AutoIP: A United Framework to Integrate Physics into Gaussian Processes

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Advanced Methods in Applied Statistics

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Modeling Physical Systems

Our goals are to:

- Minimizing misfit
- Require few training data points
- Ensuring our model is physically realistic
- Quantifying uncertainty

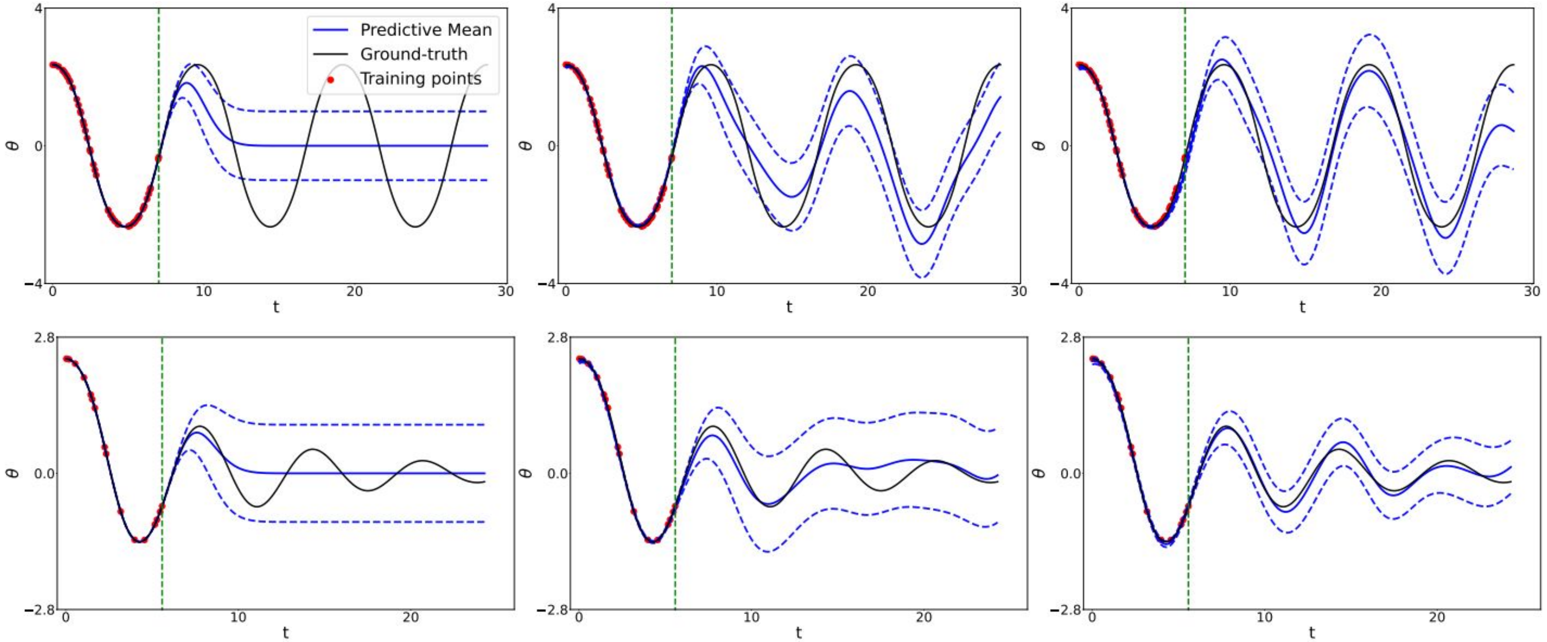
Common methods:

- Analytical Expressions
- Physics Informed Neural Networks (PINNs)

Automatically Incorporating Physics (AutoIP)

- AutoIP leverages Gaussian Processes (GPs) to predict functions that both:
  - Fits training data
  - Conforms to physically motivated partial differential equations (PDE)

