Imperial College London

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Learning Invariances in Dynamical System

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Dynamical System

$$m\frac{d^2x}{dt^2} + b\frac{dx}{dt} + kx = 0,$$

Dynamical System

$$\frac{d^n x}{dt^n} = F\left(t, x, \frac{dx}{dt}, \dots, \frac{d^{n-1}x}{dt^{n-1}}\right),$$

$$\begin{cases} \dot{x}_1 = f_1(x_1, \dots, x_n) \\ \vdots \\ \dot{x}_n = f_n(x_1, \dots, x_n) \end{cases}$$

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Planetary Evolution; Predator-Prey Dynamics, Protein mechanics, Quantum Mechanics

Symmetry and Invariances

Gaussian Process (GP)

Definition

GP is a collection of random variables, any finite number of which have a joint Gaussian distribution

Gaussian Process (GP)

$$\begin{bmatrix} f \\ f^* \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} K(X, X) & K(X, X^*) \\ K(X^*, X) & K(X^*, X^*) \end{bmatrix}\right),$$

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$$y = f + \epsilon;\ \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

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$$\begin{bmatrix} y \\ f^* \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} K(X,X) + \sigma_n^2 \mathbb{I} & K(X,X^*) \\ K(X^*,X) & K(X^*,X^*) \end{bmatrix}\right).$$

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A very important formula:

$$\text{if } \begin{bmatrix} x \\ y \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu_x \\ \mu_y \end{bmatrix}, \begin{bmatrix} A & C \\ C^T & B \end{bmatrix}\right),$$

$$x|y \sim \mathcal{N}\left(\mu_x + CB^{-1}(y-\mu_y), A - CB^{-1}C^T\right)$$

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$$f^*|X,y,X^* \sim \mathcal{N}\left(\overline{f^*}, \mathrm{cov}(f^*)\right)$$

$$\overline{f^*} = K(X^*,X)[K(X,X)+\sigma_n^2\mathbb{I}]^{-1}y$$

$$\mathrm{cov}(f^*) = K(X^*,X^*) - K(X^*,X)[K(X,X)+\sigma_n^2\mathbb{I}]^{-1}K(X,X^*)$$

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$$\log p(\mathbf{y} \mid X) = -\frac{1}{2}\mathbf{y}^\top \left(K+\sigma_n^2\mathbf{I}\right)^{-1}\mathbf{y} - \frac{1}{2}\log\left|K+\sigma_n^2\mathbf{I}\right| - \frac{n}{2}\log 2\pi.$$

Kernel

$$k_{RBF}(r) = \exp(-\frac{r^2}{2l^2})$$

$$k_{\text{Matérn}}(r) = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu} r}{\ell} \right)^{\nu} K_{\nu} \left(\frac{\sqrt{2\nu} r}{\ell} \right)$$

$$k_{periodic\ RBF}(r) = \exp\left(-\frac{2\sin^2\left(\frac{r}{2}\right)}{\ell^2} \right),$$

Kernel

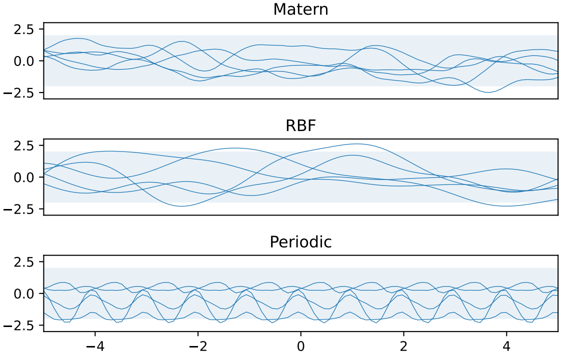

Figure 1: Samples from different GP priors of RBF, Matérn and periodic kernel.

GP regression in action

If we would like to fit a function $y = (x + x^2)\sin(x)$.

