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Physics informed Machine Learning

22 January 20120

Contributors: Romain Dupuis

Romain Dupuis
KU Leuven

KU LEUVEN

1st AIDA School in Bologna

Contents

Motivations

Why incorporating physics into ML?

- **Machine Learning shows great success**
  - Computer vision, natural language processing, autonomous vehicle
  - Medicine, engineering, fluid dynamics, materials, etc.
  - Full data-driven approach

- **Scientists can be skeptical about black-box tools**
  - Complex models: no interpretation
  - Solutions can break natural laws

- **Small amount of data**
  - Experimental data
  - Intensive simulations

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Incorporating additional knowledge

Data Informed Physics

Reduced order model

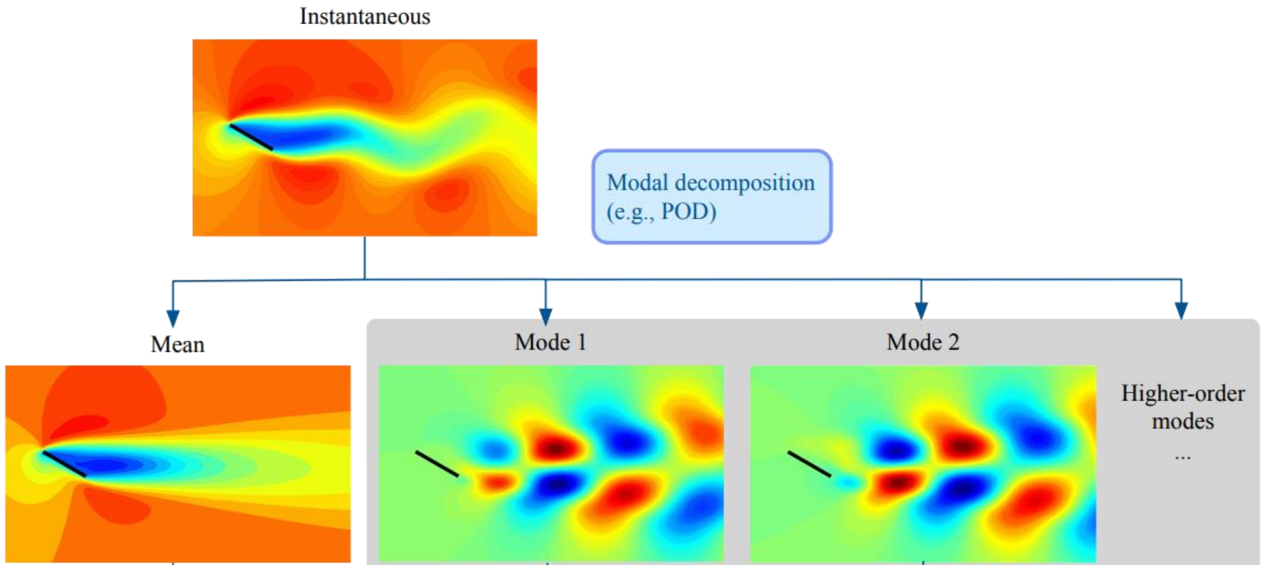
- **Non Linear dynamic system (Physics)**

$$\frac{d\boldsymbol{u}}{dt} = L\,\boldsymbol{u}(t) + N\big(\boldsymbol{u}(t)\big), \qquad \boldsymbol{u} \in \mathbb{R}^n$$

- **Extracting low-dimensional patterns (data)**

$$u(t) \approx \boldsymbol{\phi}_r \boldsymbol{a}(t), \qquad \boldsymbol{\phi}_r^T \boldsymbol{\phi}_r = \boldsymbol{I}$$

$$\boldsymbol{a} \in \mathbb{R}^r \; with \; r \ll n$$



[1] Taira et al.

- **Low rank system**

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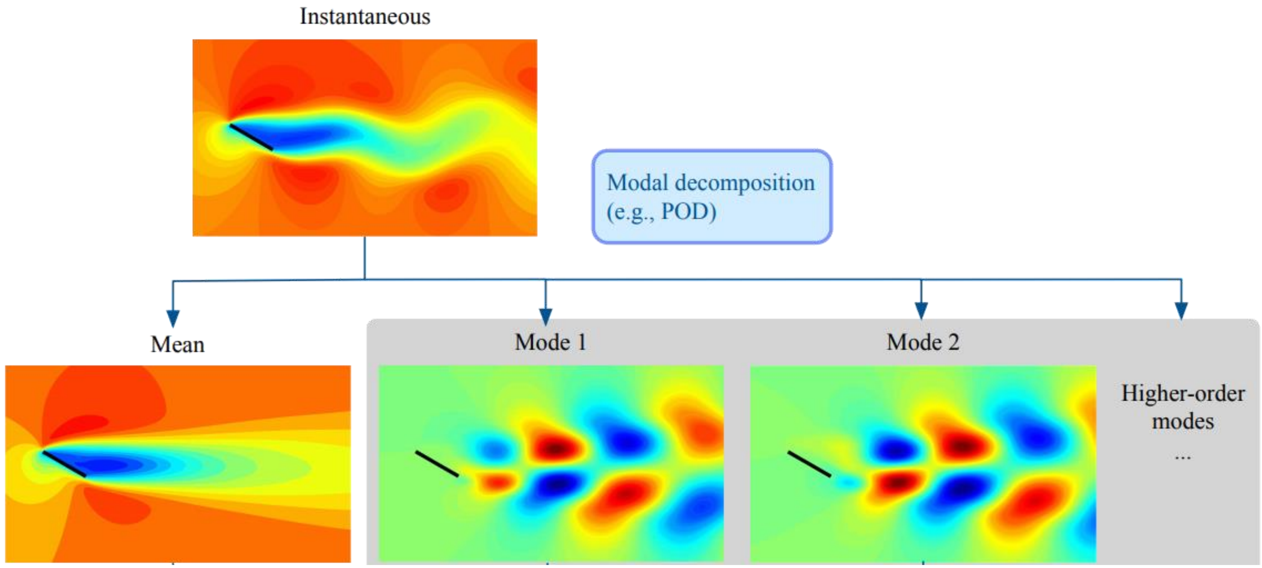

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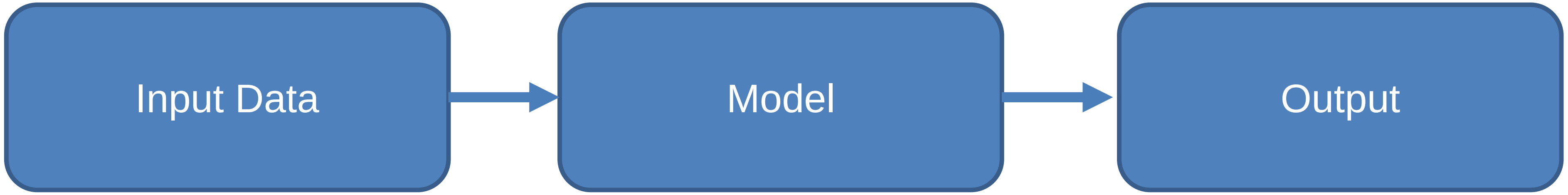
Physics-informed ML

Very large taxonomy

- **Physics informed machine learning**
- **Knowledge-based machine learning**
- **Theory-guided machine learning**
- **Physics-constrained machine learning**
- **Etc…**

Informed Machine Learning



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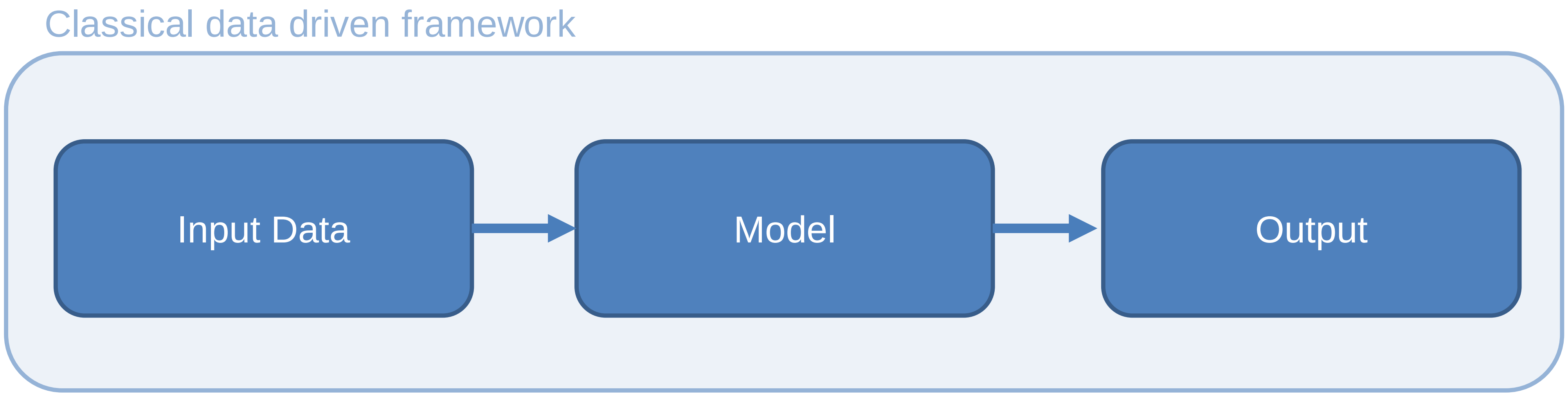

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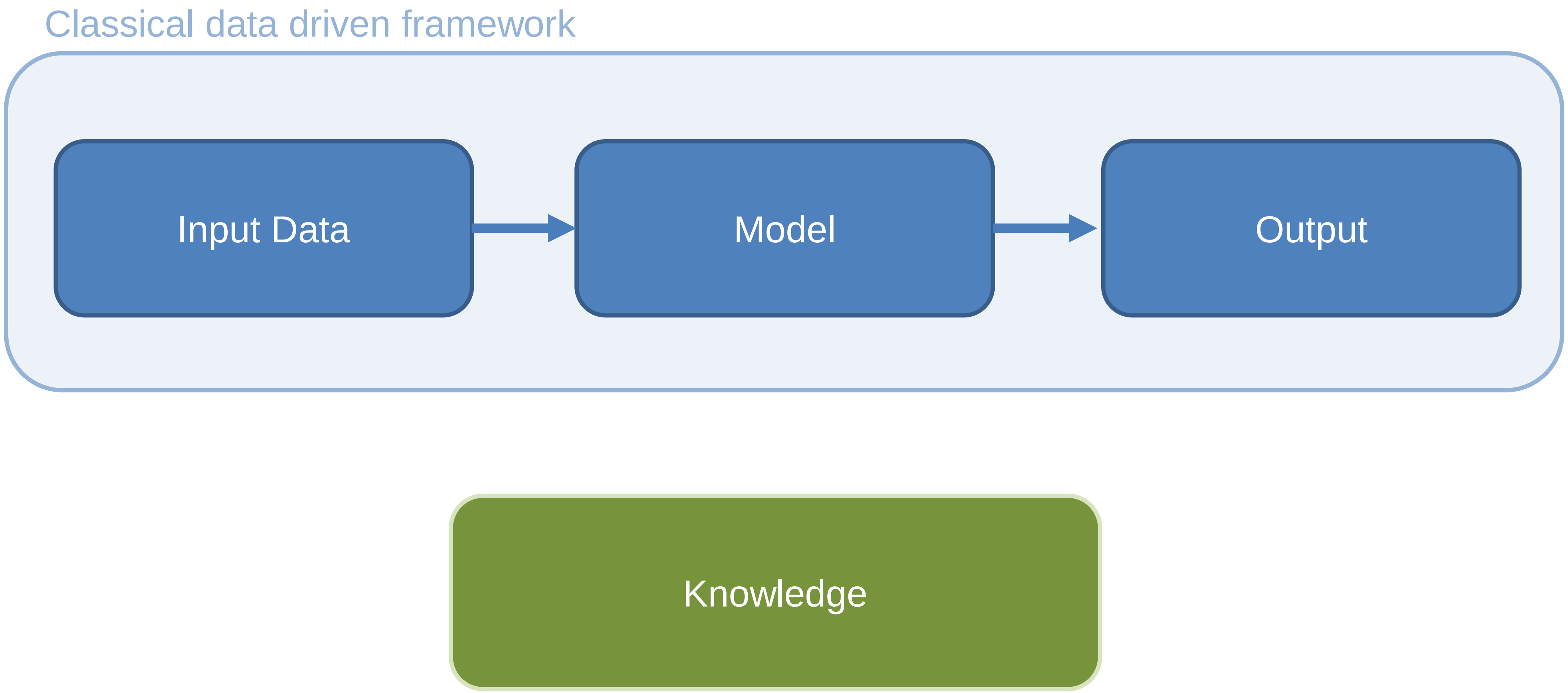

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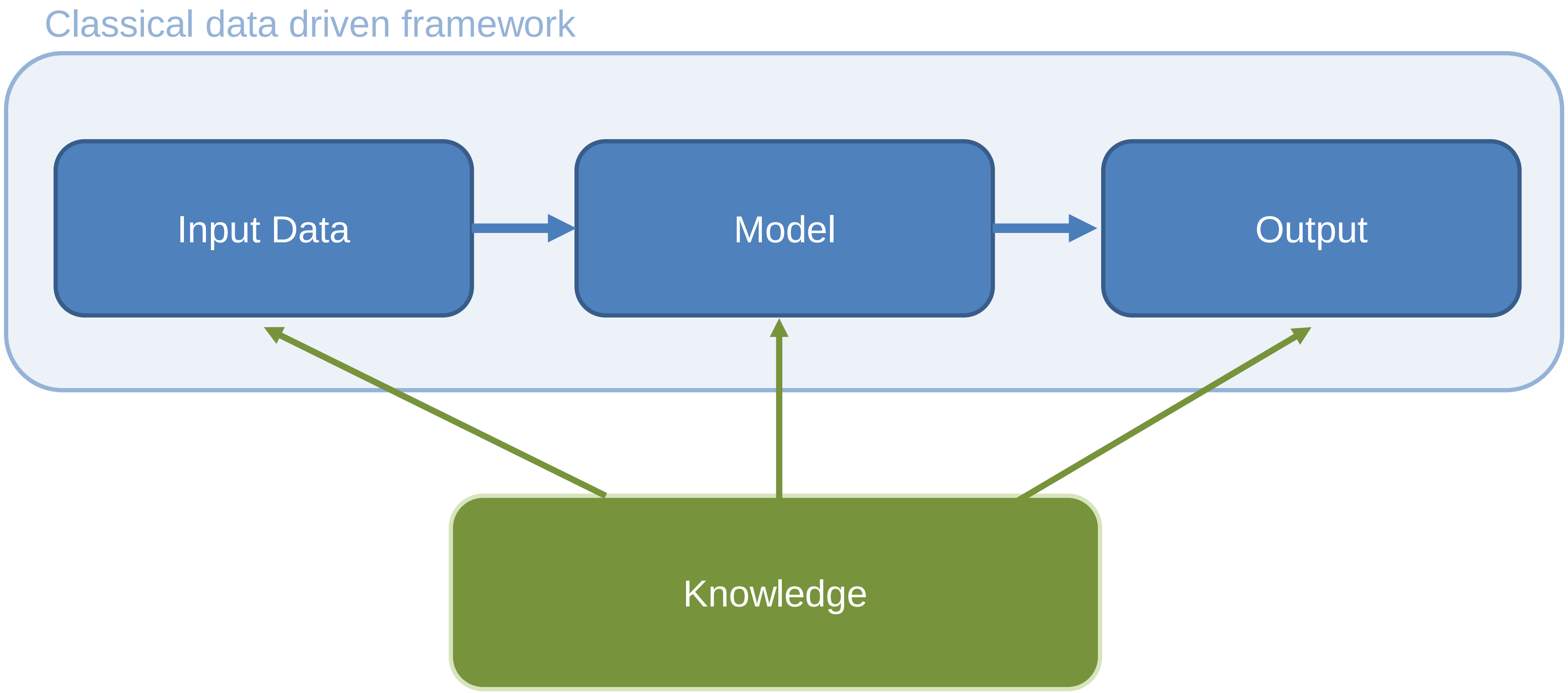
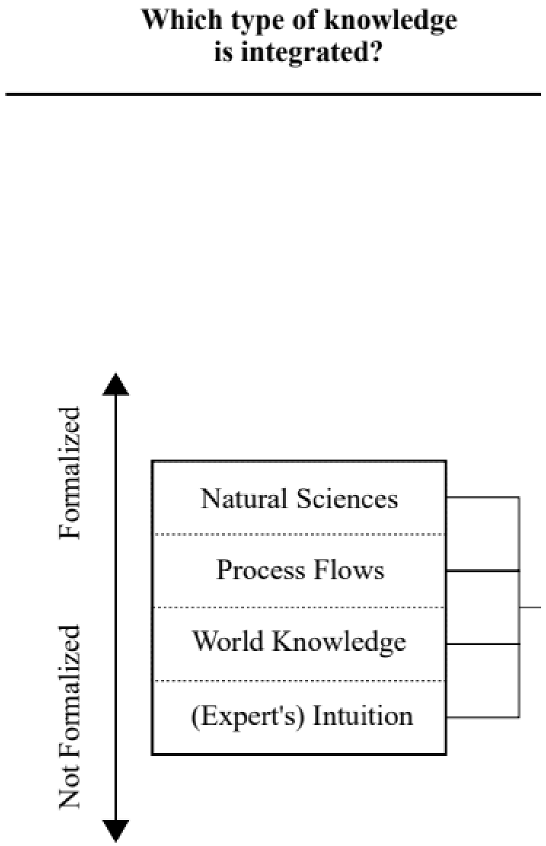


Type of knowledge



von Rued et al.