AutoIP- Predicting Pendulum Dynamics



(a) GPR (b) AutoIP-I (c) AutoIP-C

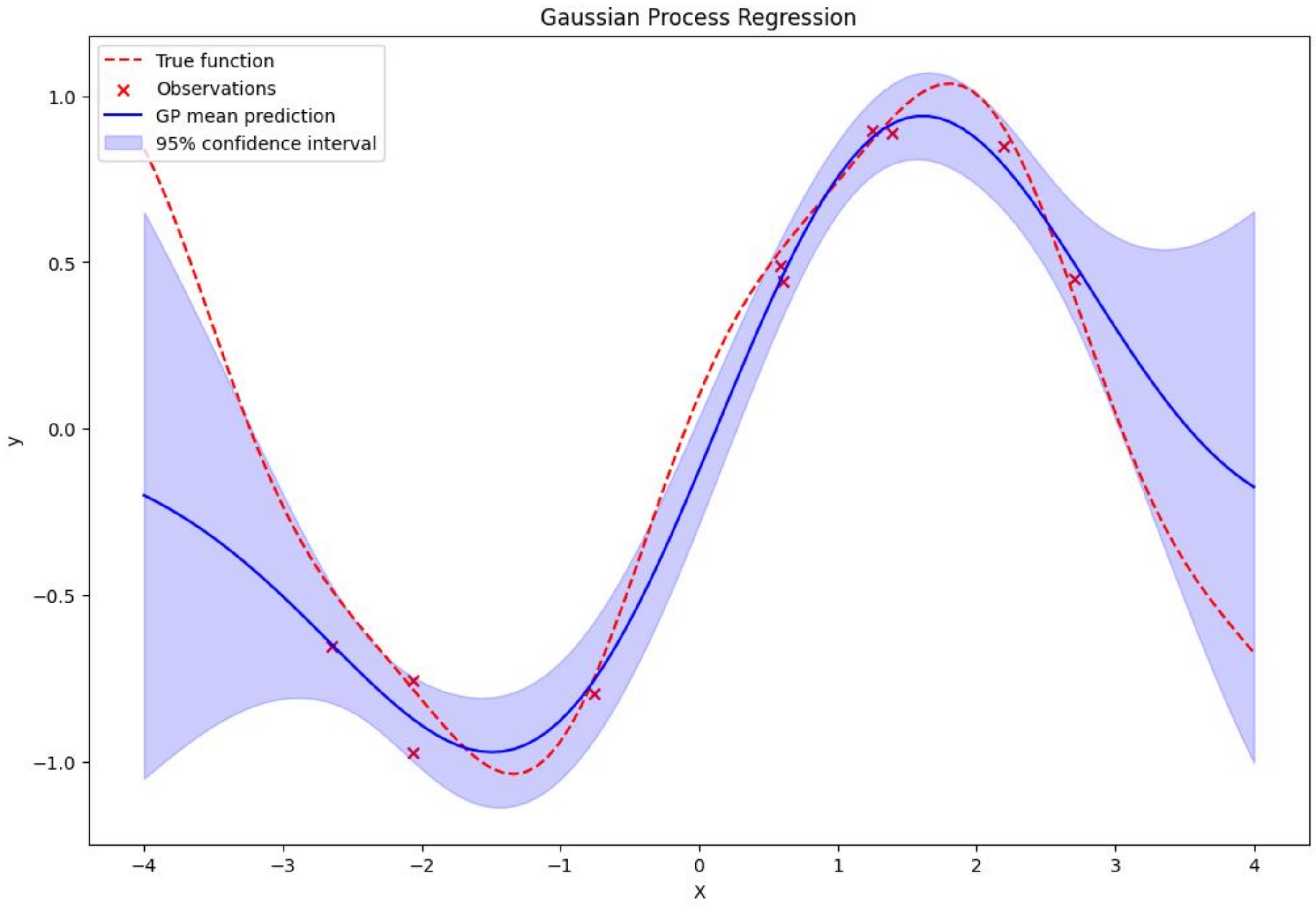
Gaussian Processes

A method that allows you to find a family of curves that fit a set of points.

Parameterized by:

- Mean Function μ(x)
  - Often set to 0
- Covariance Function
  - Kernel Function k(x, x')
  - Radial Basis Function is a

$$K(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\sigma^2}\right)$$



Gaussian Processes – Understanding the Covariance Function

- **Key idea:** Describe f(x) values over x with covariance matrices
  - Each column of covariance matrix is a separate x value.

- To illustrate this idea, we show sampling in five dimensional joint Gaussian distribution in the GIF below.

$$\boxed{f_{\mathbf{X}}(x_1,\ldots,x_k) = \frac{\exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right)}{\sqrt{(2\pi)^k|\boldsymbol{\Sigma}|}}}$$