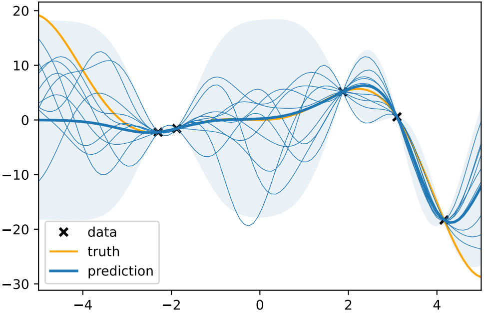

Figure 2: GP fit of the function $f = (x + x^2)\sin(x)$ with posterior samples, light shaded blue indicates 95% credible interval.

Related Work

Methods	Respect the physics laws	Learn the physics laws	Generalise beyond physics
ODE approach	X	O	O
Symbolic approach	O	O	X
Physics informed ML	O	X	X
Energy conserving NN	O	X	X
GP in dynamical system	X	O	O
Our method	O	O	O

Table 1: Comparing the capabilities of different existing approach to learning invariance in dynamical systems

Invariance Kernel I

We have a general dynamical system with coordinates $\mathbf{p}, \mathbf{q}$, then we will call the dynamics $\frac{d\mathbf{p}}{dt} = a(\mathbf{p}, \mathbf{q})$ and $\frac{d\mathbf{q}}{dt} = v(\mathbf{p}, \mathbf{q})$.

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$$\mathbf{f}(\mathbf{q}, \mathbf{p}) = \begin{pmatrix} \mathbf{a}(\mathbf{q}, \mathbf{p}) \\ \mathbf{v}(\mathbf{q}, \mathbf{p}) \end{pmatrix}$$

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$$\mathbf{f}(\mathbf{q}, \mathbf{p}) = \begin{pmatrix} \mathbf{a}(\mathbf{q}, \mathbf{p}) \\ \mathbf{v}(\mathbf{q}, \mathbf{p}) \end{pmatrix}$$

We will then put a GP prior on $\mathbf{f}$ so that

$$\mathbf{f} \sim \mathcal{GP}(m, K)$$

Invariance Kernel II

$$X \equiv \begin{pmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{pmatrix} = \begin{pmatrix} q_{11} & q_{21} & \dots & q_{d1} & p_{11} & p_{21} & \dots & p_{d1} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ q_{1n} & q_{2n} & \dots & q_{dn} & p_{1n} & p_{2n} & \dots & p_{dn} \end{pmatrix}.$$

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$$\mathbf{f}(X) = \begin{pmatrix} a_1(\mathbf{x}_1) \\ \vdots \\ a_1(\mathbf{x}_n) \\ \vdots \\ a_d(\mathbf{x}_n) \\ v_1(\mathbf{x}_1) \\ \vdots \\ v_d(\mathbf{x}_n) \end{pmatrix}$$

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Invariance Kernel II

$$K = \mathrm{Cov}(\mathbf{f}(X), \mathbf{f}(X')) =$$

$$\begin{pmatrix} K_{a_1}(X, X') & \dots & \dots & \dots & 0 \\ \vdots & \ddots & \dots & \ddots & \vdots \\ 0 & \dots & K_{a_d}(X, X') & \dots & 0 \\ \vdots & \ddots & \vdots & K_{v_1}(X, X') & \vdots \\ 0 & \dots & 0 & \dots & K_{v_d}(X, X') \end{pmatrix},$$

where each K_f is an RBF kernel

Invariance Kernel III

$$\mathcal{L}[E] \equiv \frac{dE}{dt} = \sum_{i=1}^{d} \frac{\partial E}{\partial p_i}\frac{\partial p_i}{\partial t} + \sum_{i=1}^{d} \frac{\partial E}{\partial q_i}\frac{\partial q_i}{\partial t}$$

$$= \sum_{i=1}^{d} \frac{\partial E}{\partial p_i} a_i(\mathbf{p}, \mathbf{q}) + \sum_{i=1}^{d} \frac{\partial E}{\partial q_i} v_i(\mathbf{p}, \mathbf{q}) = L[\mathbf{f}]$$

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$$\begin{pmatrix} \mathbf{f}(X) \\ L[\mathbf{f}(X_L)] \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} \mathbf{0}_{2nd} \\ \mathbf{0}_{\ell} \end{pmatrix}, \begin{pmatrix} K & LK \\ KL^T & LKL^T \end{pmatrix} \right)$$