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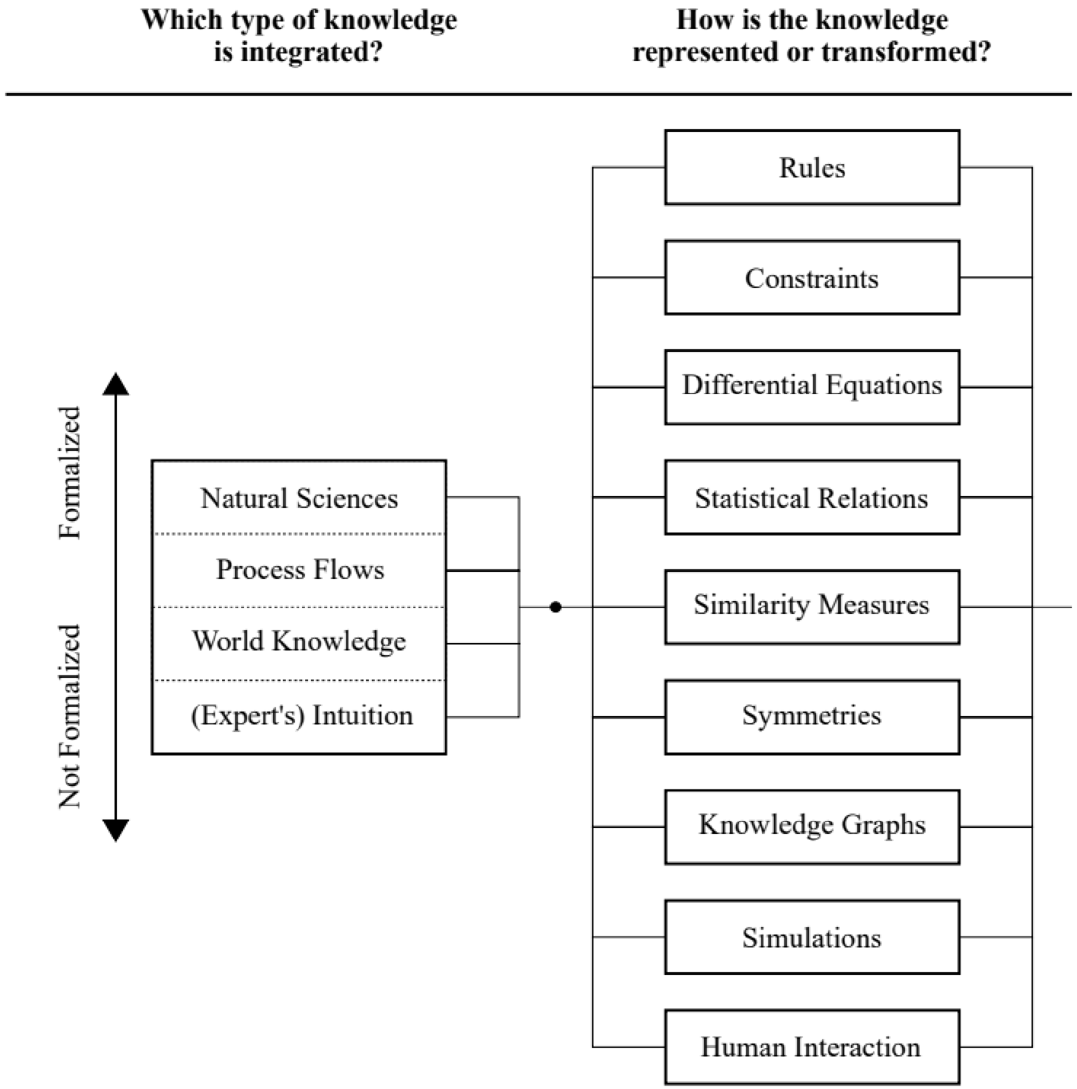

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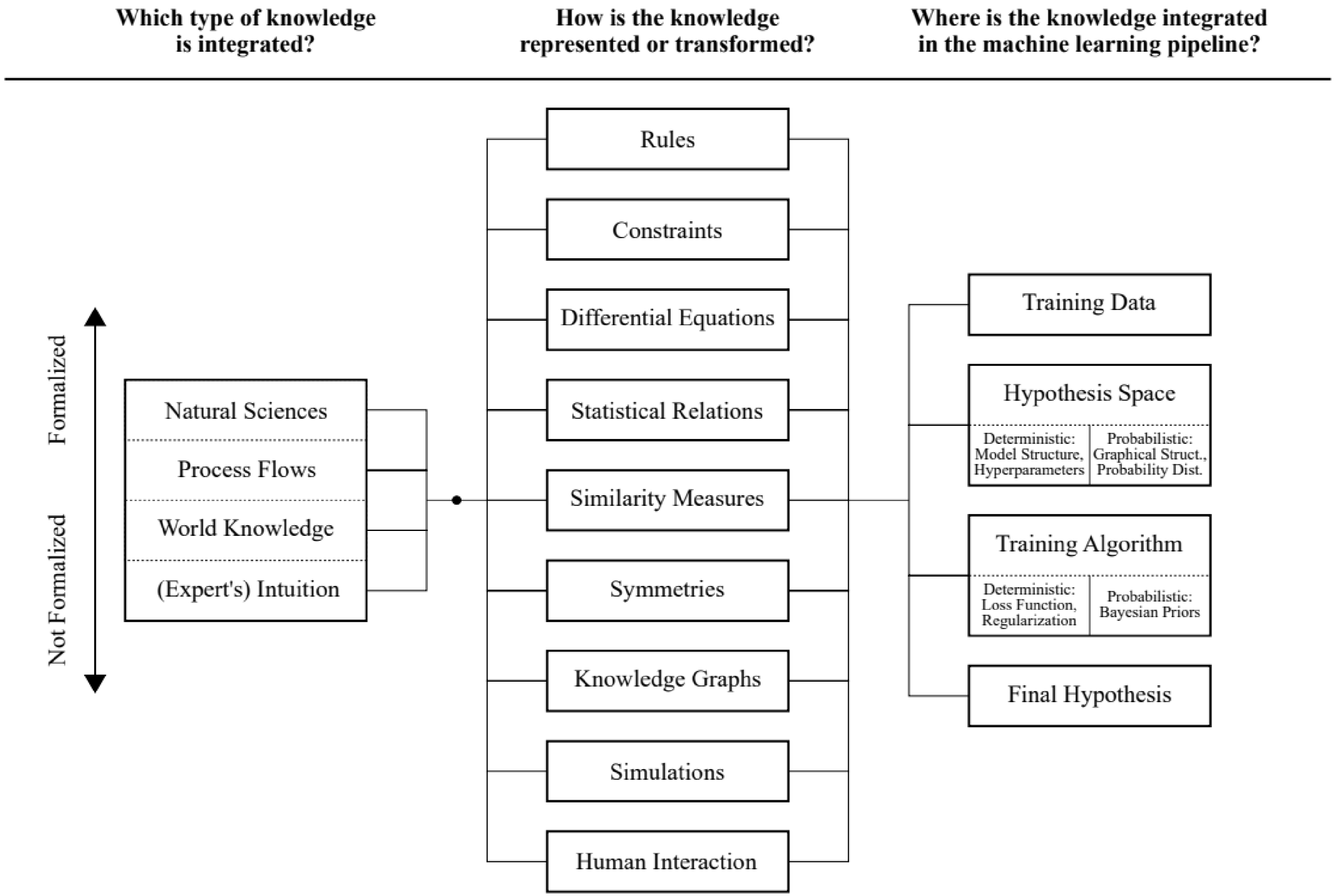

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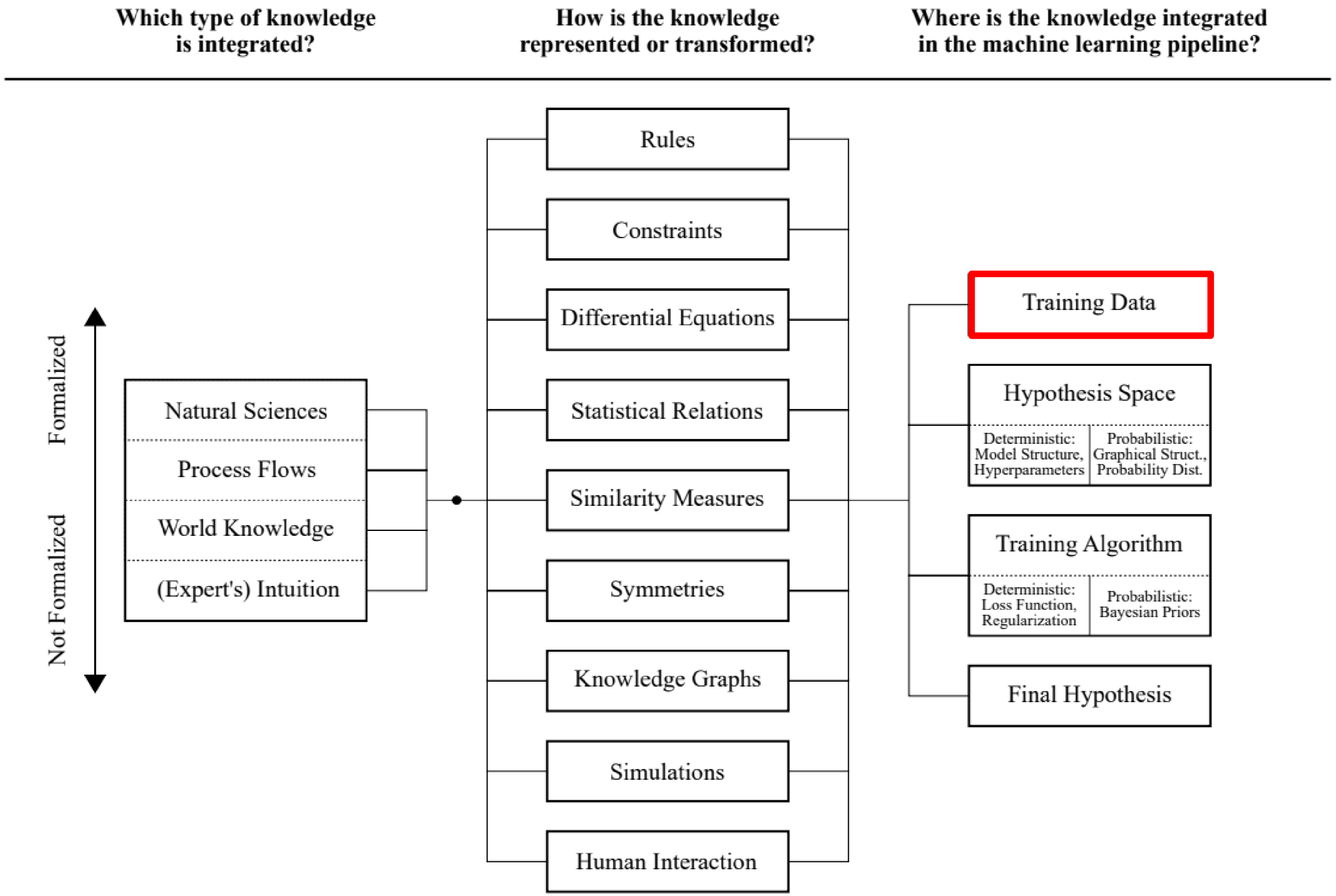
Data augmentation



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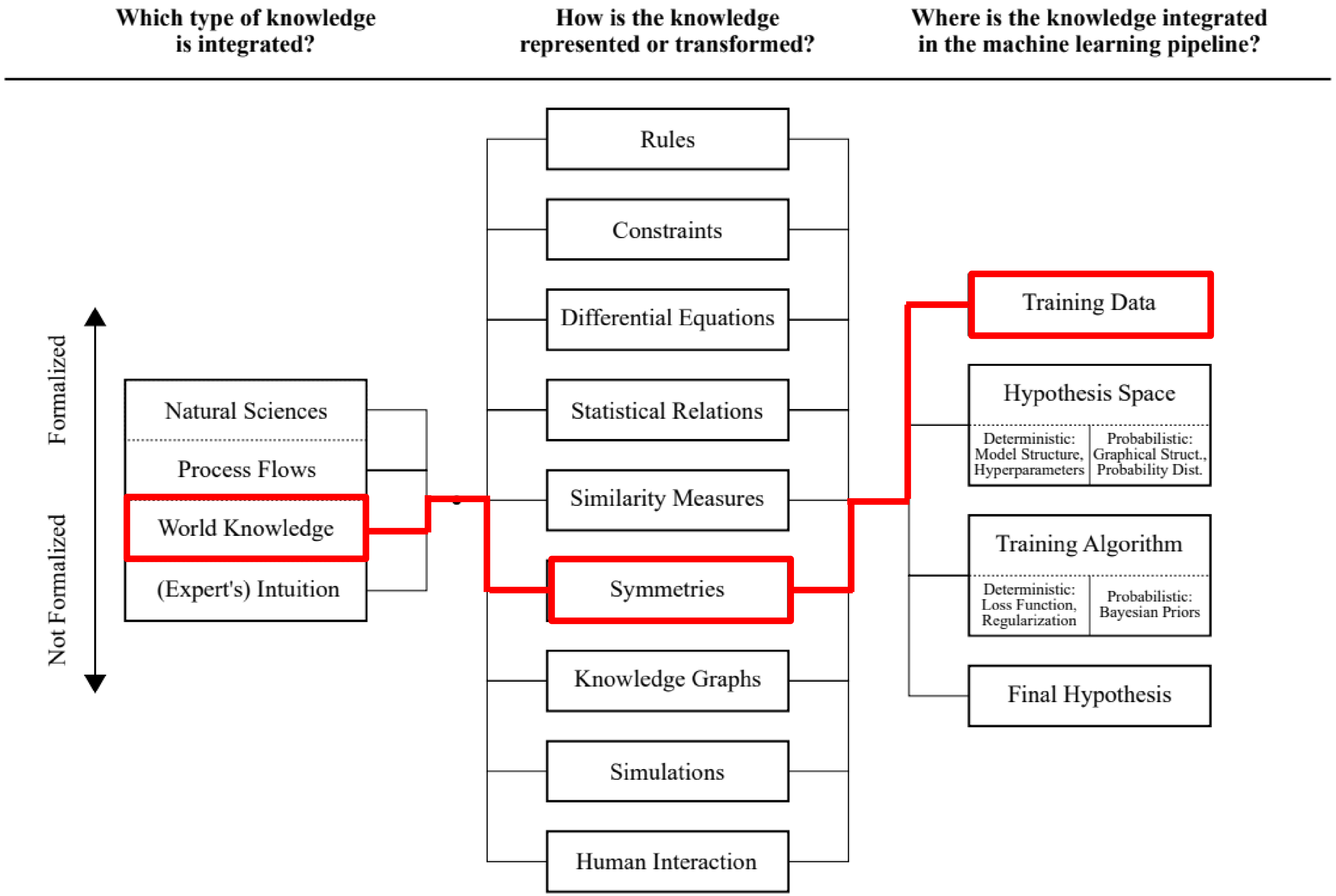

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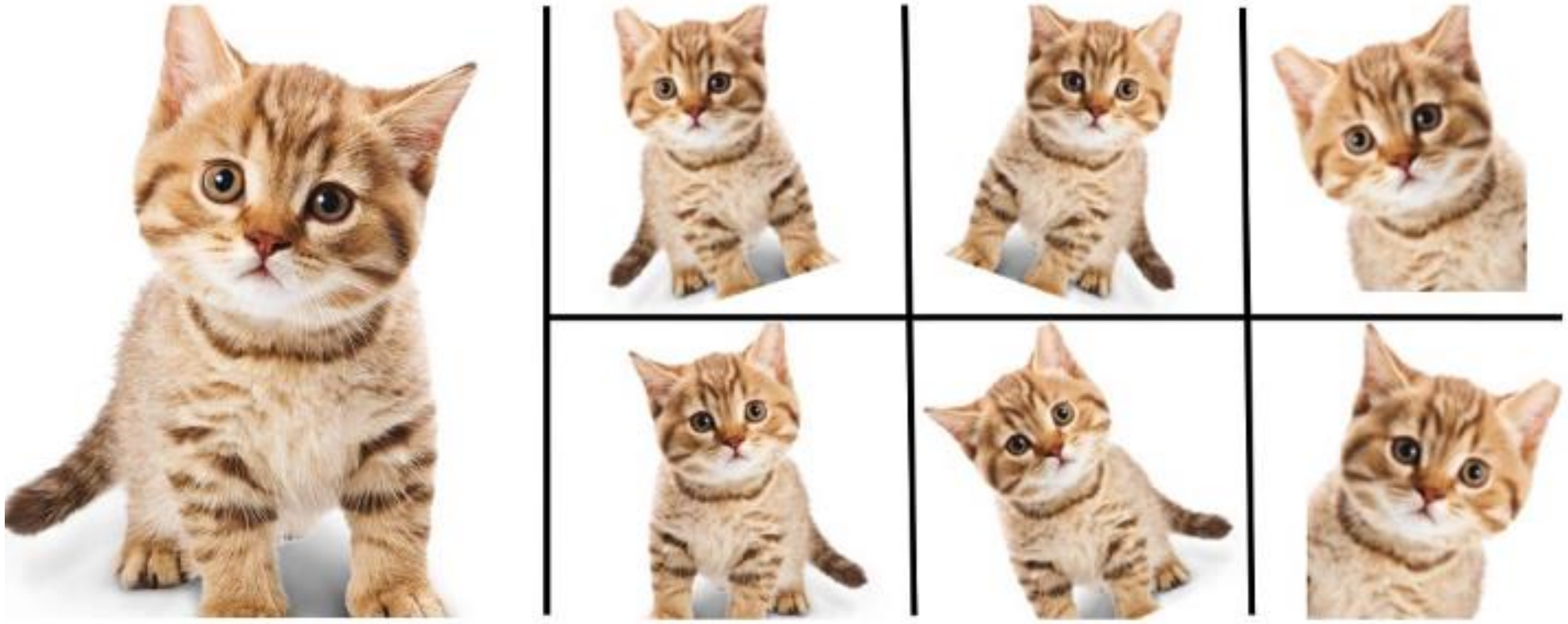
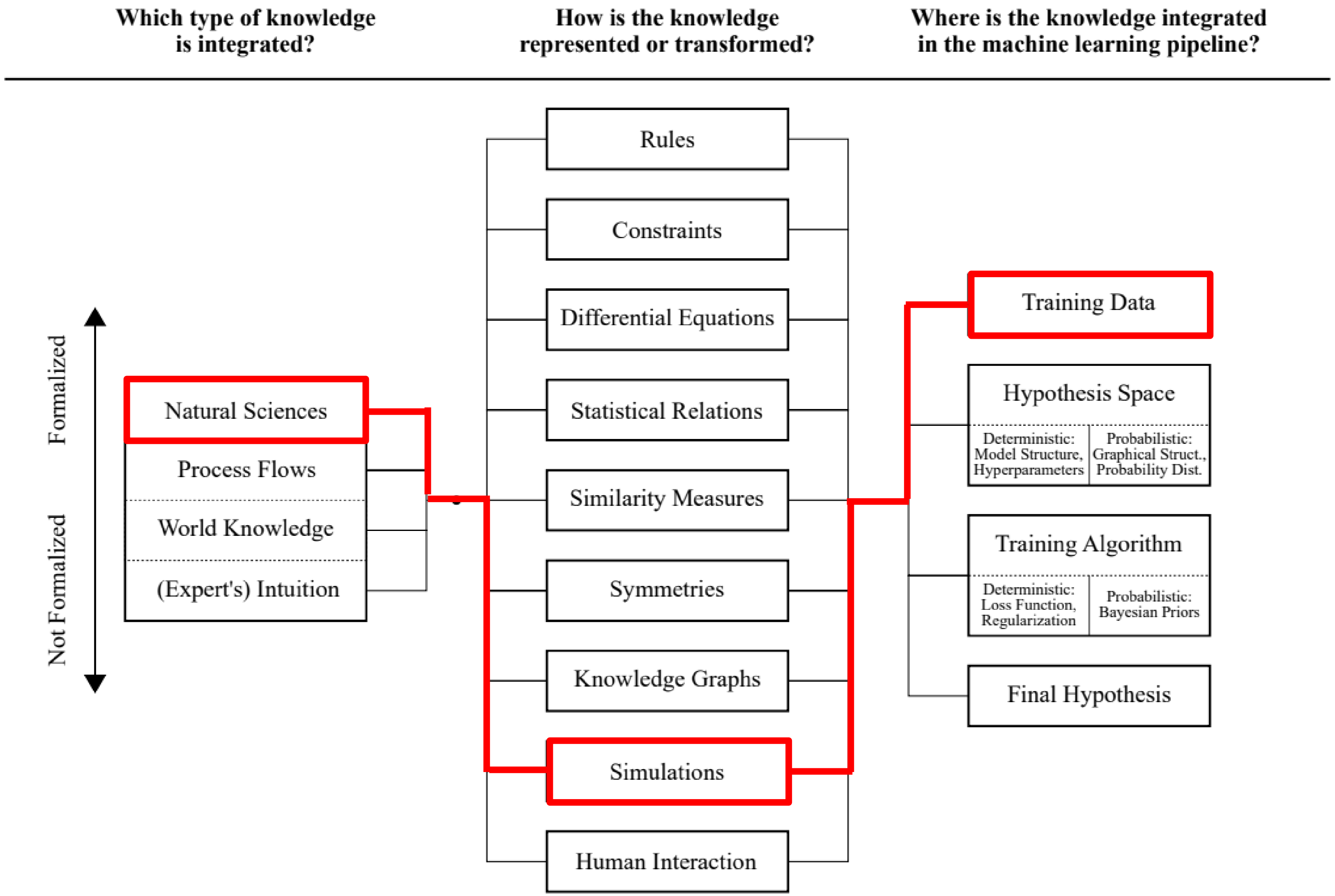