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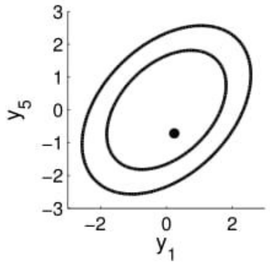
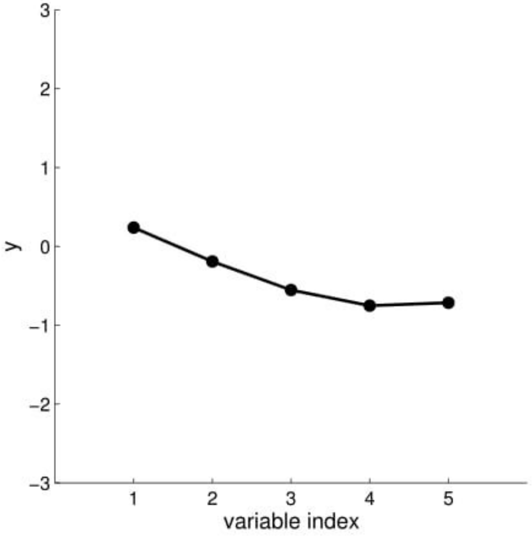


$$\Sigma = \begin{bmatrix} 1 & .9 & .8 & .6 & .4 \\ .9 & 1 & .9 & .8 & .6 \\ .8 & .9 & 1 & .9 & .8 \\ .6 & .8 & .9 & 1 & .9 \\ .4 & .6 & .8 & .9 & 1 \end{bmatrix}$$



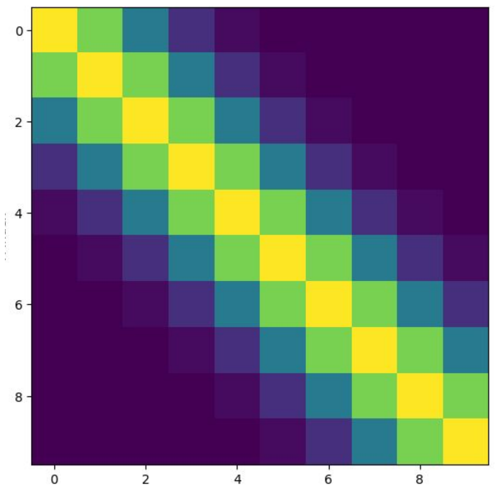
[Gaussian Processes, Not Quite for Dummies]

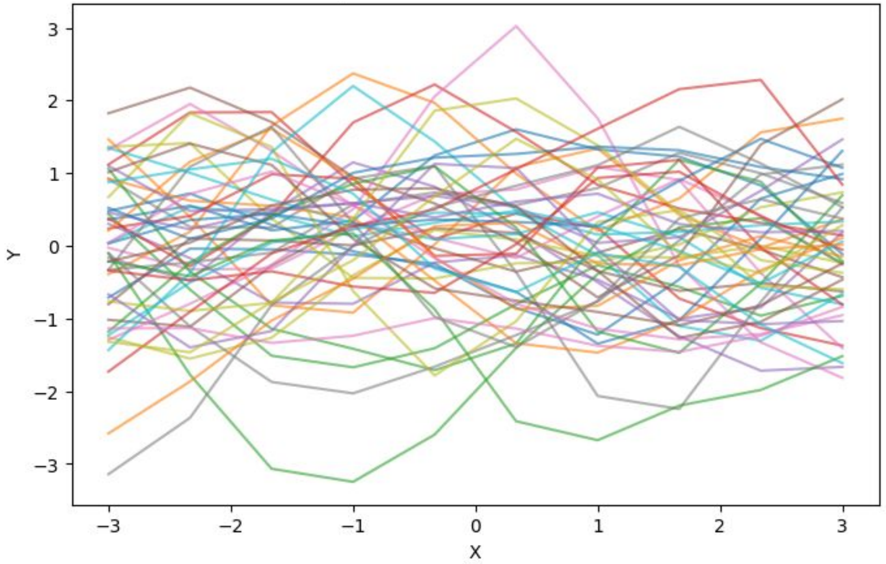
Gaussian Processes – Understanding the Covariance Function

