic

Tommy Li website:

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www.tbeckers.com

https://peilun-tommy-li.github.io

T. Beckers. “Data-driven Bayesian Control of Port-Hamiltonian Systems”.In: *Proceedings of the Conference on Decision and Control*. 2023

T. Beckers, T. Z. Jiahao, and G. J. Pappas. “Learning Switching Port-Hamiltonian Systems with Uncertainty Quantification”. In: *Proceedings of the IFAC World Congress*. 2023.

T. Beckers, J. H. Seidman, P. Perdikaris, and G. J. Pappas. “Gaussian Process Port-Hamiltonian Systems: Bayesian Learning with Physics Prior”. In: Proceedings of the Conference on Decision and Control. 2022.