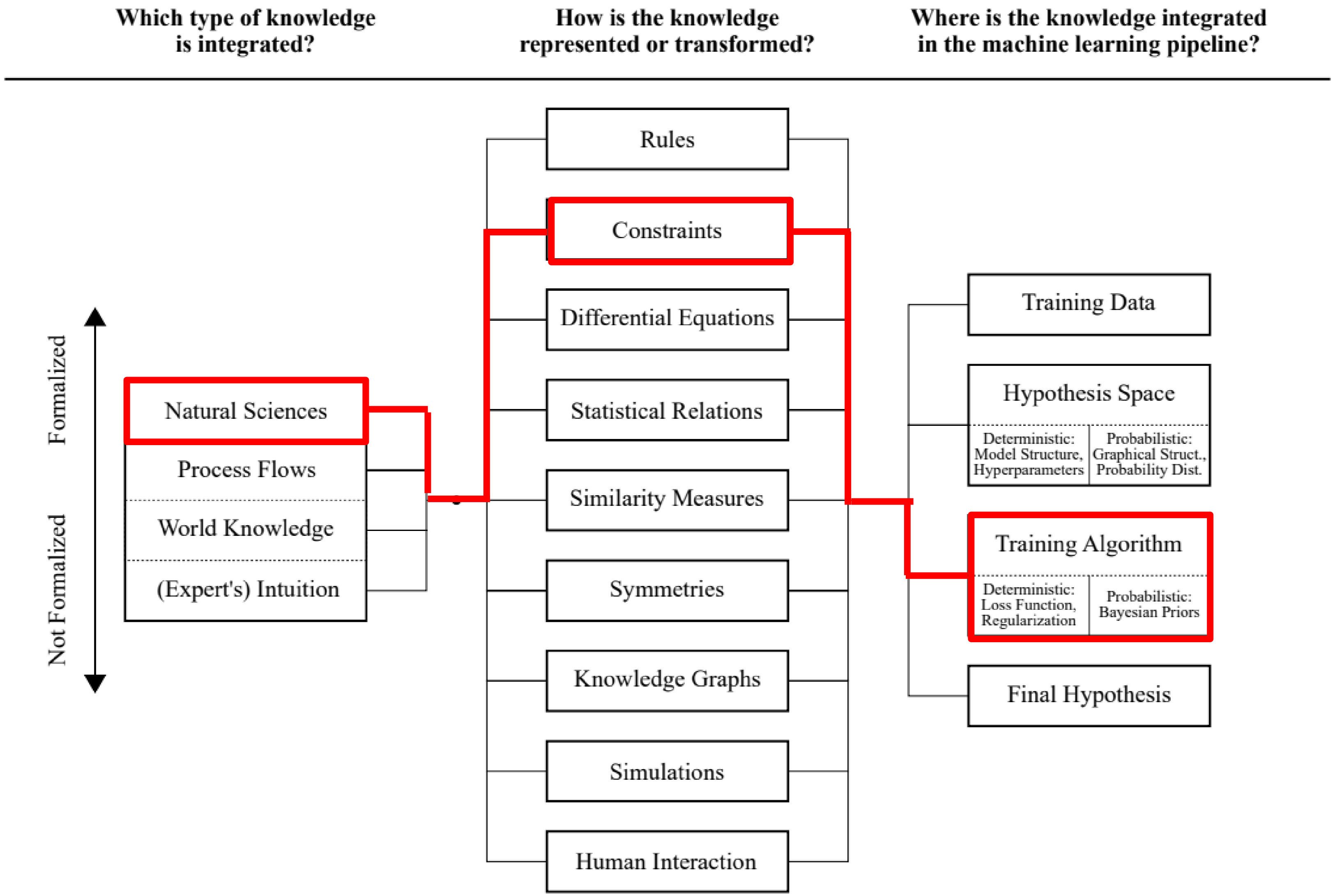
Credit https://nanonets.com/blog/data-augmentation-how-to-use-deep-learning-when-you-have-limited-data-part-2/

Data augmentation with simulations



von Rued et al.

Constraining the solution with the loss function



von Rued et al.

Physics guided Neural Network (Karpatne et al.)

- **Initial problem**
  - Approximate $f: X \rightarrow Y$ by a neural network f_{nn}
  - $\tilde{Y}$ is the predictor of f

- **Classical loss function**
  - $\underset{f_{nn}}{argmin}\, Loss(\tilde{Y}, Y) + \lambda R(f_{nn})$
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- **Finding temperature profile of lakes**
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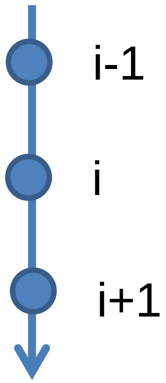
  - Physical relationship between the temperature, density, and depth of water
  - Relationship between ρ and T is known
  - Density-depth relationship: ρ cannot decrease with depth d: $\Delta\rho(i,t) = \tilde{\rho}(d_i,t) - \tilde{\rho}(d_{i+1},t) \leq 0$



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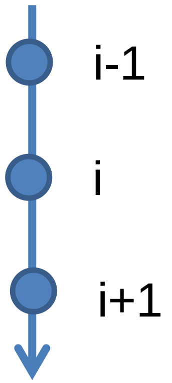

$$\boxed{L_{phy} = \frac{1}{n_t(n_d - 1)} \sum_{t=1}^{n_t} \sum_{i=1}^{n_d - 1} ReLU(\Delta\rho(i,t))}$$

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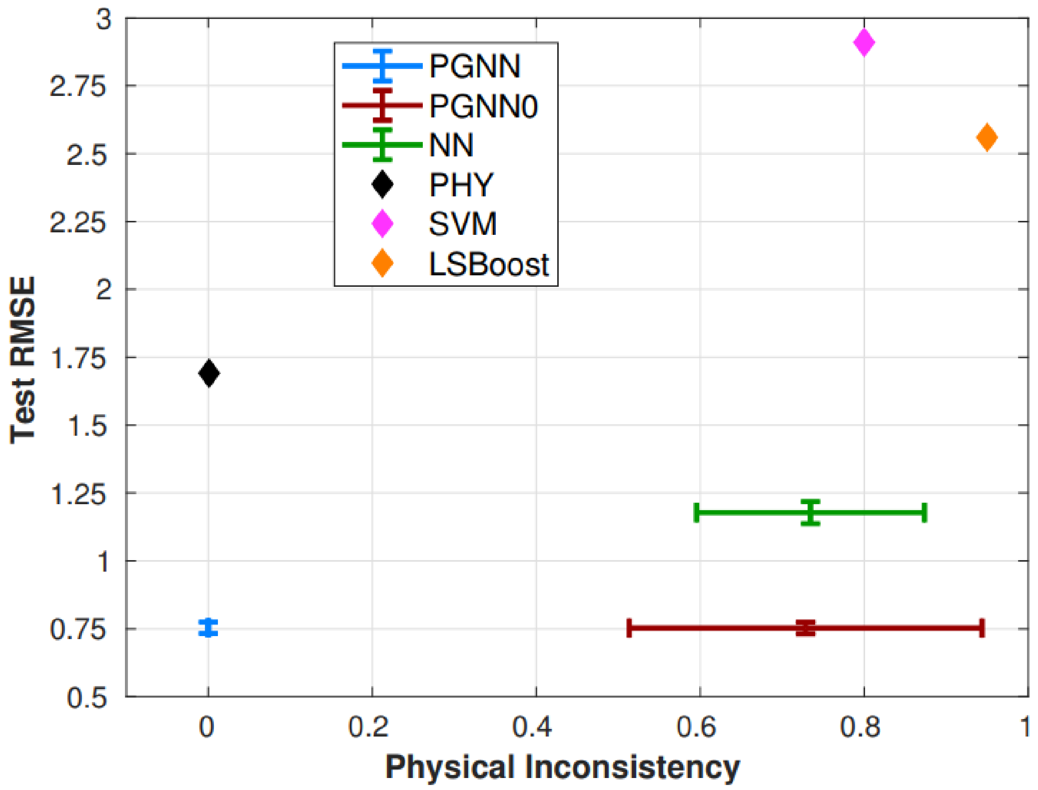
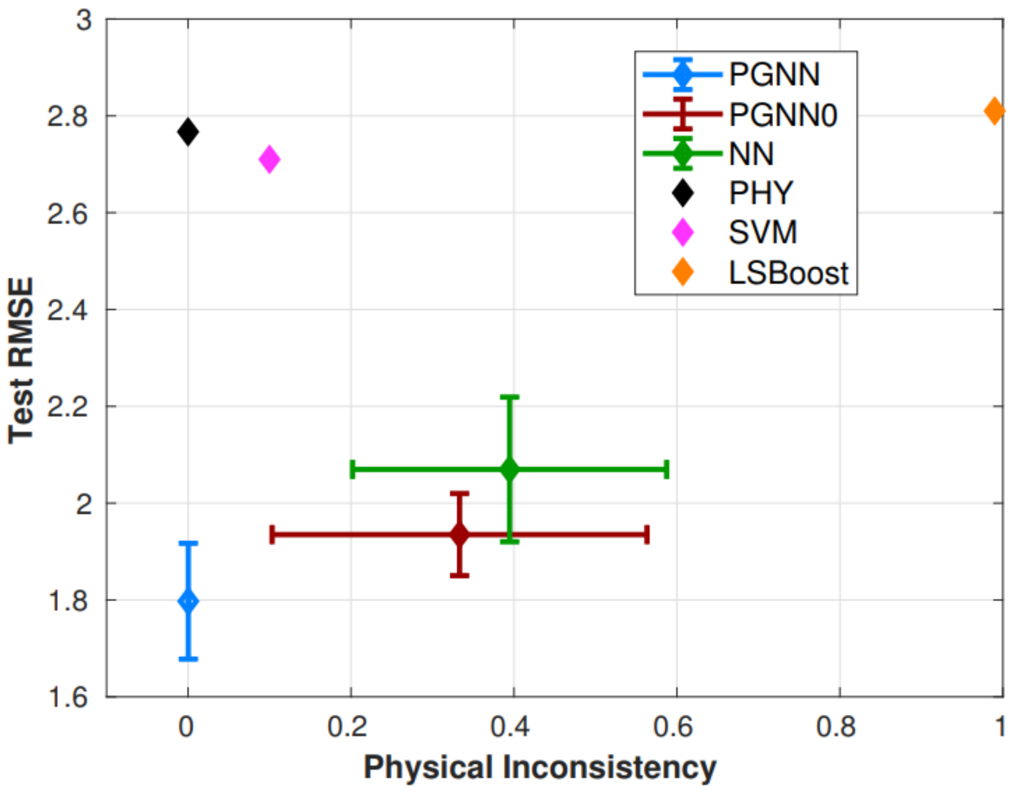


(a) Results on Lake Mille Lacs



(b) Results on Lake Mendota

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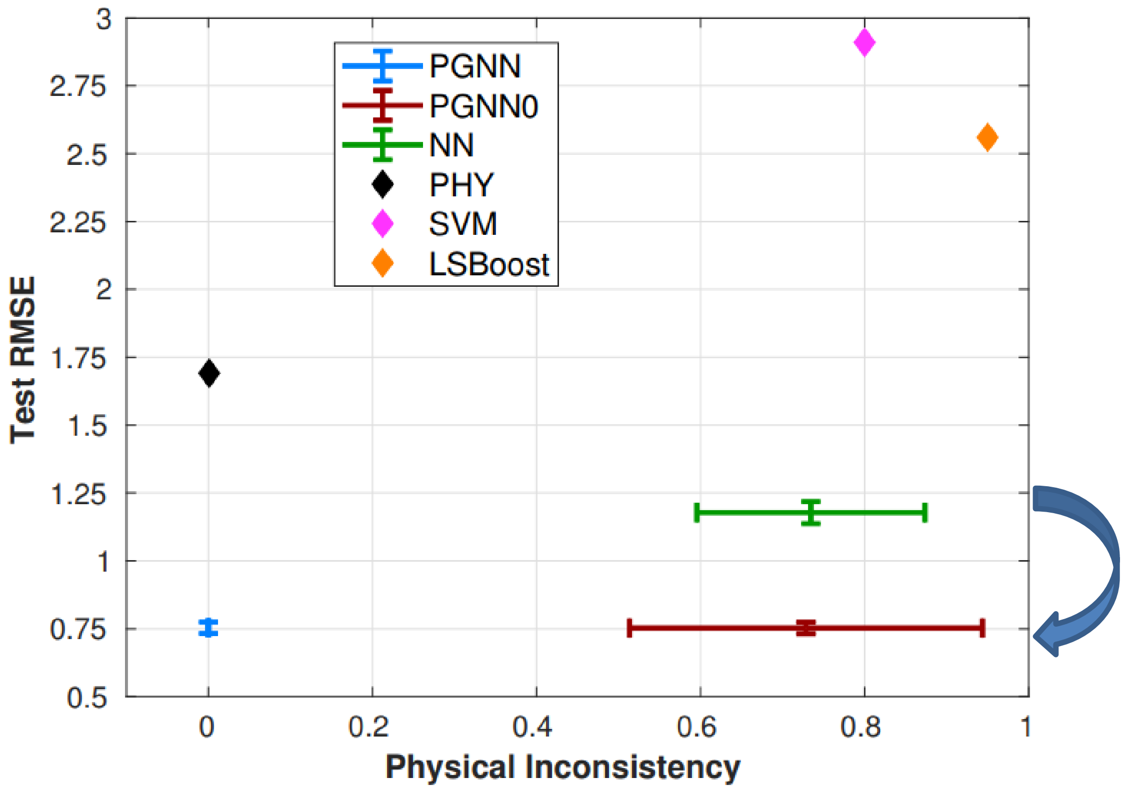

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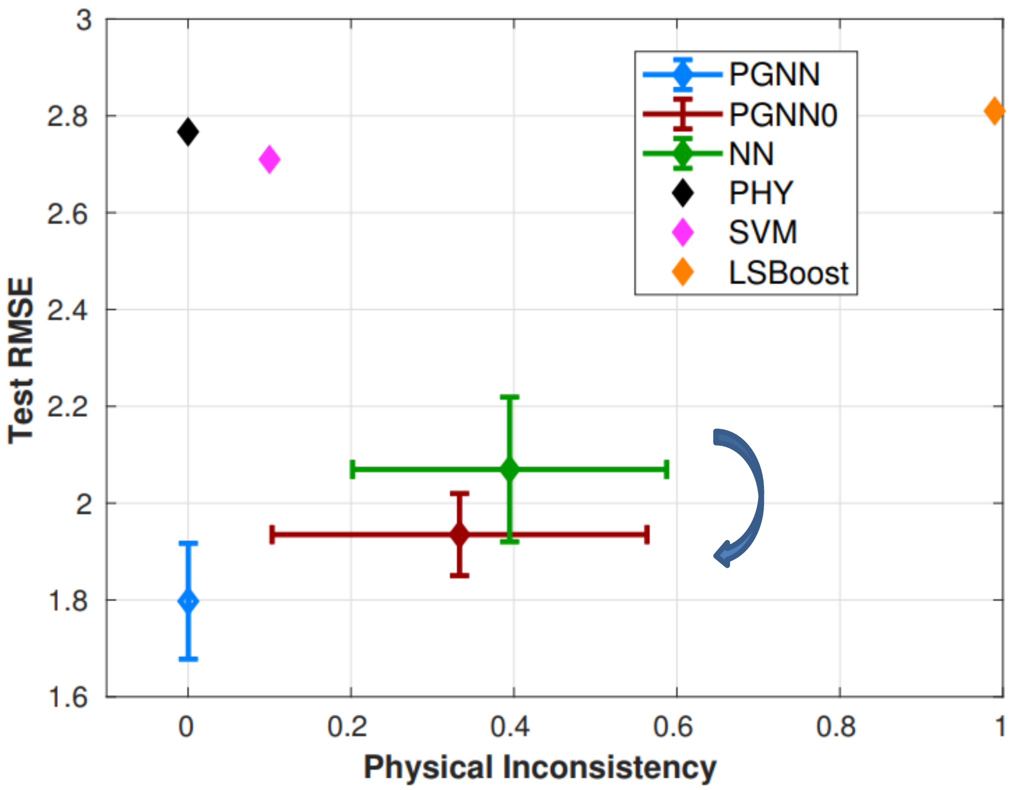