Covariance matrices

Sampled Functions

10 Indices

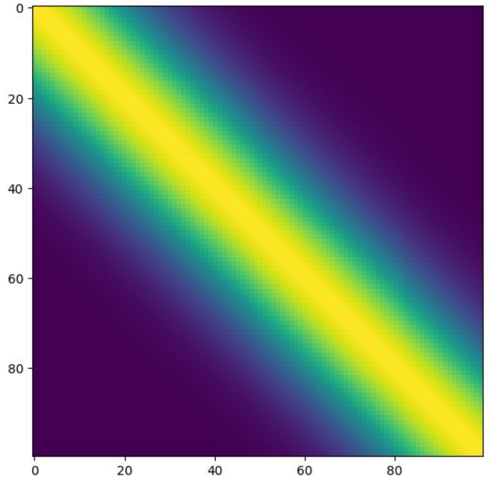


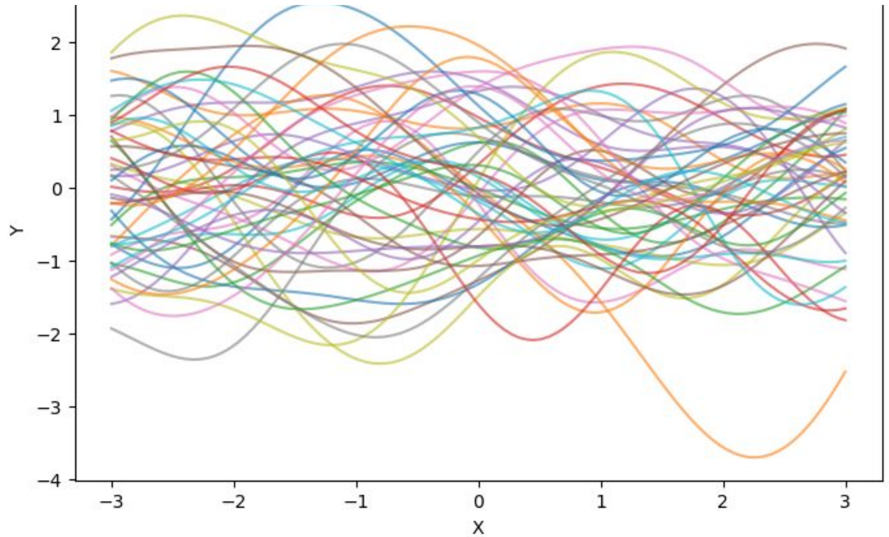


Low N prior samples

Rugged functions

100 Indices





High N prior samples

Smooth functions

Gaussian Processes Regression

What if we wish to infer function values on unseen points X*?

We create a joint distribution function p(f,f*|X*,X) and then marginalize over p(f)

Joint gaussian distribution

- Adding unknown observations

$\mathbf{K} = K(\mathbf{X},\mathbf{X}),\ \ \mathbf{K}_* = K(\mathbf{X},\mathbf{X}_*)\ \text{ and }\ \mathbf{K}_{**} = K(\mathbf{X}_*,\mathbf{X}_*)$