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$$\mathbf{f}(X) | L[\mathbf{f}(X_L)] = 0 \sim \mathcal{N}\left(\mathbf{0}_{2nd}, \left(K - LK(LKL^T)^{-1} KL^T\right)\right)$$

Learning Invariance

$$\mathcal{L}[E] = \sum_{i=1}^{d} \frac{\partial E}{\partial p_i} a_i(\mathbf{p}, \mathbf{q}) + \sum_{i=1}^{d} \frac{\partial E}{\partial q_i} v_i(\mathbf{p}, \mathbf{q})$$

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- One dimensional:

$$L[\mathbf{f}] = f(p)a + g(q)v$$

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- One dimensional:

$$L[\mathbf{f}] = f(p)a + g(q)v$$

- Two dimensional:

$$\begin{aligned} L[\mathbf{f}] = {} & f_1(q_1, q_2, p_1, p_2)a_1 + f_2(q_1, q_2, p_1, p_2)a_2 \\ & + g_1(q_1, q_2, p_1, p_2)v_1 + g_2(q_1, q_2, p_1, p_2)v_2 \end{aligned}$$

Damped System- Approximate Invariance

we have $L[\mathbf{f}(X_L)] = \epsilon$, where $\epsilon \sim \mathcal{N}(m_L, \sigma_L^2)$

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$$\begin{pmatrix} \mathbf{f}(X) \\ L[\mathbf{f}(X_L)] \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} \mathbf{0}_{2nd} \\ \mathbf{m}_\ell \end{pmatrix}, \begin{pmatrix} K & LK \\ KL^T & LKL^T + \sigma_L^2 \mathbb{I} \end{pmatrix} \right),$$

Damped System- Latent Dynamics

$$\mathcal{L}[E] + z = \frac{dE}{dt} + z = \sum_{i=1}^{d} \frac{\partial E}{\partial p_i}\frac{\partial p_i}{\partial t} + \sum_{i=1}^{d} \frac{\partial E}{\partial q_i}\frac{\partial q_i}{\partial t} + z =$$

$$\sum_{i=1}^{d} \frac{\partial E}{\partial p_i} a_i + \sum_{i=1}^{d} \frac{\partial E}{\partial q_i} v_i + z = L_\gamma[\mathbf{f}_\gamma] = 0$$

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$$\begin{pmatrix} \begin{pmatrix} \mathbf{f}(X) \\ z(X) \end{pmatrix} \\ L_\gamma[\mathbf{f}(X_L), z(X_L)] \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} \mathbf{0}_{3nd} \\ \mathbf{0}_\ell \end{pmatrix}, \begin{pmatrix} K & L_\gamma K \\ K L_\gamma^T & L_\gamma K L_\gamma^T \end{pmatrix} \right),$$

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Experiments

1. Data Generation
2. Evaluation Methods
3. Implementation Techicalities

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Simple Harmonic Motion (SHM)

$$\frac{d^2x}{dt^2} = -\frac{kx}{m}$$

$$x = A\sin(\omega_0 t + \phi)$$

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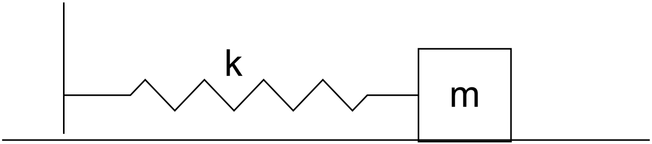

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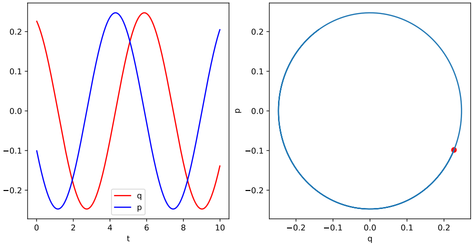

SHM Invariance Kernel- I

We had $\mathcal{L}[E] \equiv \frac{dE}{dt} = \sum_{i=1}^{d} \frac{\partial E}{\partial p_i} a_i(\mathbf{p}, \mathbf{q}) + \sum_{i=1}^{d} \frac{\partial E}{\partial q_i} v_i(\mathbf{p}, \mathbf{q}) = L[\mathbf{f}]$