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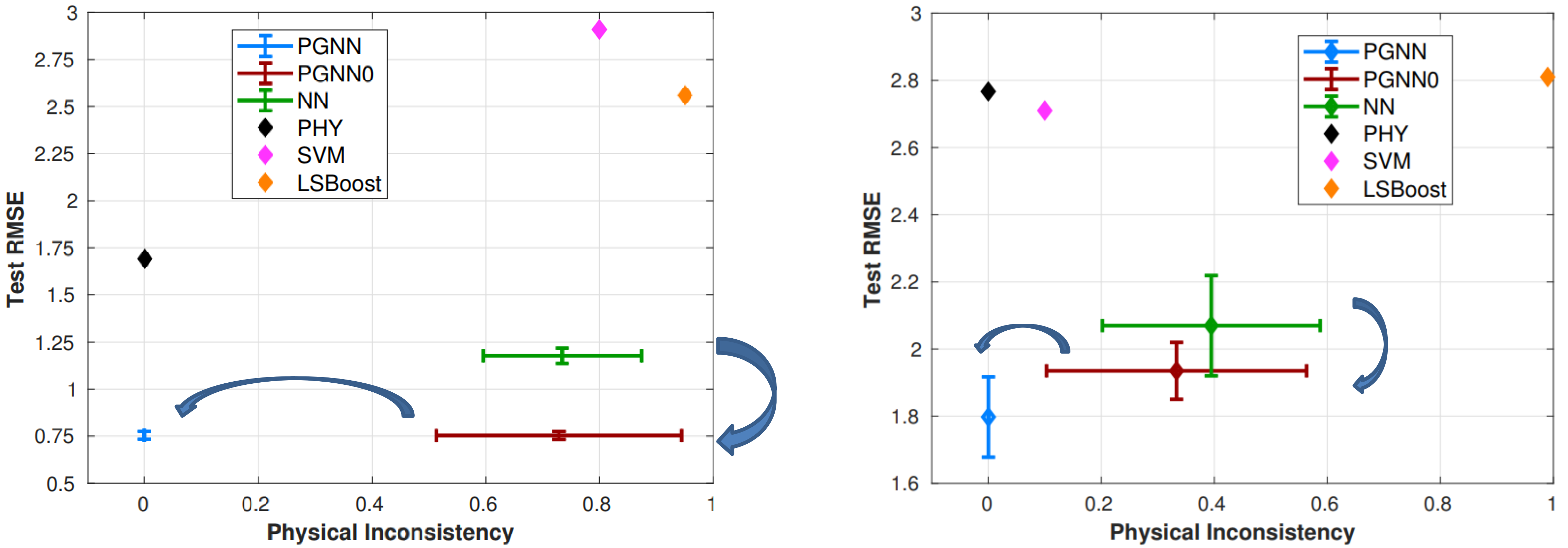

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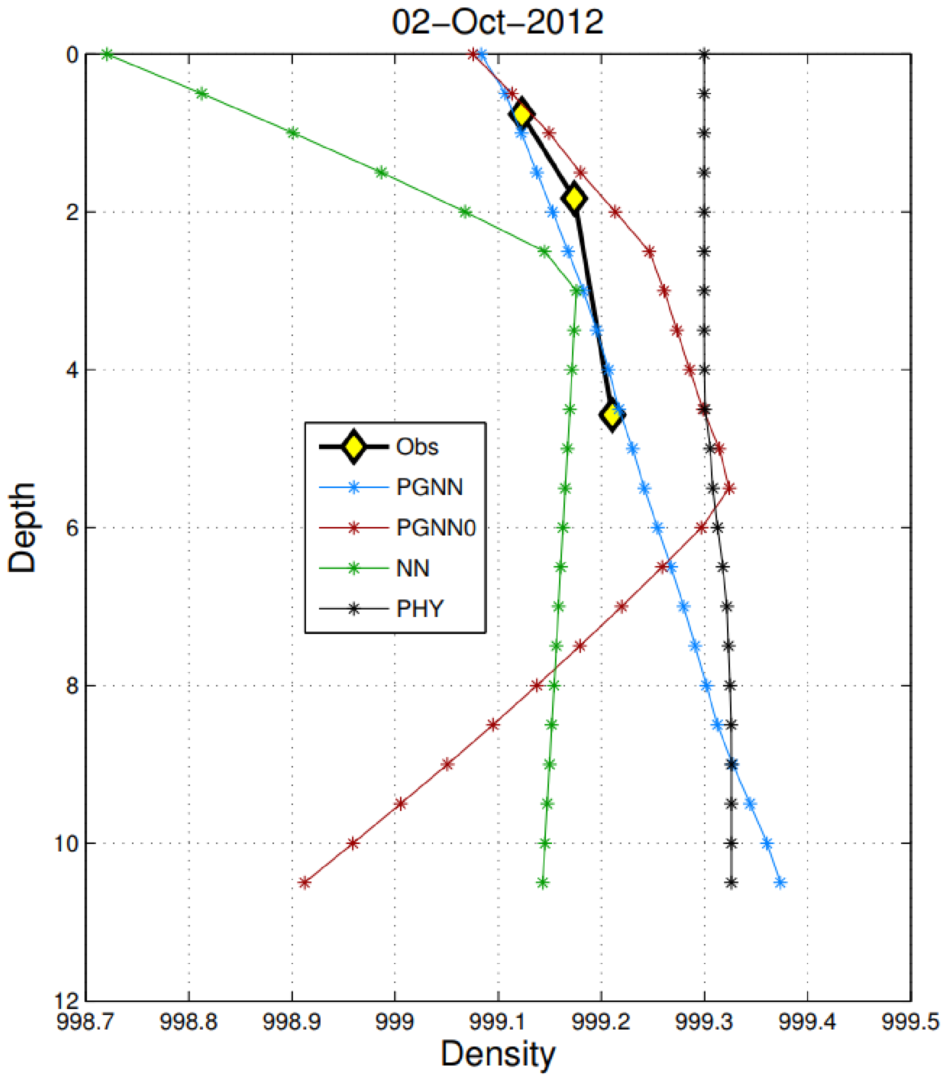
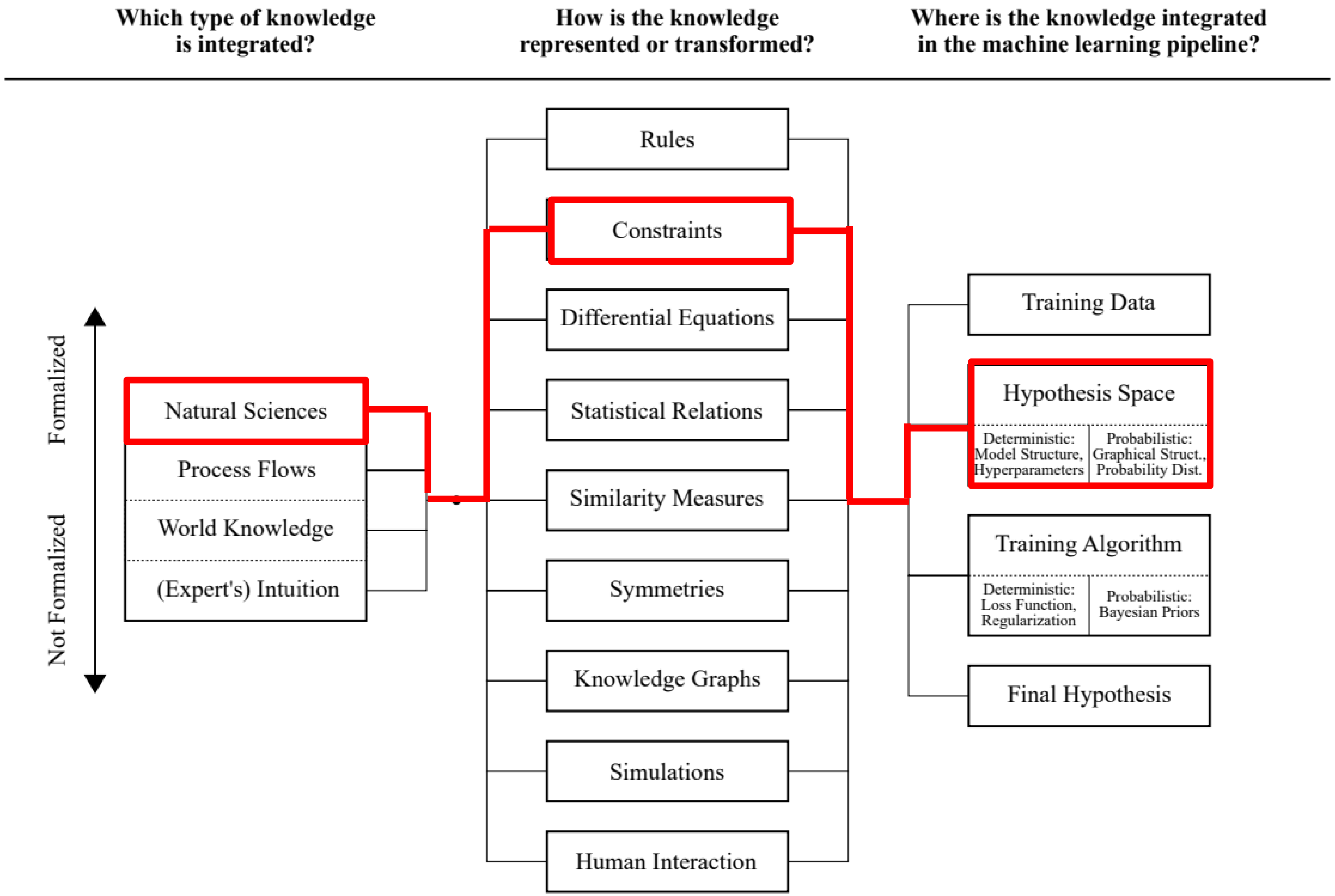


(a) Lake Mille Lacs on 02-October-2012

Limiting the model space



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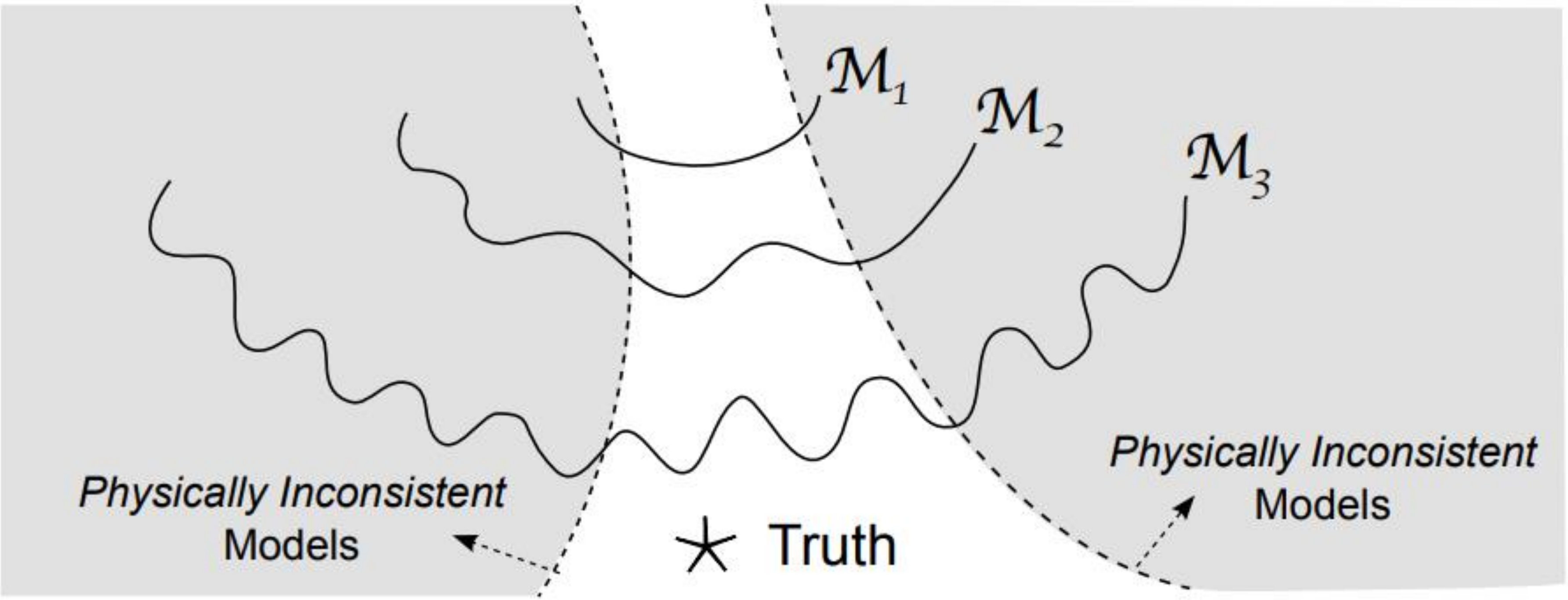

Karpatne et al

Scientific knowledge can reduce the model variance
- removing physically inconsistent solutions
- without likely affecting their bias.

Gaussian Process Regression

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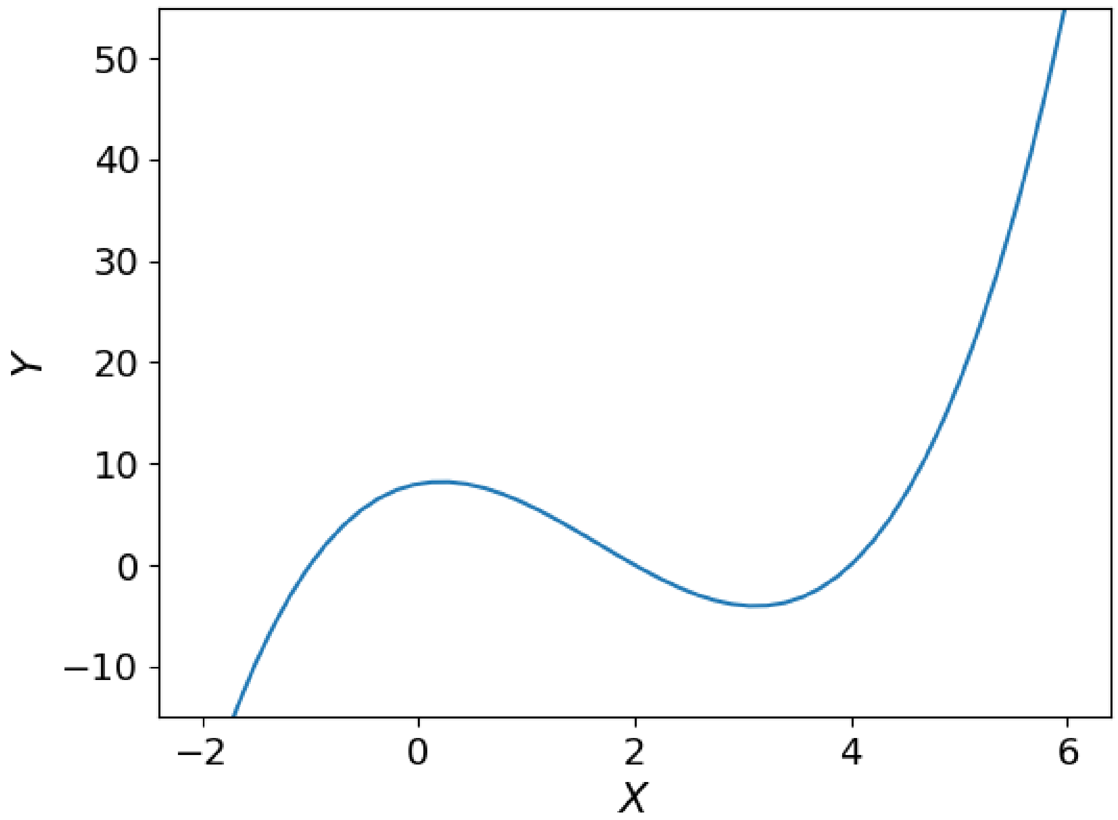