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

Apply Bayes' Rule

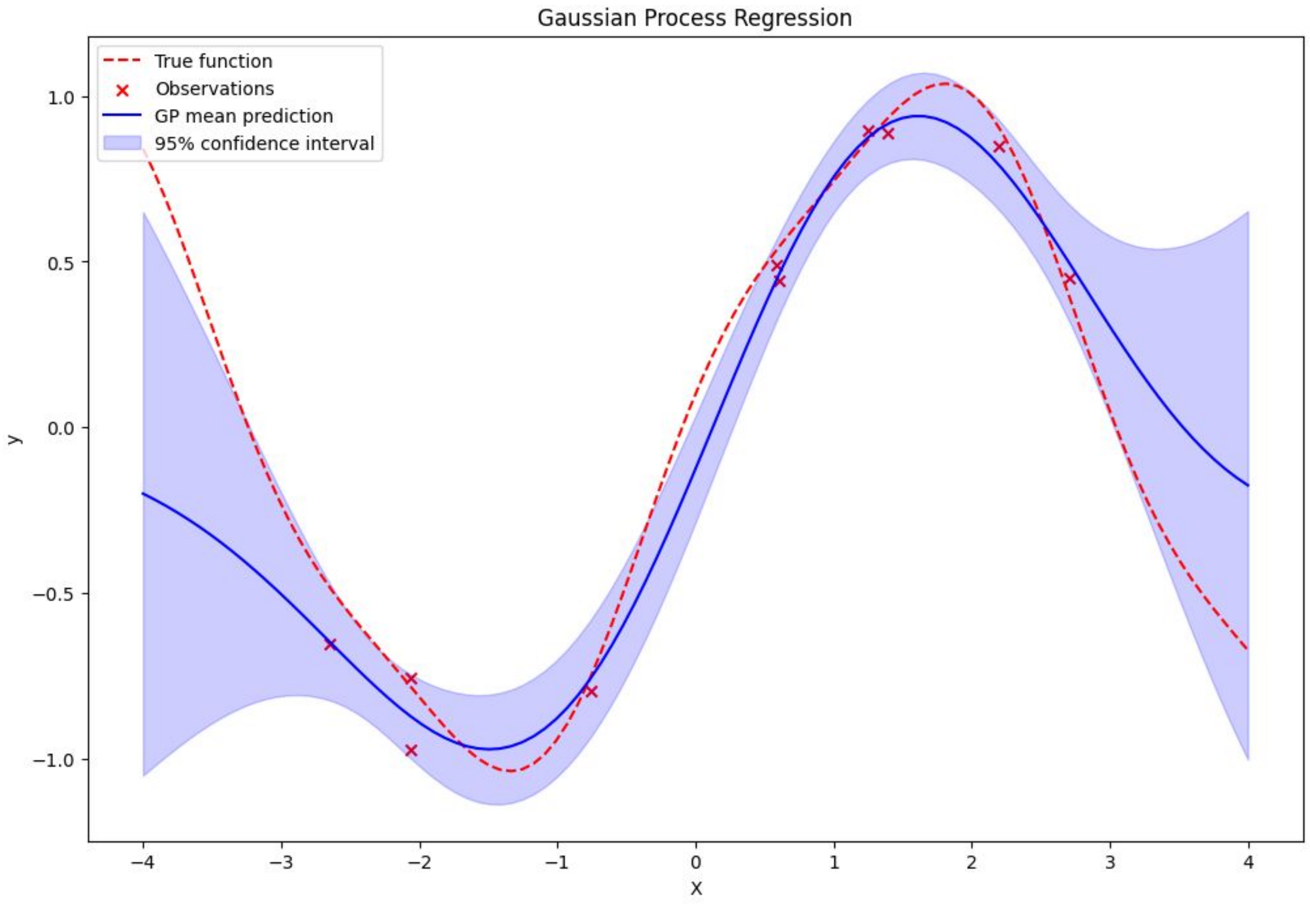
$$p(f^*|f) = \frac{p(f^*, f)}{p(f)}$$

Solve for Posterior

$$\mathbf{f}_* \mid \mathbf{f}, \mathbf{X}, \mathbf{X}_* \sim \mathcal{N}\left(\mathbf{K}_*^\top \mathbf{K}^{-1}\mathbf{f},\ \mathbf{K}_{**} - \mathbf{K}_*^\top \mathbf{K}^{-1}\mathbf{K}_*\right)$$

Gaussian Processes Regression

$$\mathbf{f}_* \mid \mathbf{f}, \mathbf{X}, \mathbf{X}_* \sim \mathcal{N}\Big(\underbrace{\mathbf{K}_*^\top \mathbf{K}^{-1}\mathbf{f}}_{\text{Mean}},\ \underbrace{\mathbf{K}_{**} - \mathbf{K}_*^\top \mathbf{K}^{-1}\mathbf{K}_*}_{\text{Variance}}\Big)$$



AutoIP

- Restricting Gaussian Process to a PDE

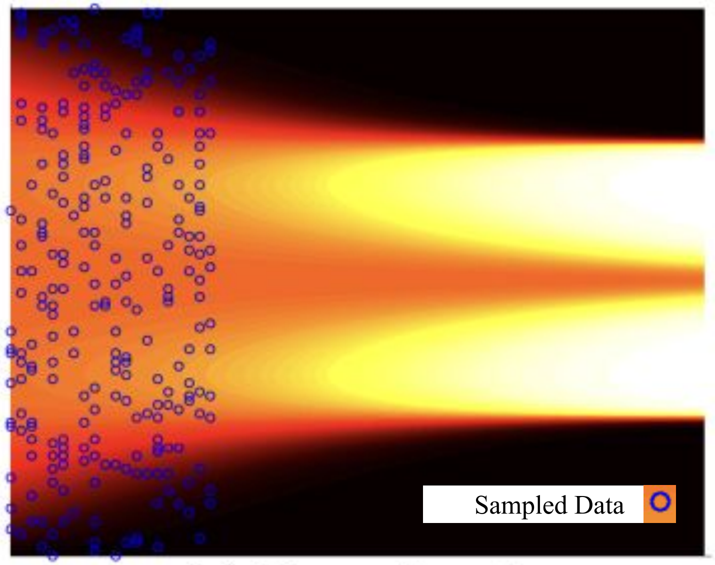
Example: Reaction-Diffusion System

Data Points Collected $(\mathbf{z}_1, y_1) \longrightarrow \mathbf{z}_n = (x_n, t_n)$

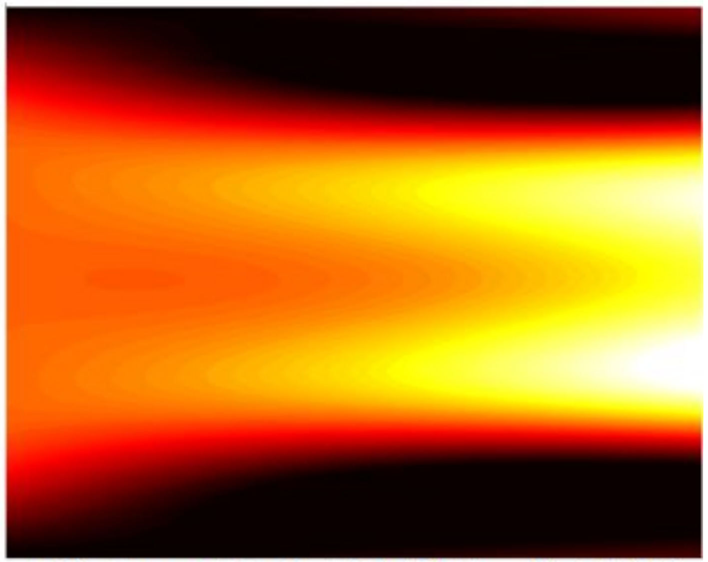
Collocation points selected $\widehat{\mathcal{Z}} = \{\widehat{\mathbf{z}}_1, \ldots, \widehat{\mathbf{z}}_M\}$