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$$E = \frac{kq^2}{2} + \frac{mp^2}{2}$$

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So we have

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So we have

$$L[\mathbf{f}] = mpa + kvp = 0$$

$$L([\mathbf{f}(X_L)]) = \begin{pmatrix} mp_{L,1}a(q_{L,1}, p_{L,1}) + kq_{L,1}v(q_{L,1}, p_{L,1}) \\ \vdots \\ mp_{L,\ell}a(q_{L,\ell}, p_{L,\ell}) + kq_{L,\ell}v(q_{L,\ell}, p_{L,\ell}) \end{pmatrix},$$

SHM Invariance Kernel- II

$$\begin{pmatrix} \mathbf{f}(X) \\ L([\mathbf{f}(X_L)]) \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} 0_{2n} \\ 0_\ell \end{pmatrix}, \begin{pmatrix} A & B \\ C & D \end{pmatrix} \right)$$

$$\mathbf{f}(X) | L[\mathbf{f}(X_L)] = 0 \sim \mathcal{N}(0_{2n}, A - BD^{-1}C),$$

SHM Invariance Kernel- II

$$A = K(X,X), B = \begin{pmatrix} K_a(X,X_L) \\ K_v(X,X_L) \end{pmatrix} \odot \begin{pmatrix} mP_L \\ kQ_L \end{pmatrix}, C = B^T,$$

$$D = K_a(X_L,X_L) \odot m^2(p_L \otimes p_L) + K_v(X_L,X_L) \odot k^2(q_L \otimes q_L),$$

$$P_L = \begin{pmatrix} p_{L,1} & \cdots & p_{L,\ell} \\ \vdots & \text{repeats n rows} & \vdots \\ p_{L,1} & \cdots & p_{L,\ell} \end{pmatrix},$$

$$p_L \otimes p_L = \begin{pmatrix} p_{L,1}^2 & p_{L,1}p_{L,2} & \cdots & p_{L,1}p_{L,\ell} \\ \vdots & \vdots & \vdots & \vdots \\ p_{L,\ell}p_{L,1} & p_{L,\ell}p_{L,2} & \cdots & p_{L,\ell}^2 \end{pmatrix},$$

SHM Invariance Kernel- III

$$
\begin{aligned}
B_{ij} &= \mathrm{Cov}(\mathbf{f}(X), L[\mathbf{f}(X_L)])_{ij} \\
&= \mathrm{Cov}(\mathbf{f}(X)_i, L[\mathbf{f}(X_L)]_j) \\
&= \begin{cases} \mathrm{Cov}(a(q_i,p_i), mp_{L,j}a(q_{L,j},p_{L,j}) + kq_{L,j}v(q_{L,j},p_{L,j})) & i \leq n \\ \mathrm{Cov}(v(q_i,p_i), mp_{L,j}a(q_{L,j},p_{L,j}) + kq_{L,j}v(q_{L,j},p_{L,j})) & i > n \end{cases} \\
&= \begin{cases} K_{RBF,a}(\mathbf{x}_i,\mathbf{x}_{L,j})mp_{L,j} & i \leq n \\ K_{RBF,v}(\mathbf{x}_i,\mathbf{x}_{L,j})kq_{L,j} & i > n \end{cases},
\end{aligned}
$$

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SHM Invariance Kernel- III

$$
\begin{aligned}
D_{ij} &= \mathrm{Cov}(L[\mathbf{f}(X_L)], L[\mathbf{f}(X_L)])_{ij} \\
&= \mathrm{Cov}(mp_{L,i}a(q_{L,i}, p_{L,i}) + kq_{L,i}v(q_{L,i}, p_{L,i}), mp_{L,i}a(q_{L,i}, p_{L,i}) + kq_{L,i}v(\\
&= m^2 p_{L,i} p_{L,j} K_{RBF,a}(\mathbf{x}_{L,i}, \mathbf{x}_{L,j}) + k^2 q_{L,i} q_{L,j} K_{RBF,v}(\mathbf{x}_{L,i}, \mathbf{x}_{L,j})
\end{aligned}
$$