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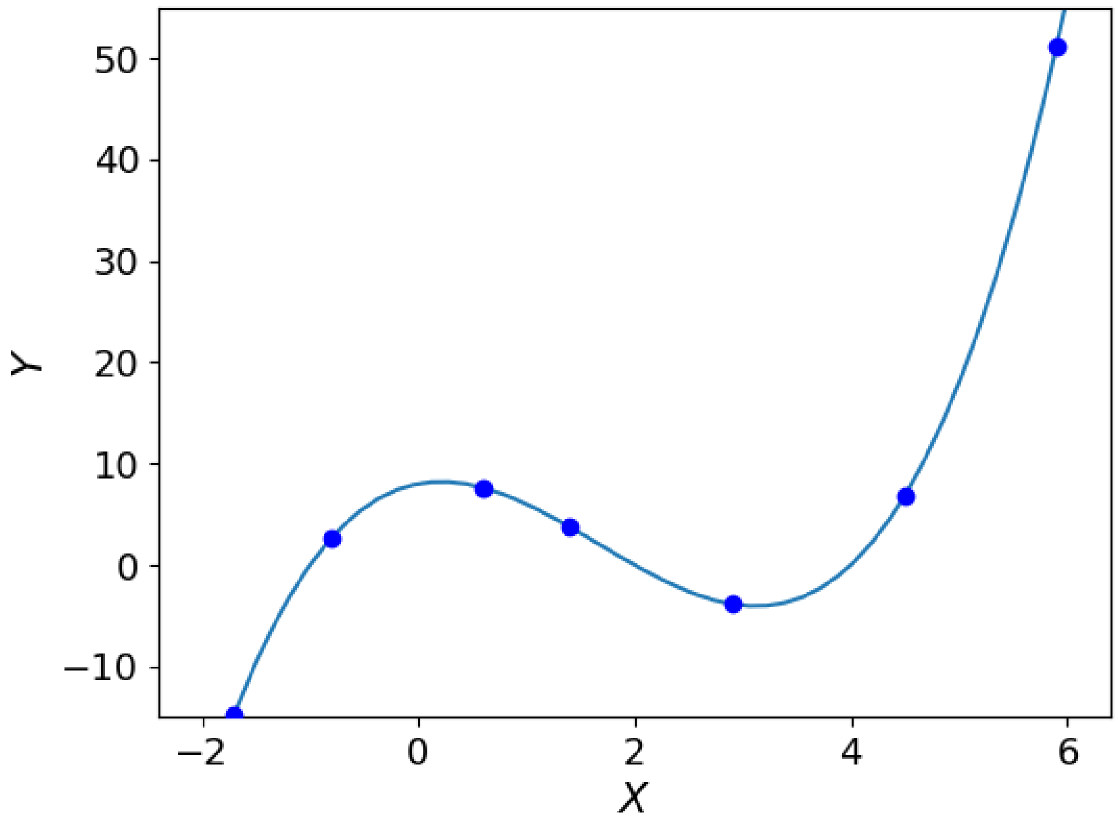

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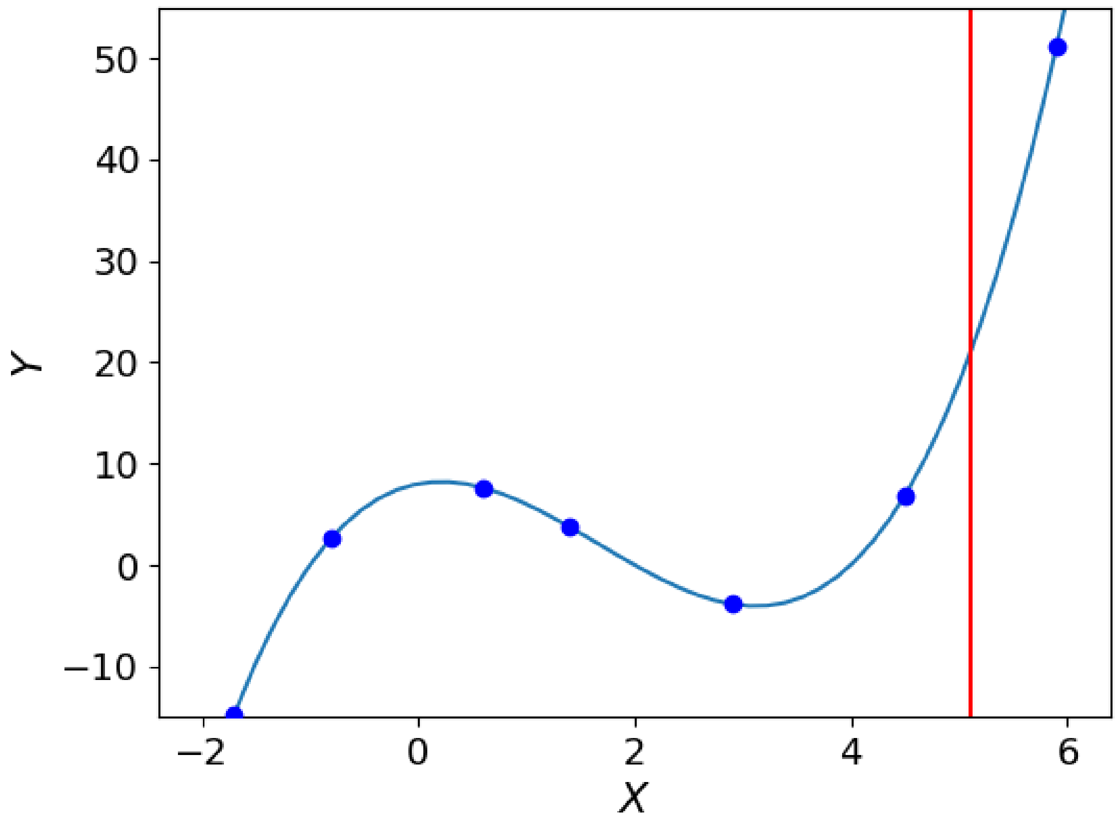

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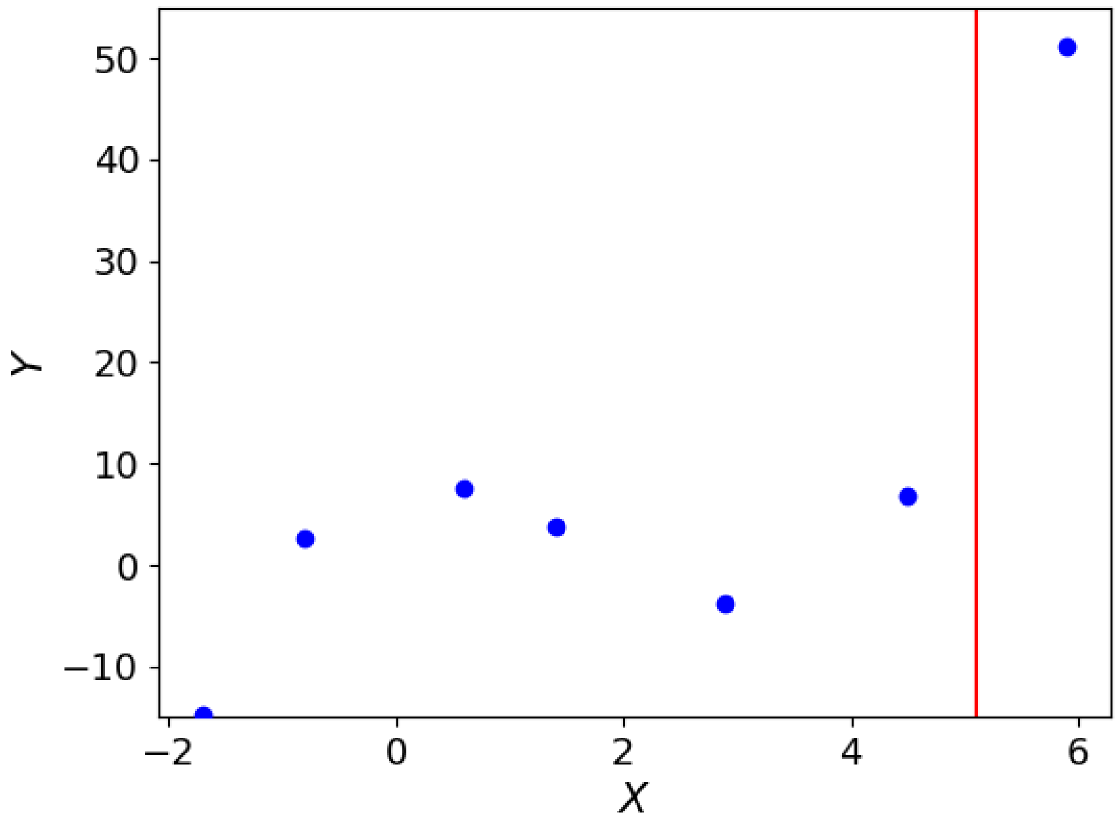

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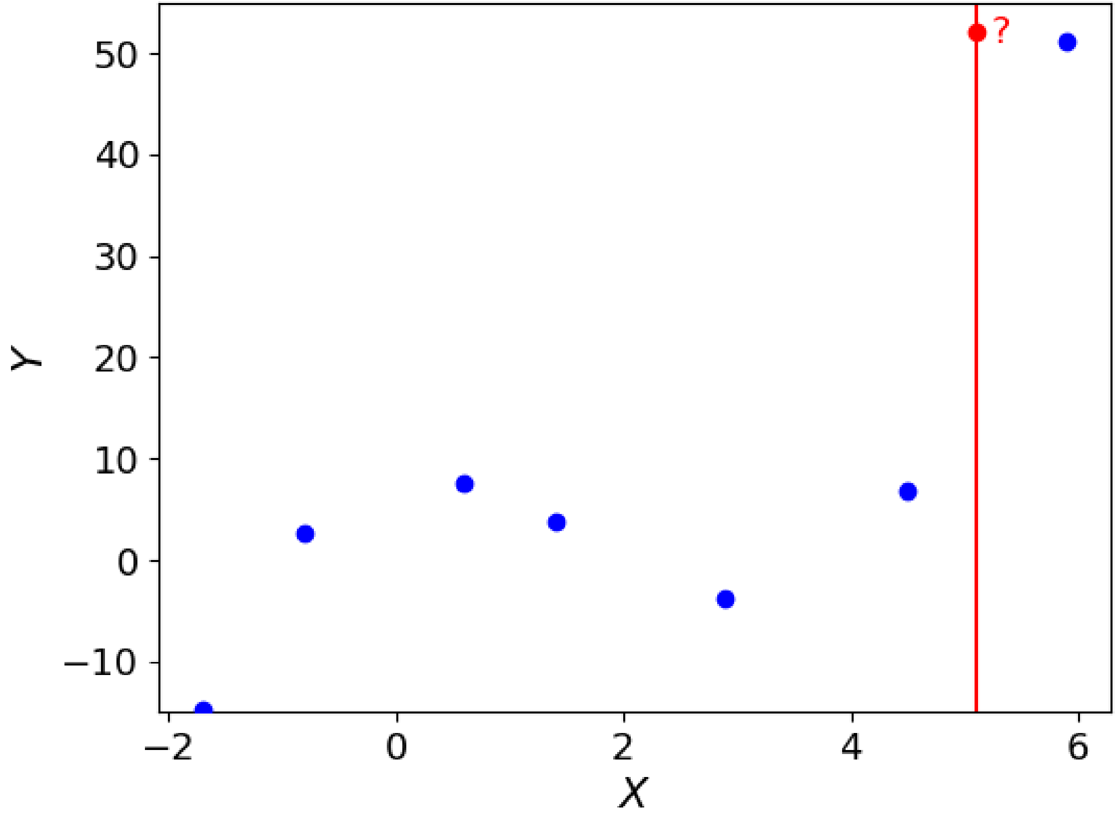

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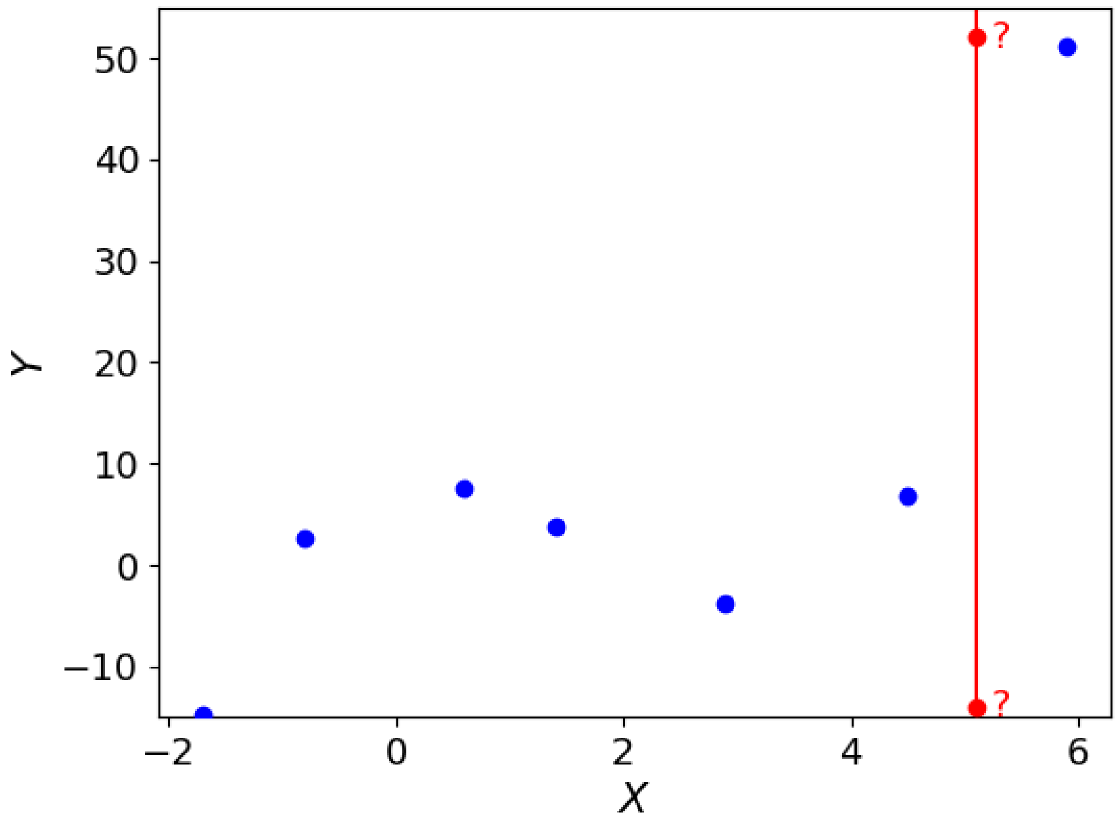

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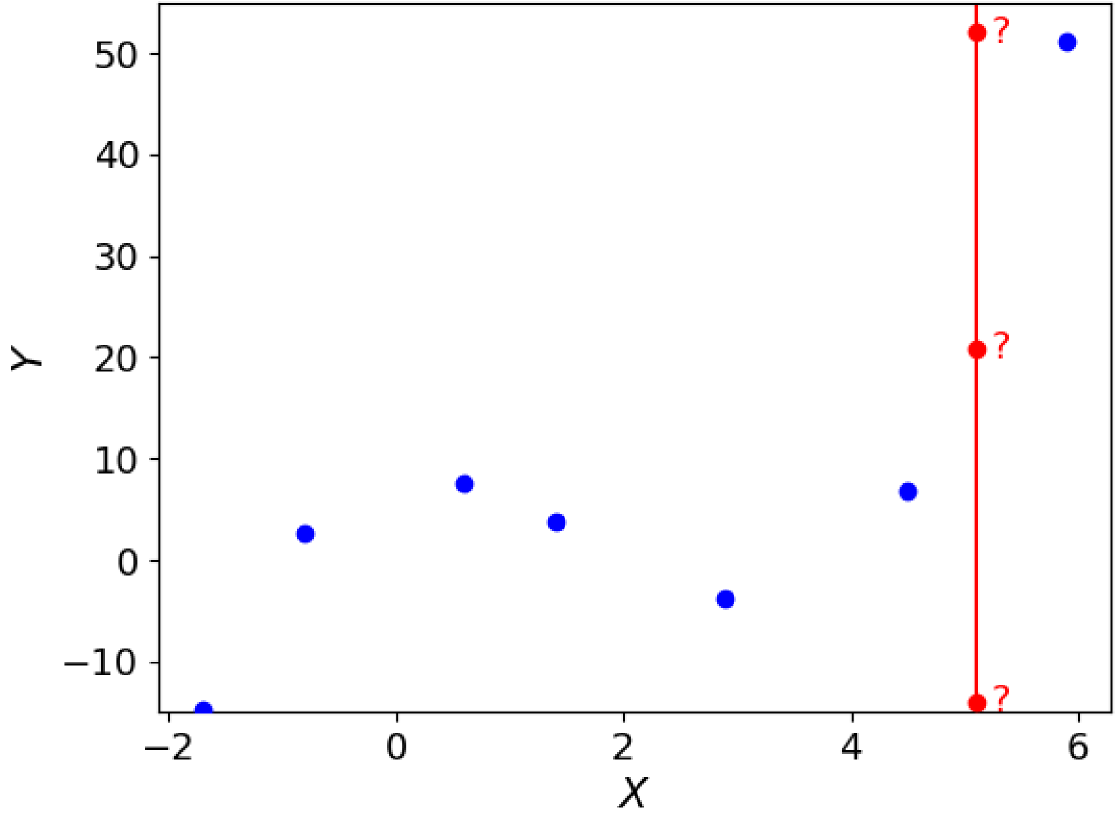

Gaussian Process Regression

- **Context**
  - Function to learn $f : \mathbb{R}^d \rightarrow \mathbb{R}$
  - Given set of inputs $\mathbf{X} = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_n\}$ associated to $y_1, \dots, y_n$ such as $y_i = f(\boldsymbol{x}_i)$