Incomplete Allen-Cahn Equation

$$\partial_t u - \nu \cdot \partial_x^2 u + \gamma \cdot u(u^2 - 1) + g(x,t) = 0$$



(a) Ground-truth


(d) AutoIP-C: RMSE = 0.1865

AutoIP

How do we incorporate derivatives into GP's?

Construct GP prior over u and g

$$u \sim \mathcal{GP}\left(0, \kappa_u(\cdot,\cdot)\right) \quad g \sim \mathcal{GP}\left(0, \kappa_g(\cdot,\cdot)\right)$$

Getting derivatives from kernel differentiation

$$\text{cov}(\hat{A}u(z_1), \hat{B}u(z_2)) = \hat{A}\hat{B}\kappa(z_1, z_2)$$

Examples of Kernel Derived Derivatives

$$\text{cov}\left(u(\mathbf{z}_1), u(\mathbf{z}_2)\right) = \kappa_u(\mathbf{z}_1, \mathbf{z}_2),$$

$$\text{cov}\left(\partial_t u(\mathbf{z}_1), \partial_t u(\mathbf{z}_2)\right) = \frac{\partial^2 \kappa_u(\mathbf{z}_1, \mathbf{z}_2)}{\partial t_1 \partial t_2},$$

Constructing Gaussian Prior <u>with derivatives</u>

$$\mathbf{f} = [\mathbf{u}; \widehat{\mathbf{u}}; \widehat{\mathbf{u}}_t; \widehat{\mathbf{u}}_{xx}; \mathbf{g}] \Longrightarrow p(\mathbf{f}) = \mathcal{N}(\mathbf{f}|\mathbf{0}, \mathbf{\Sigma})$$

AutoIP - Construct Joint Prior

Next, we feed the joint prior to two likelihoods:

I. To fit the actual observations from a Gaussian noise model

$$p(\mathbf{y}|\mathbf{f}) = \mathcal{N}(\mathbf{y}|\mathbf{u}, \beta^{-1}\mathbf{I})$$

II. A virtual Gaussian likelihood that integrates the physics into the differential equation

$$p(\mathbf{0}|\mathbf{f}) = \mathcal{N}(\mathbf{0}|\widehat{\mathbf{u}}_t - \nu\widehat{\mathbf{u}}_{xx} + \gamma\widehat{\mathbf{u}} \circ (\widehat{\mathbf{u}} \circ \widehat{\mathbf{u}} - \mathbf{1}) + \mathbf{g}, v\mathbf{I})$$

AutoIP

Next, construct the Joint Probability for the model:

$$p(\mathbf{f}, \mathbf{y}, \mathbf{0}) = \mathcal{N}(\mathbf{f}|\mathbf{0}, \boldsymbol{\Sigma})\mathcal{N}(\mathbf{y}|\mathbf{u}, \beta^{-1}\mathbf{I}) \cdot \mathcal{N}(\mathbf{0}|\widehat{\mathbf{u}}_t - \nu\widehat{\mathbf{u}}_{xx} + \gamma\widehat{\mathbf{u}} \circ (\widehat{\mathbf{u}} \circ \widehat{\mathbf{u}} - \mathbf{1}) + \mathbf{g}, v\mathbf{I})$$

This joint probability distribution is maximized using a stochastic variational learning algorithm.