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Learning Invariance

$$\mathcal{L}[E] \equiv \frac{dE}{dt} = \sum_{i=1}^{d} \frac{\partial E}{\partial p_i} a_i(\mathbf{p}, \mathbf{q}) + \sum_{i=1}^{d} \frac{\partial E}{\partial q_i} v_i(\mathbf{p}, \mathbf{q}) = L[\mathbf{f}]$$

$$L[\mathbf{f}] = f(p)a + g(q)v$$

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Learning Invariance

$$L[\mathbf{f}] = f(p)a + g(q)v$$

$$A = K(X, X), B = \begin{pmatrix} K_a(X, X_L) \\ K_v(X, X_L) \end{pmatrix} \odot \begin{pmatrix} f(P_L) \\ g(Q_L) \end{pmatrix}, C = B^T,$$

$$D = K_a(X_L, X_L) \odot (f(p_L) \otimes f(p_L)) + K_v(X_L, X_L) \odot (g(q_L) \otimes g(q_L)),$$

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$$L[\mathbf{f}] = f(p)a + g(q)v$$

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$$D = K_a(X_L,X_L) \odot (f(p_L) \otimes f(p_L)) + K_v(X_L,X_L) \odot (g(q_L) \otimes g(q_L)),$$

$$f(P_L) = \begin{pmatrix} f(p_{L,1}) & \dots & f(p_{L,\ell}) \\ \vdots & \text{repeats n rows} & \vdots \\ f(p_{L,1}) & \dots & f(p_{L,\ell}) \end{pmatrix},$$

$$f(p_L) \otimes f(p_L) = \begin{pmatrix} f(p_{L,1})^2 & f(p_{L,1})f(p_{L,2}) & \dots & f(p_{L,1})f(p_{L,\ell}) \\ \vdots & \vdots & \vdots & \vdots \\ f(p_{L,\ell})f(p_{L,1}) & f(p_{L,\ell})f(p_{L,2}) & \dots & f(p_{L,\ell})^2 \end{pmatrix},$$

Results for SHM

Method	RBF	Known Invariance	Learnt Invariance
Log Marginal Likelihood	67.67	82.00	79.24
MSE	0.0950	0.0017	0.0027

Table 2: SHM performance.

Results for SHM

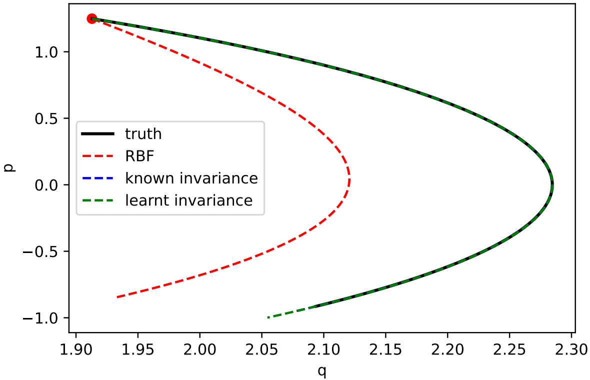

Figure 3: One SHM predicted trajectory.

Results for SHM

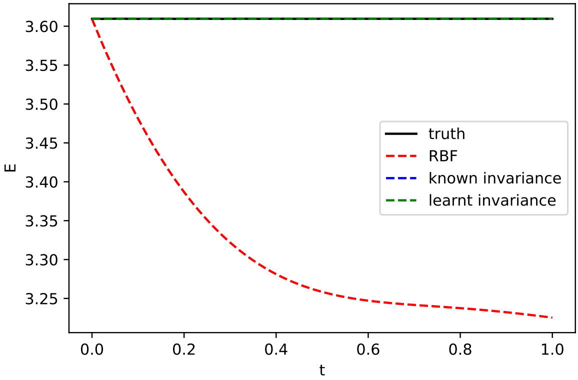

Figure 3: The energy along the trajectory.