- **Definition of a Gaussian Process**
  - All values $\left(f(\boldsymbol{x}_1), \dots, f(\boldsymbol{x}_n)\right)$ are normally distributed
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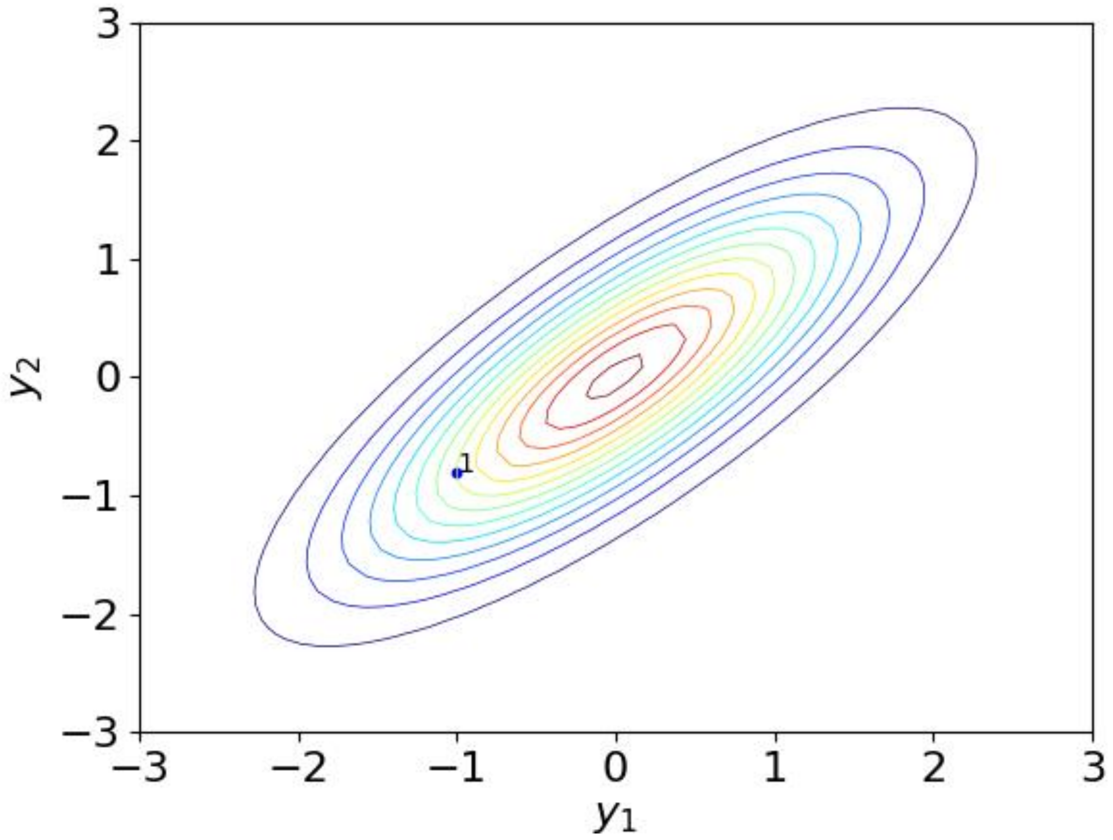
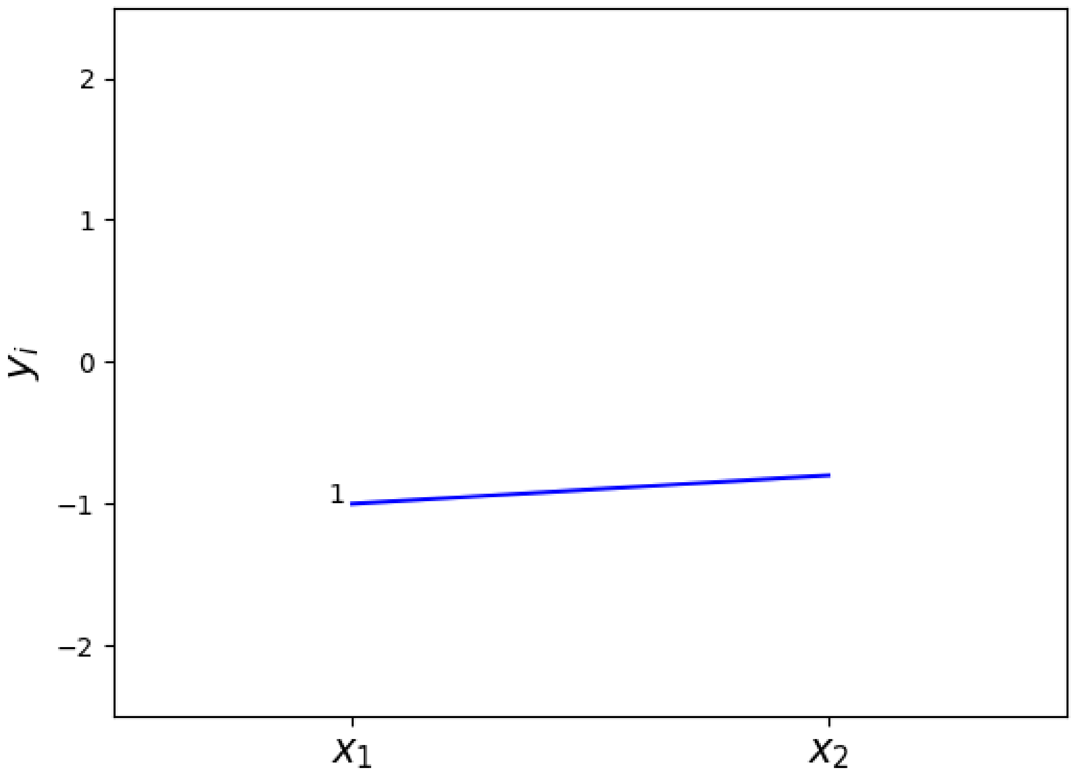
- **Full definition**
  - Mean : $\mathbb{E}[f(\boldsymbol{x})] = \mu(\boldsymbol{x})$ usually can be 0
  - Covariance function $Cov\left(f(\boldsymbol{x}), f(\boldsymbol{x}')\right) = k(\boldsymbol{x}, \boldsymbol{x}')$ with k a function called kernel
  - $\mathrm{f}(\mathbf{x}) \sim GP(0, k(\boldsymbol{x}, \boldsymbol{x}'))$

$$\begin{bmatrix} f(\boldsymbol{x}) \\ f(\boldsymbol{x}') \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} k(\boldsymbol{x}, \boldsymbol{x}) & k(\boldsymbol{x}, \boldsymbol{x}') \\ k(\boldsymbol{x}', \boldsymbol{x}) & k(\boldsymbol{x}', \boldsymbol{x}') \end{bmatrix}\right.$$

Gaussian Process Regression: 2D example





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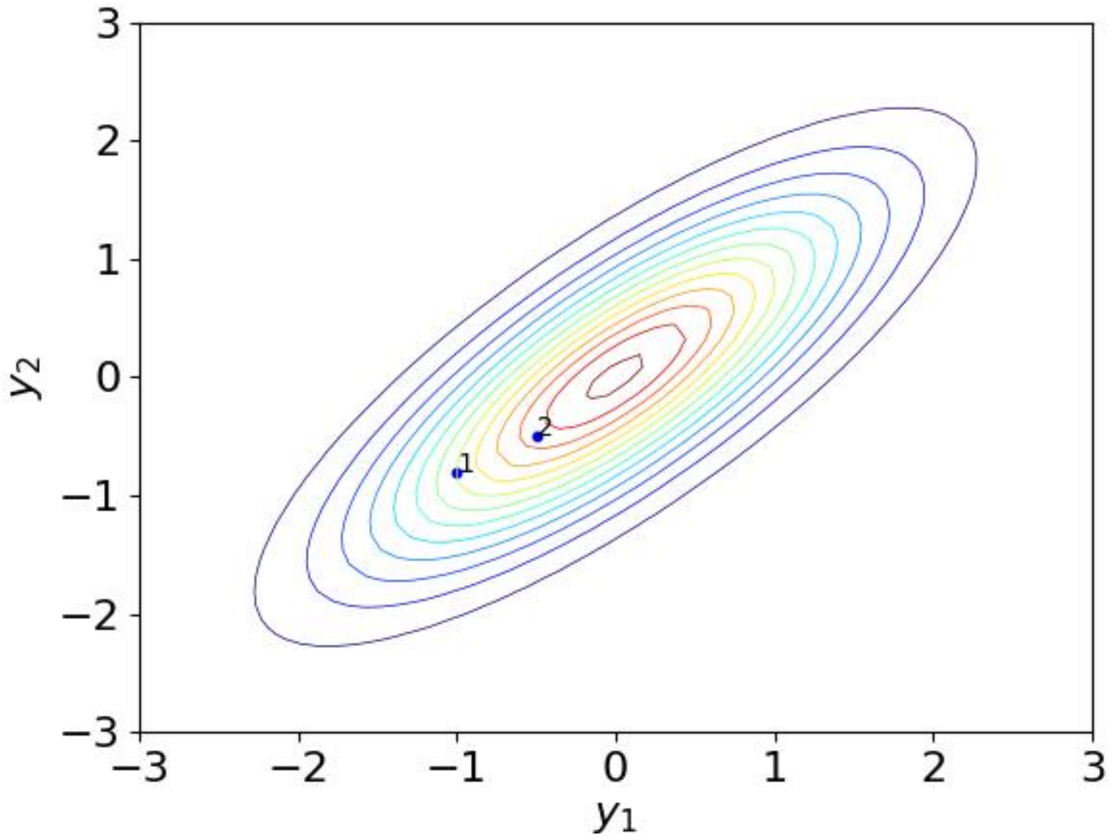

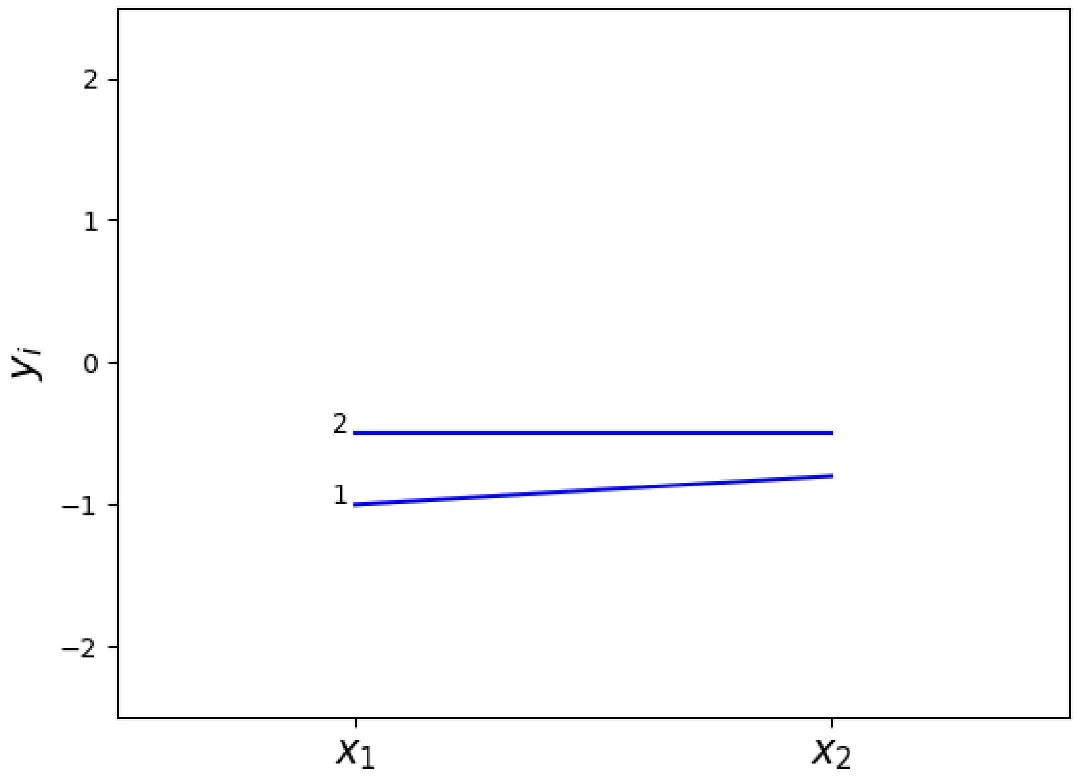

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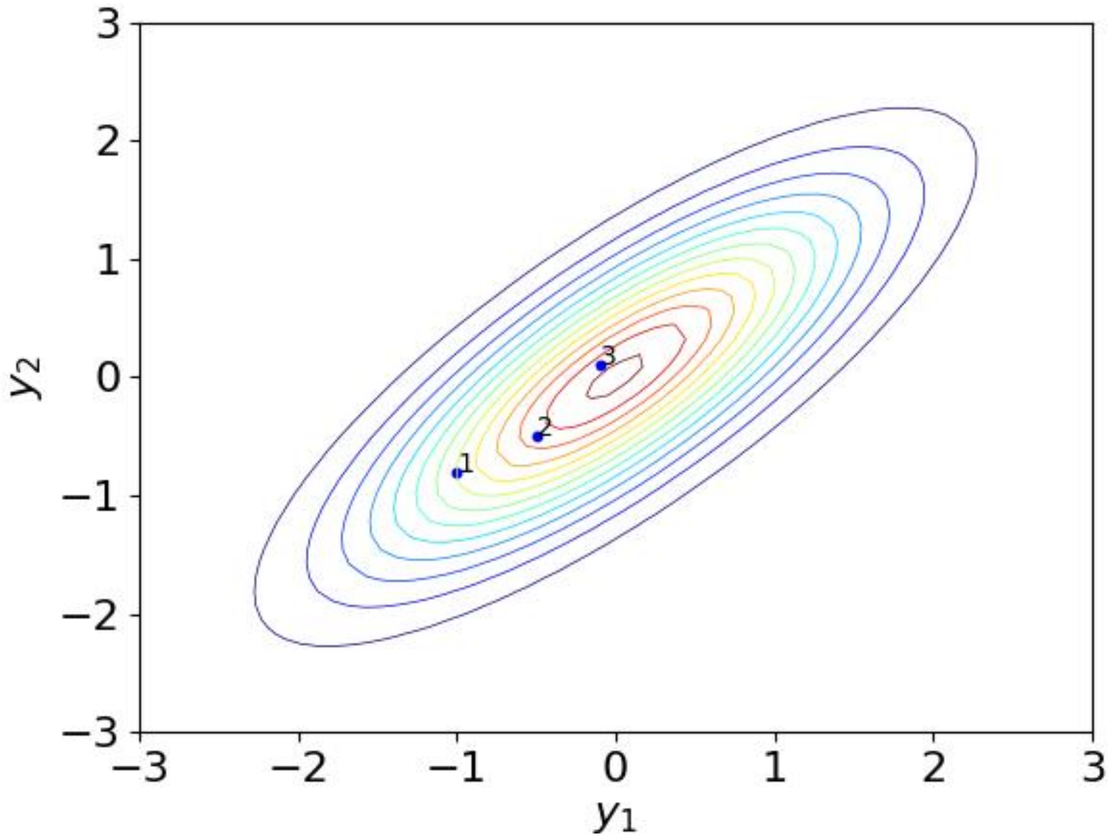

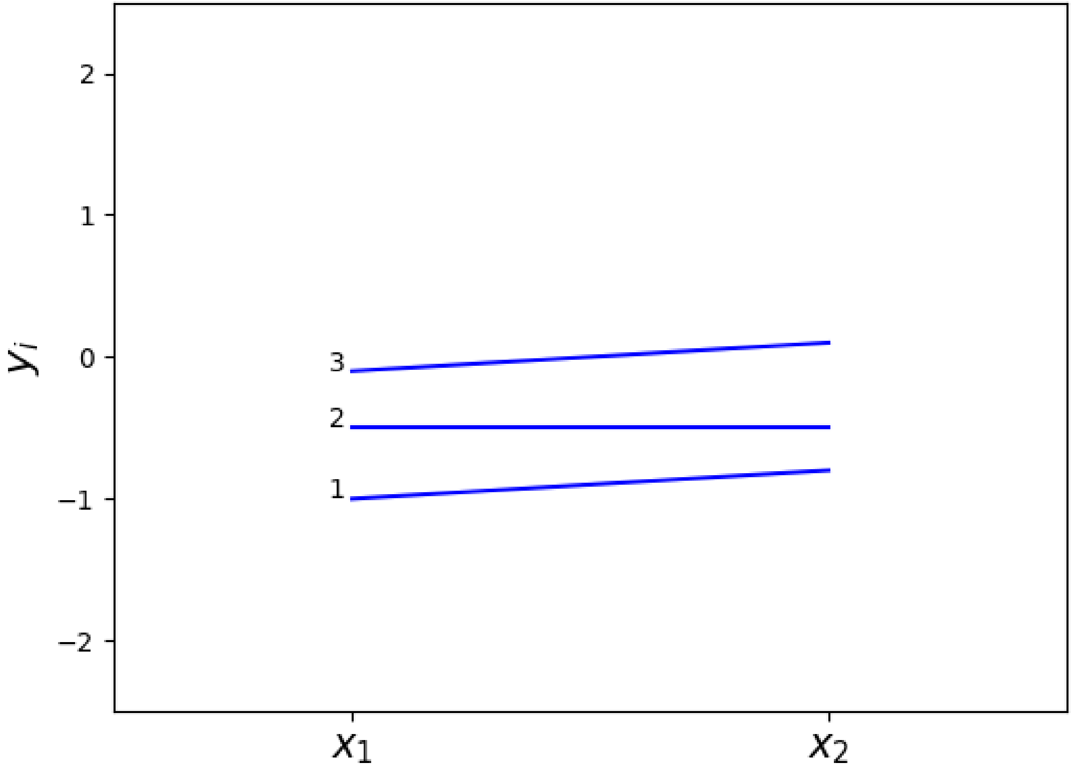

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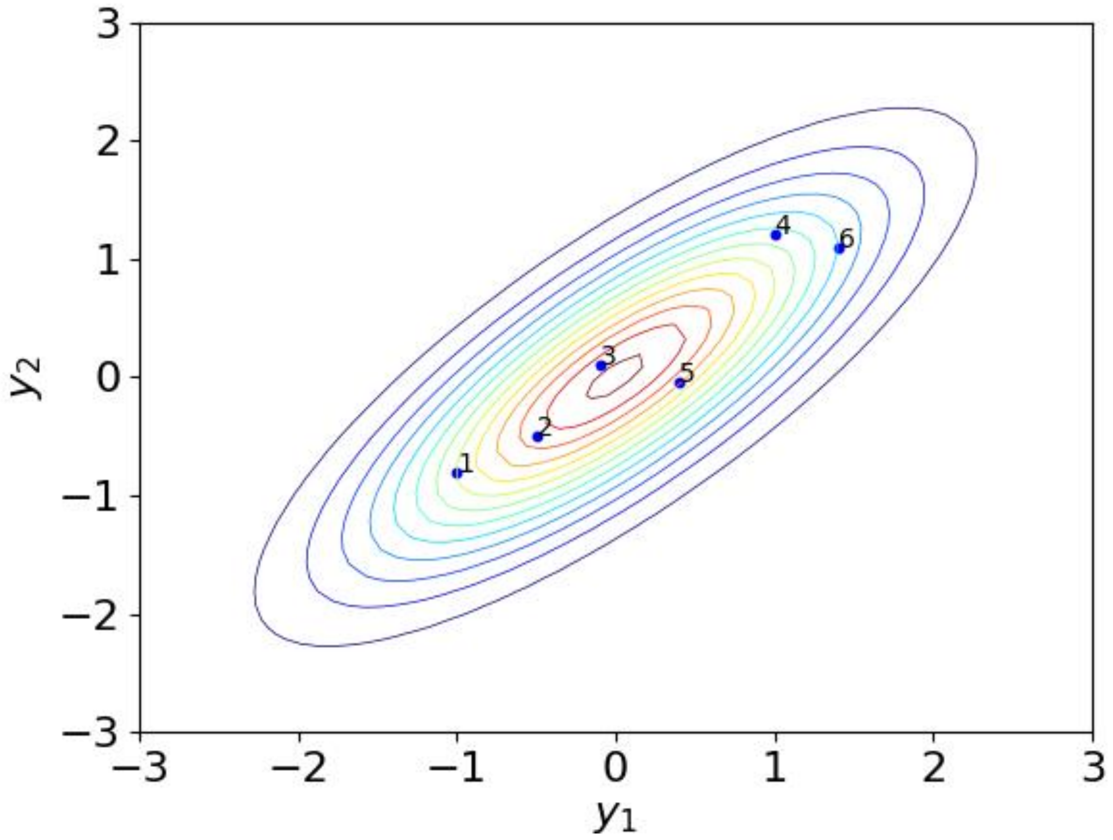