Experimenting with AutoIP - Reaction Diffusion Equations

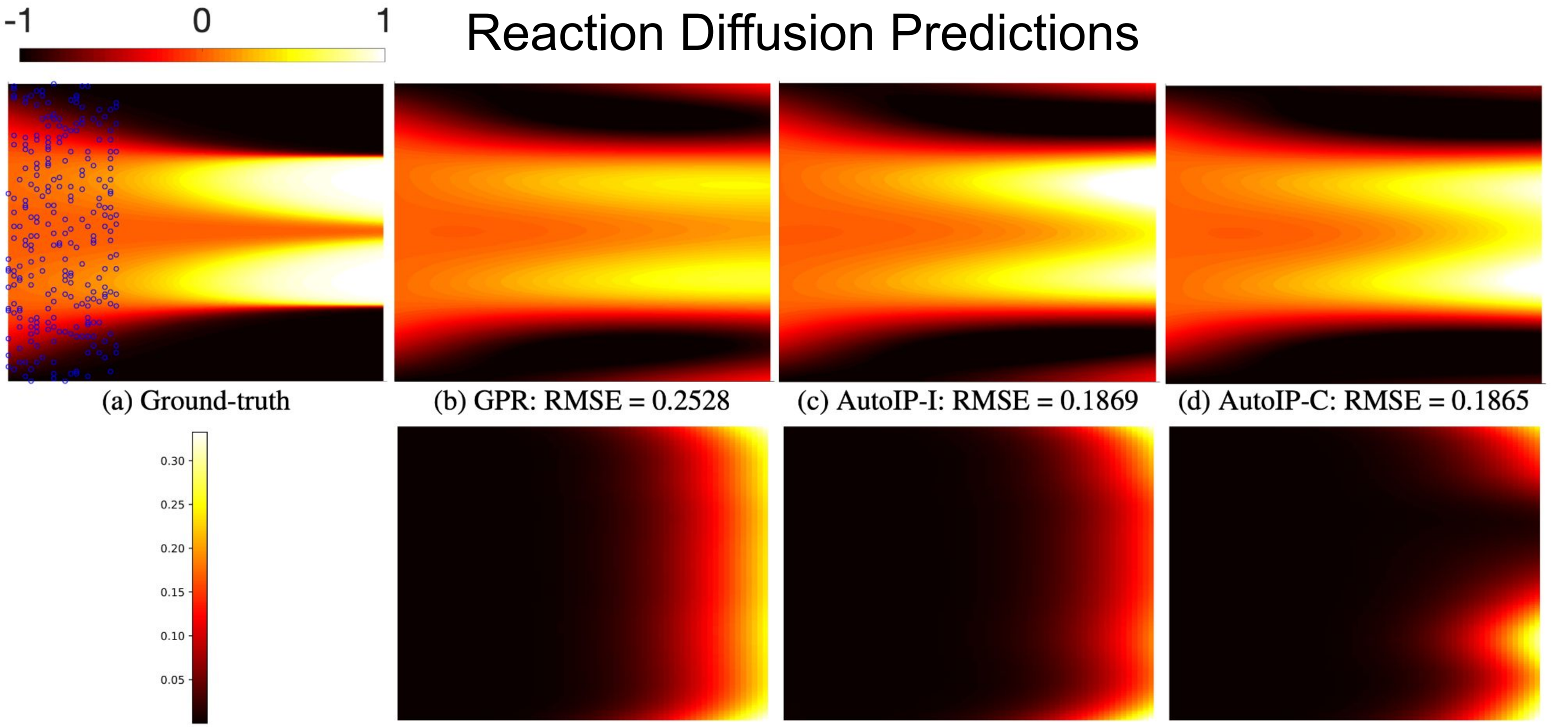
Complete Equation (AutoIP-C) $$\frac{\partial u}{\partial t} - 0.0001\frac{\partial^2 u}{\partial x^2} + 5u^3 - 5u = 0,$$

Incomplete Equation (AutoIP-I) $$\frac{\partial u}{\partial t} - 0.0001\frac{\partial^2 u}{\partial x^2} + g(x,t) = 0,$$

Comparing Modeling Methods

	GPR	AutoIP-I	AutoIP-C	PINN (100)	PINN (10K)
RMSE	0.2528	0.1869	0.1865	0.4388	**0.0169**
# Collocation Points	**100**	**100**	**100**	**100**	**10,000**

Reaction Diffusion Predictions



(a) Ground-truth (b) GPR: RMSE = 0.2528 (c) AutoIP-I: RMSE = 0.1869 (d) AutoIP-C: RMSE = 0.1865

(e) GPR predictive variance (f) AutoIP-I predictive variance (g) AutoIP-C predictive variance