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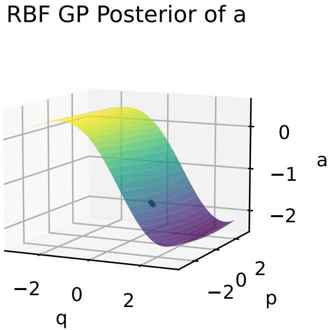
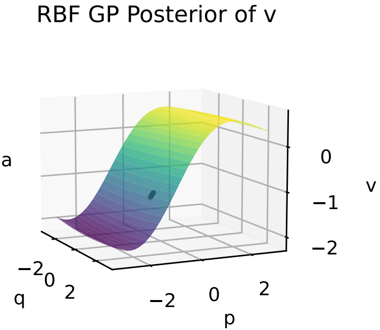
Results for SHM





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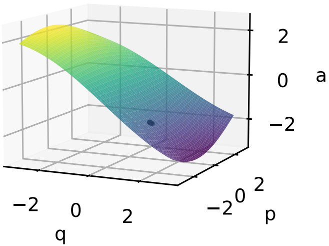
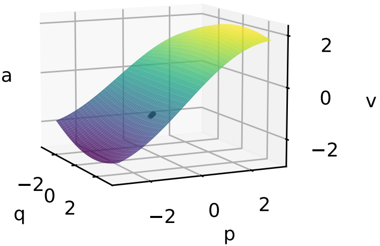
Results for SHM

Invariance GP Posterior of a



Invariance GP Posterior of v



Results for SHM

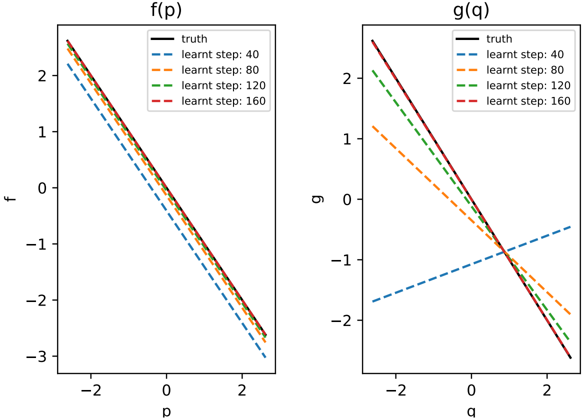


Figure 3: Learnt invariance for SHM.

Pendulum

$$\frac{d^2q}{dt^2} = -\frac{g}{\ell}\sin q,$$

Pendulum

$$\frac{d^2q}{dt^2} = -\frac{g}{\ell}\sin q,$$

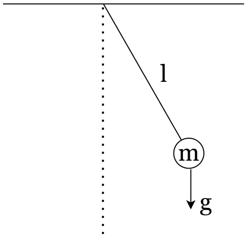


Figure 4: A pendulum is a simple system that is nonlinear.

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Pendulum

$$\frac{d^2q}{dt^2} = -\frac{g}{\ell}\sin q,$$

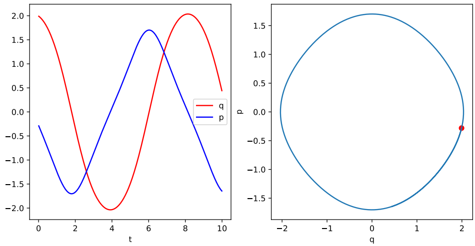

Figure 4: Example trajectory of pendulum.

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Pendulum Invariance

$$\mathcal{L}[E] \equiv \frac{dE}{dt} = \sum_{i=1}^{d} \frac{\partial E}{\partial p_i} a_i(\mathbf{p}, \mathbf{q}) + \sum_{i=1}^{d} \frac{\partial E}{\partial q_i} v_i(\mathbf{p}, \mathbf{q}) = L[\mathbf{f}]$$