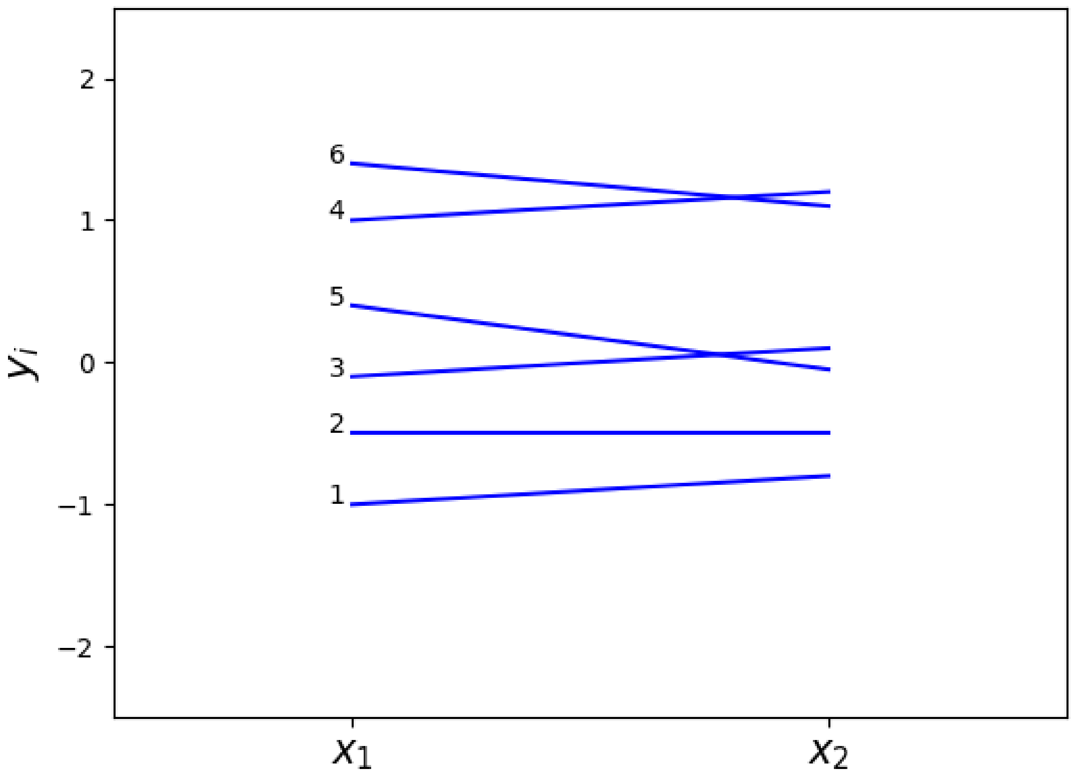

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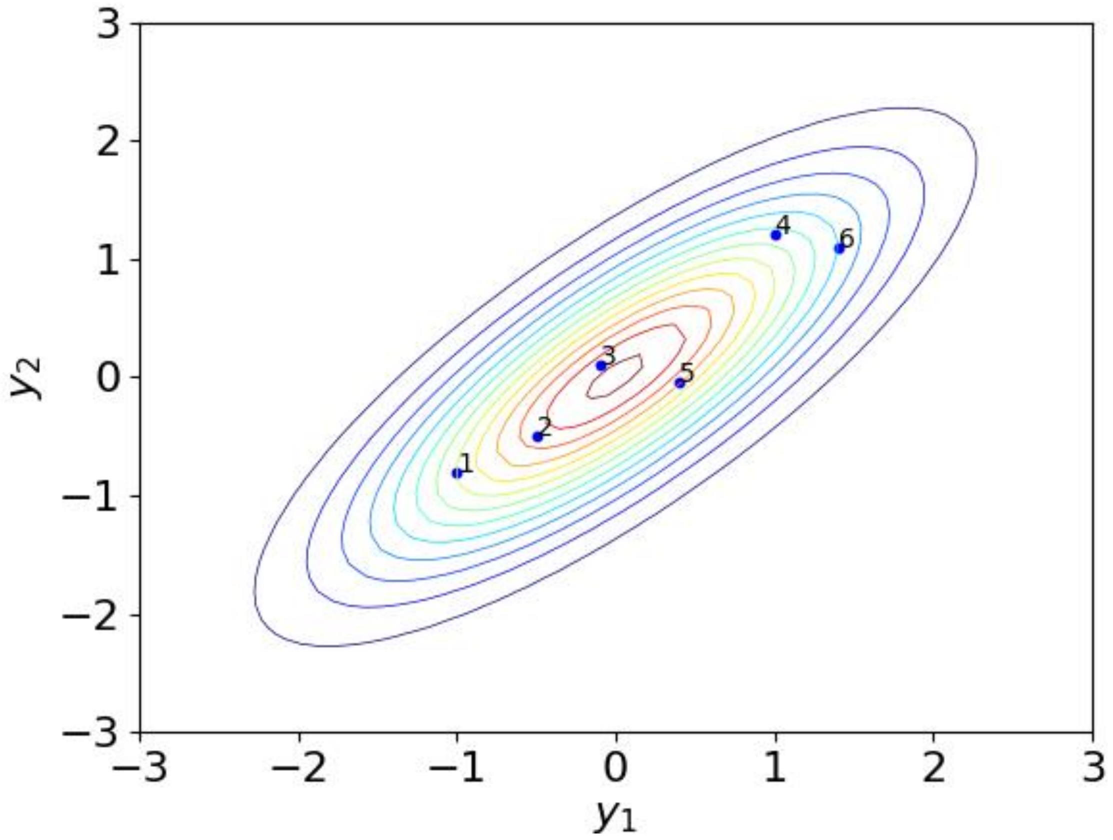

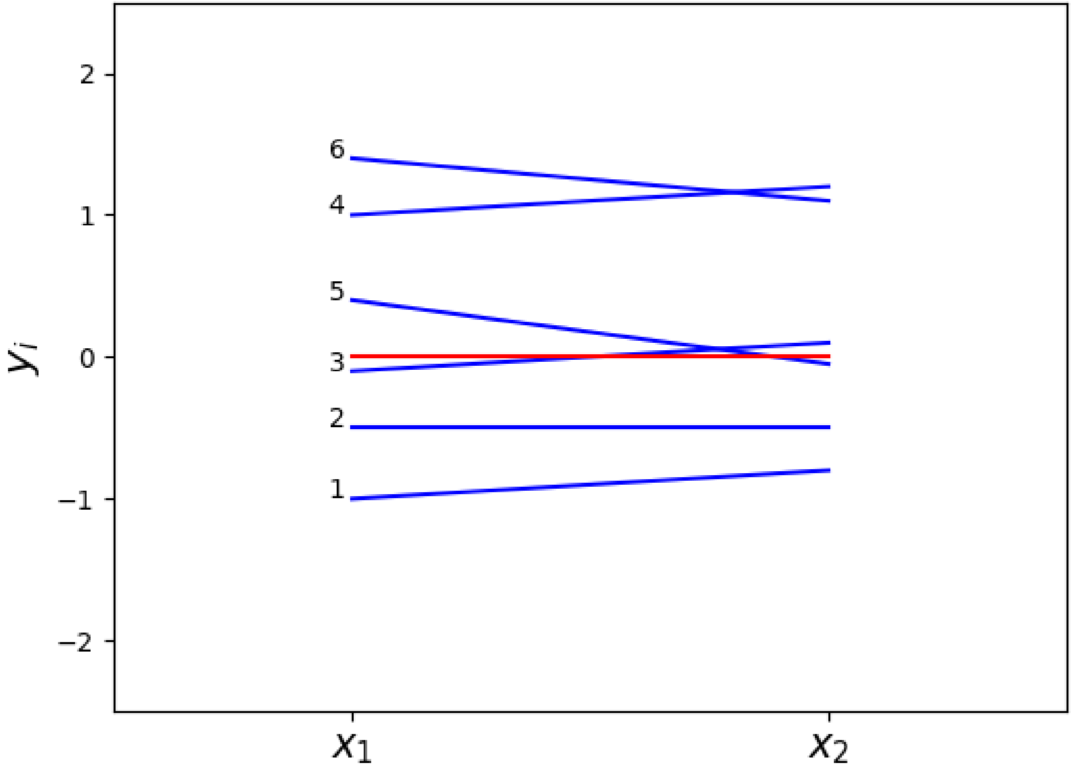

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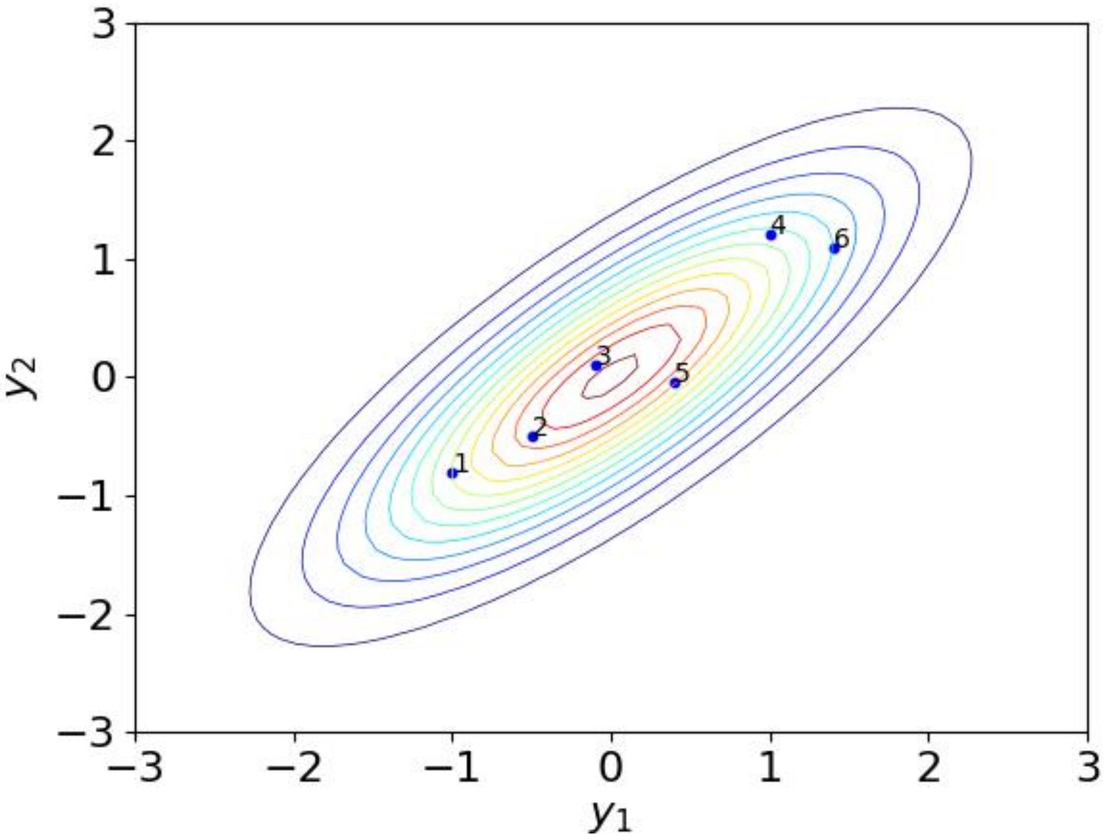
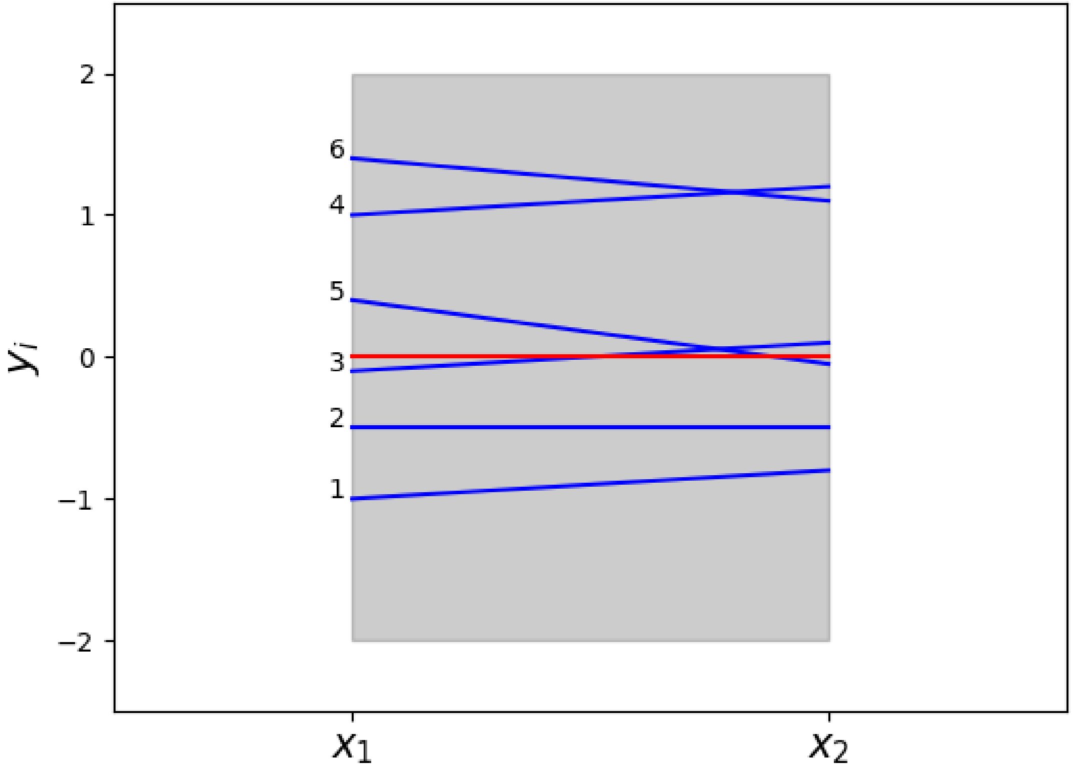
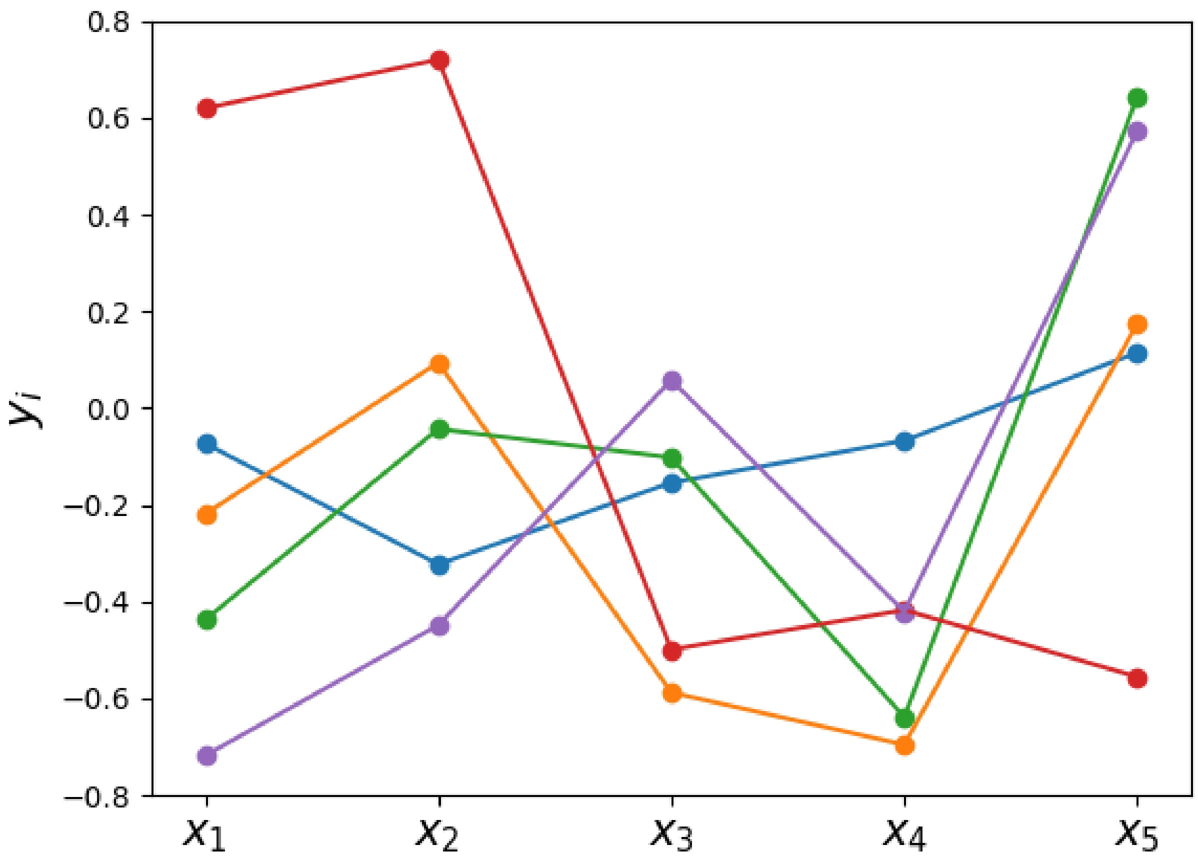
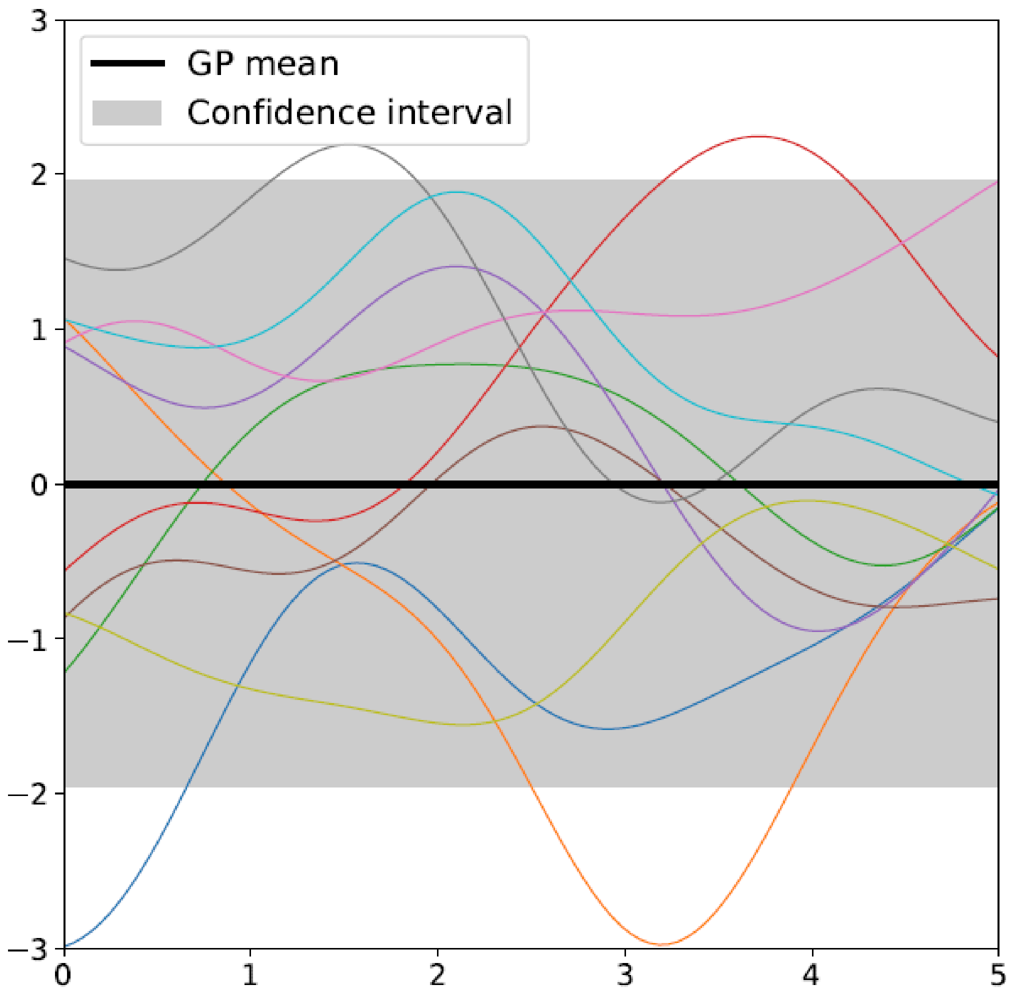