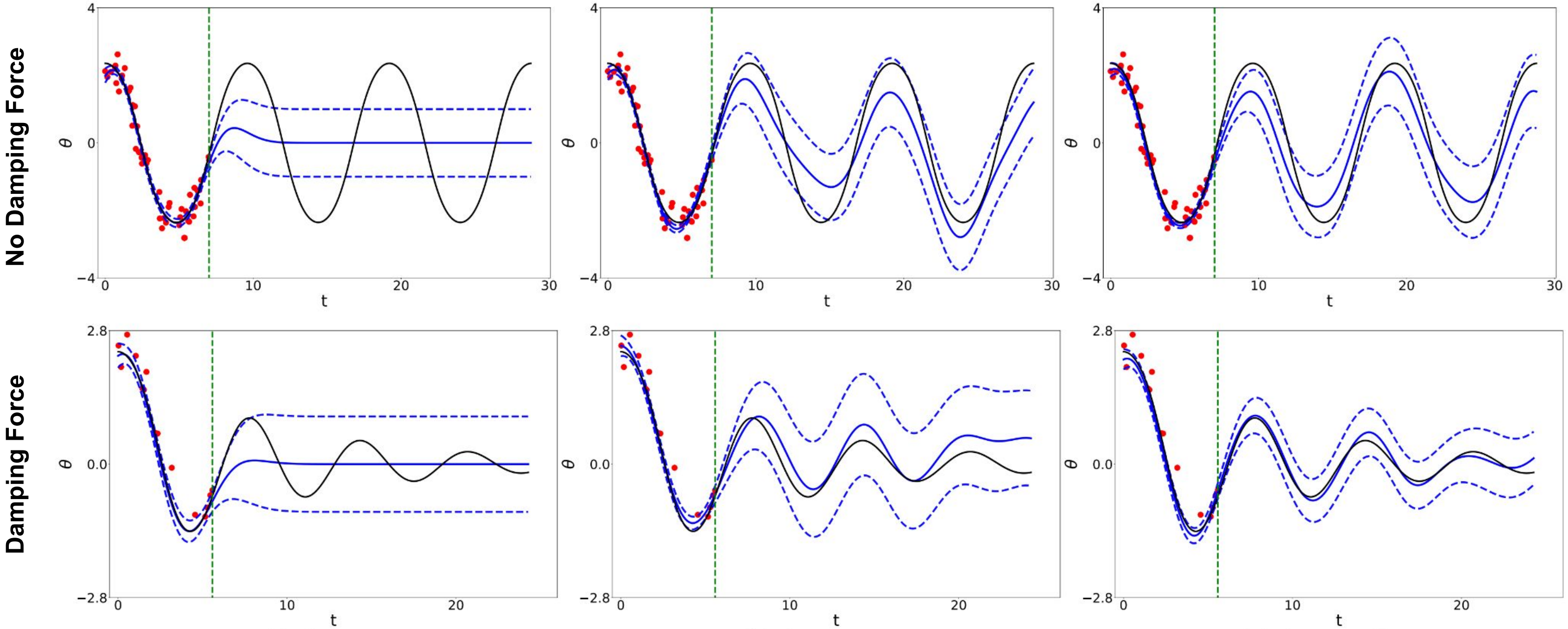
Experimenting with AutoIP - Nonlinear Pendulum

Method (CL Points)	No damping/Exact training	No damping/Noisy training	Damping/Exact training	Damping/Noisy training
PINN-50 (10k)	1.367 ± 0.575	1.658 ± 0.074	$\mathbf{0.00007 \pm 0.00001}$	0.157 ± 0.051
PINN-100 (10k)	1.862 ± 0.584	1.993 ± 0.357	$\mathbf{0.00007 \pm 0.00002}$	0.186 ± 0.045
AutoIP-I (20)	0.585 ± 0.017	0.691 ± 0.030	0.212 ± 0.014	0.268 ± 0.013
AutoIP-C (20)	$\mathbf{0.416 \pm 0.050}$	$\mathbf{0.488 \pm 0.036}$	0.096 ± 0.004	$\mathbf{0.133 \pm 0.010}$

AutoIP-C $$\frac{\mathrm{d}^2\theta}{\mathrm{d}t^2} + \sin(\theta) + b\frac{\mathrm{d}\theta}{\mathrm{d}t} = 0,$$

AutoIP-I $$\frac{\mathrm{d}^2\theta}{\mathrm{d}t^2} + g(t) = 0.$$

Nonlinear Pendulum Predictions



(a) GPR (b) AutoIP-I (c) AutoIP-C

No damping	RMSE
GPR	1.354 ± 0.005
AutoIP-I	0.585 ± 0.017
AutoIP-C	$\mathbf{0.416 \pm 0.050}$
With damping	
GPR	0.262 ± 0.0003
AutoIP-I	0.212 ± 0.014
AutoIP-C	$\mathbf{0.096 \pm 0.0035}$

Remarks

- Adding physical constraints to GPs improves performance and ability to extrapolate outside of training regions
- Adding more collocation points improves performance
- This method scales with at least O(N^3) points, making it computationally expensive for large datasets.
- AutoIP outperformed PINNs on sparse and noisy data