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Pendulum Invariance

$$\mathcal{L}[E] \equiv \frac{dE}{dt} = \sum_{i=1}^{d} \frac{\partial E}{\partial p_i} a_i(\mathbf{p}, \mathbf{q}) + \sum_{i=1}^{d} \frac{\partial E}{\partial q_i} v_i(\mathbf{p}, \mathbf{q}) = L[\mathbf{f}]$$

$$E = \frac{m\ell^2 p^2}{2} + mg\ell(1 - \cos q)$$

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Pendulum Invariance

$$\mathcal{L}[E] \equiv \frac{dE}{dt} = \sum_{i=1}^{d} \frac{\partial E}{\partial p_i} a_i(\mathbf{p}, \mathbf{q}) + \sum_{i=1}^{d} \frac{\partial E}{\partial q_i} v_i(\mathbf{p}, \mathbf{q}) = L[\mathbf{f}]$$

$$E = \frac{m\ell^2 p^2}{2} + mg\ell(1 - \cos q)$$

$$L[\mathbf{f}] = \ell pa + g(\sin q)v = 0$$

Pendulum Invariance

$$L[\mathbf{f}] = \ell pa + g(\sin q)v = 0$$

$$B = \begin{pmatrix} K_a(X, X_L) \\ K_v(X, X_L) \end{pmatrix} \odot \begin{pmatrix} \ell P_L \\ g\sin(Q_L) \end{pmatrix},$$

$$D = K_a(X_L, X_L) \odot \ell^2(p_L \otimes p_L) + K_v(X_L, X_L) \odot g^2(\sin(q_L) \otimes \sin(q_L)),$$

Pendulum Invariance

$$L[\mathbf{f}] = \ell pa + g(\sin q)v = 0$$

$$B = \begin{pmatrix} K_a(X, X_L) \\ K_v(X, X_L) \end{pmatrix} \odot \begin{pmatrix} \ell P_L \\ g\sin(Q_L) \end{pmatrix},$$

$$D = K_a(X_L, X_L) \odot \ell^2 (p_L \otimes p_L) + K_v(X_L, X_L) \odot g^2 (\sin(q_L) \otimes \sin(q_L)),$$

$$\sin(Q_L) = g \begin{pmatrix} \sin(q_{L,1}) & \dots & \sin(q_{L,\ell}) \\ \vdots & \text{reqeats n rows} & \vdots \\ \sin(q_{L,1}) & \dots & \sin(q_{L,\ell}) \end{pmatrix},$$

$$\sin(q_L) \otimes \sin(q_L) = \begin{pmatrix} \sin(q_{L,1})^2 \dots & \sin(q_{L,1})\sin(q_{L,\ell}) & \\ \vdots & \vdots & \vdots \\ \sin(q_{L,\ell})\sin(q_{L,1}) & \dots & \sin(q_{L,\ell})^2 \end{pmatrix},$$

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Results for Pendulum

Method	RBF	Known Invariance	Learnt Invariance
Log Marginal Likelihood	299.12	331.66	325.76
MSE	0.0021	0.0009	0.0006

Table 2: Pendulum performance.

Results for Pendulum

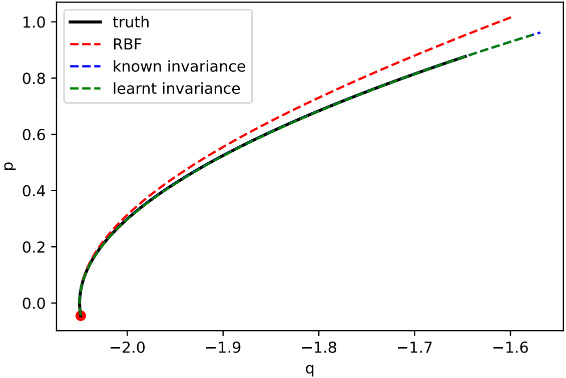

Figure 5: Pendulum predicted trajectory.

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Results for Pendulum

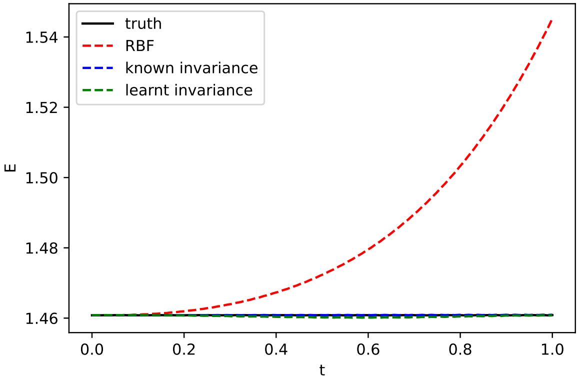

Figure 5: The energy along the trajectory.

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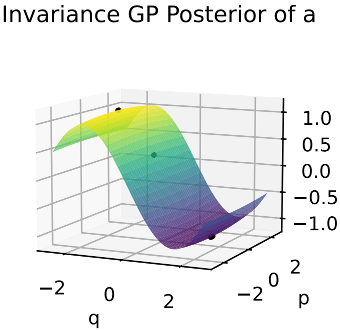
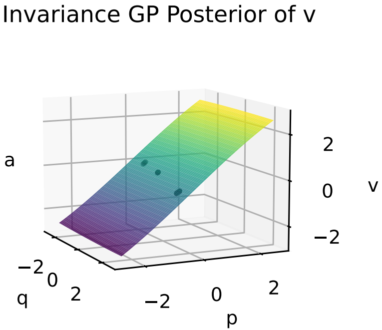
Results for Pendulum





Results for Pendulum

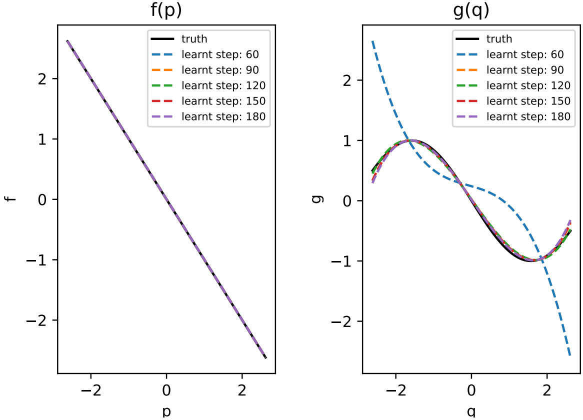


Figure 5: Learnt invariance for pendulum.

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Damped Systems

$$\frac{d^2q}{dt^2} + 2\gamma\frac{dq}{dt} + \omega_0^2 q = 0; \;\; \frac{d^2q}{dt^2} + 2\gamma\frac{dq}{dt} + \omega_0^2 \sin q = 0,$$

Two Figures aside

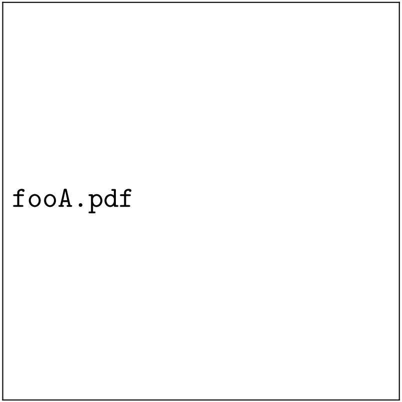

Figure 6: Caption of Figure A

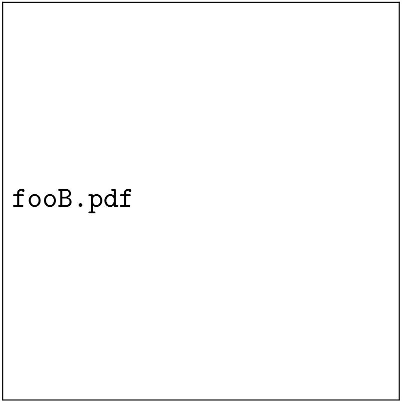

Figure 7: Caption of Figure B

Text and Figure aside

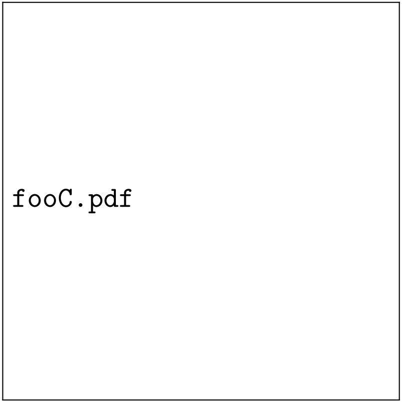

Figure 8: Caption of Figure C

Some text and a bullet point list

- ItemA
- ItemB
- ItemC
- ItemD

One Figure

`fooD.pdf`

Figure 9: Caption of Figure D