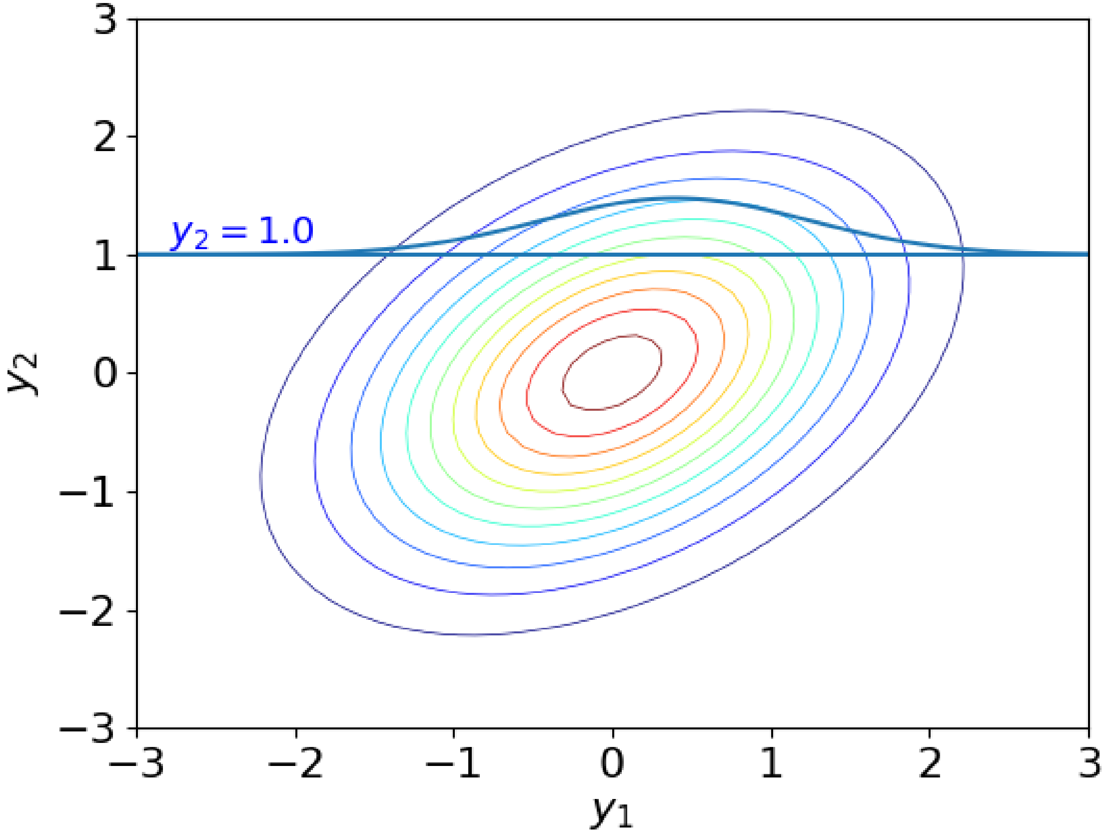
Gaussian Process Regression: 5D example



Gaussian Process Regression: infinite dimension



Gaussian Process Regression: conditional sampling



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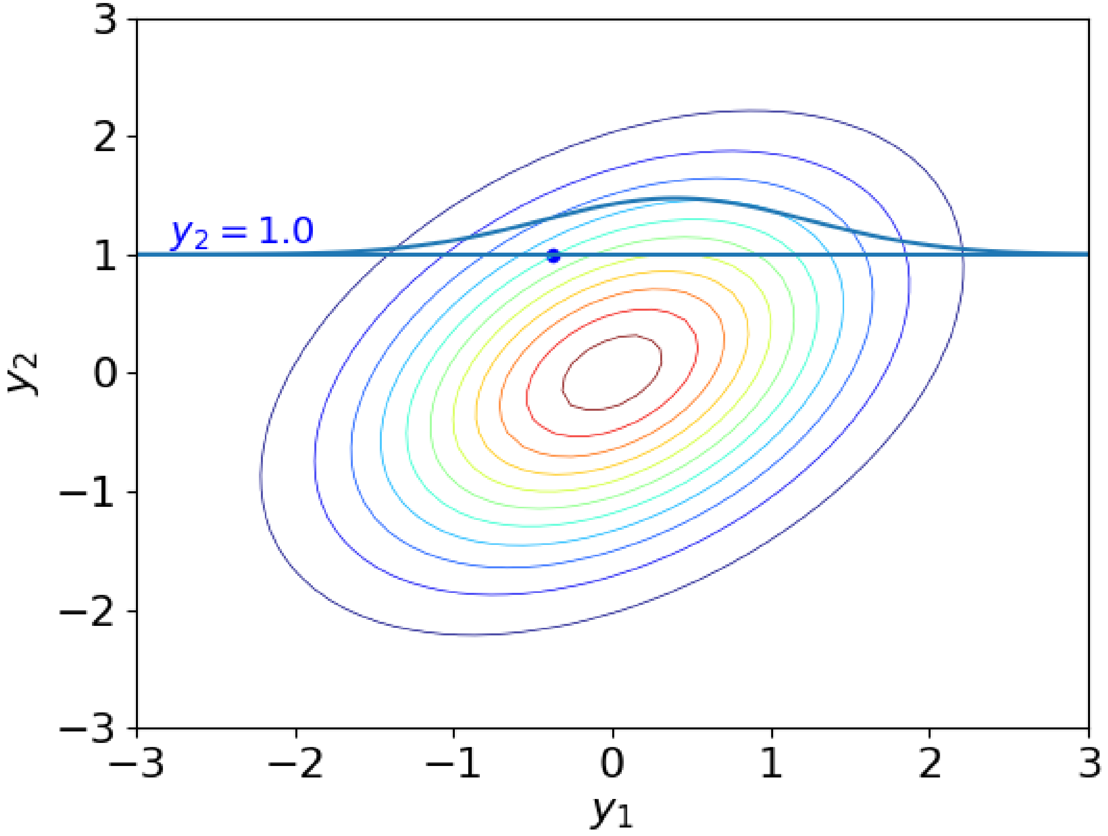

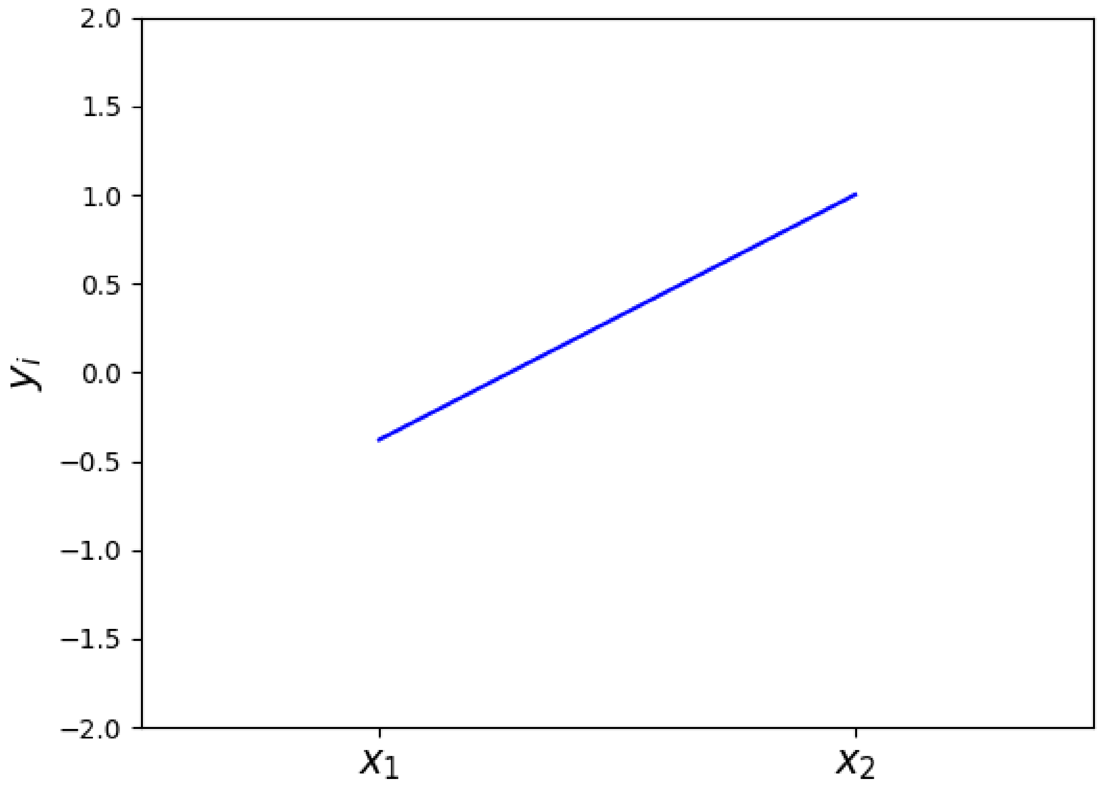

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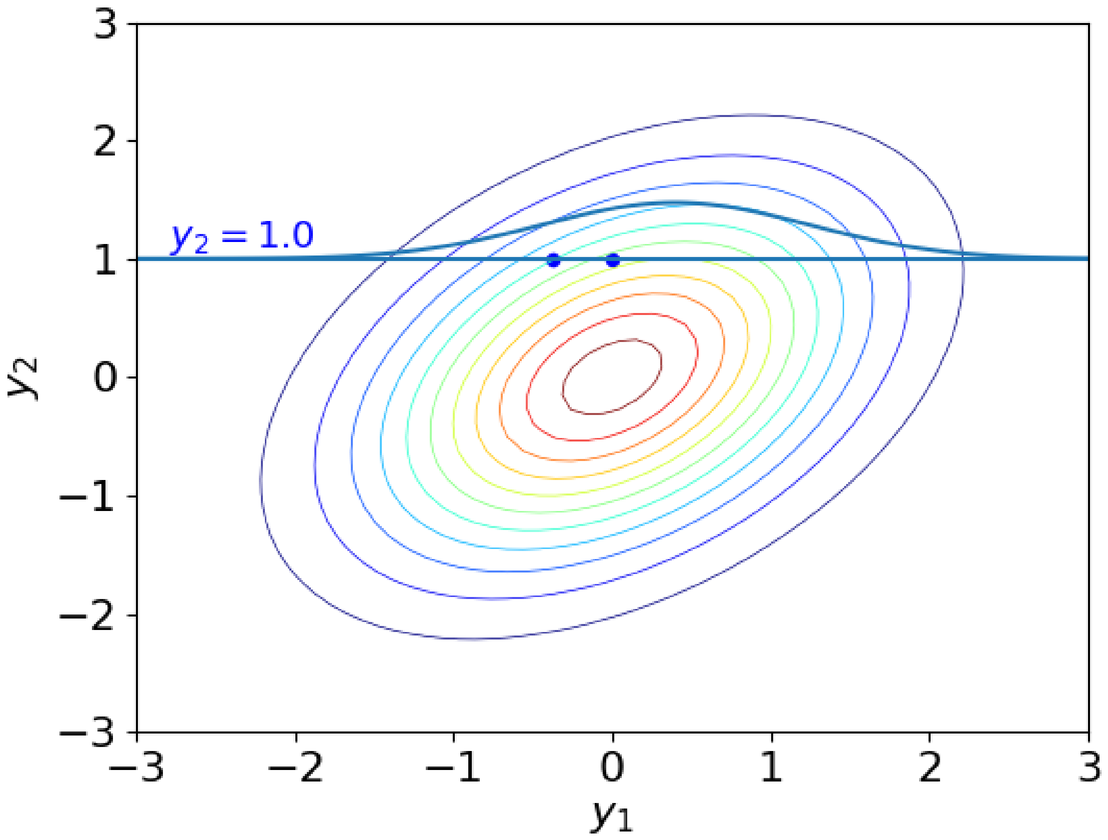

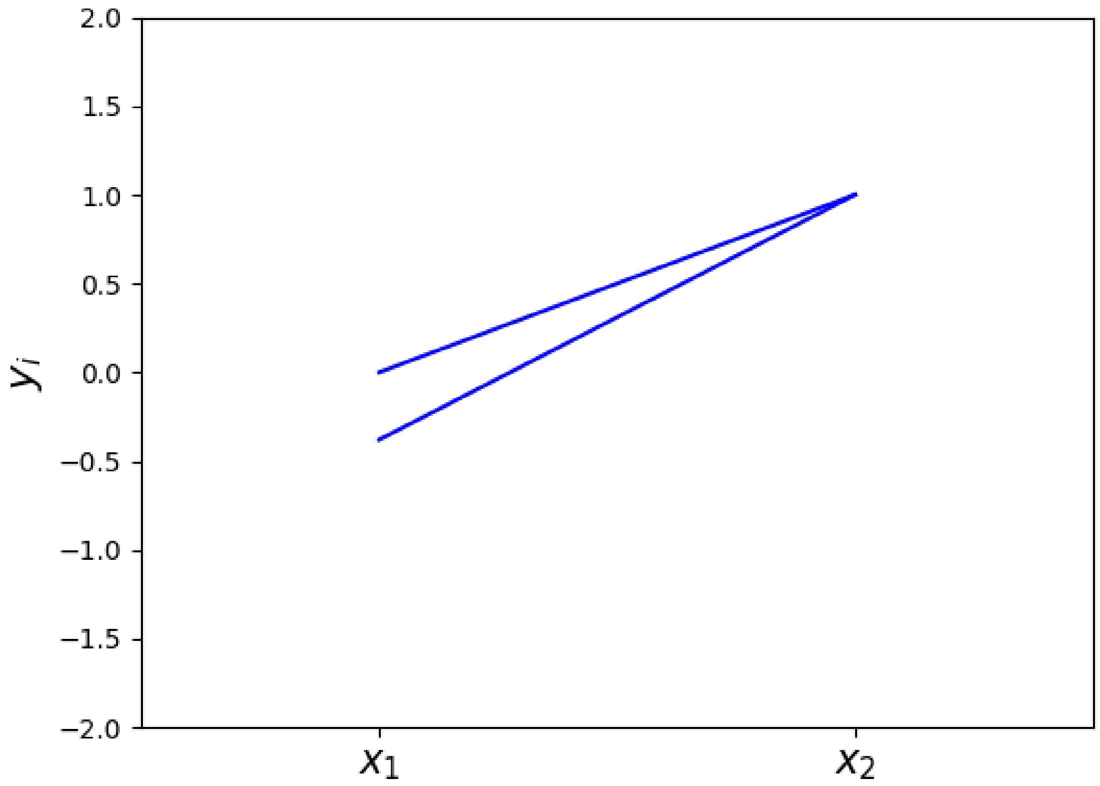

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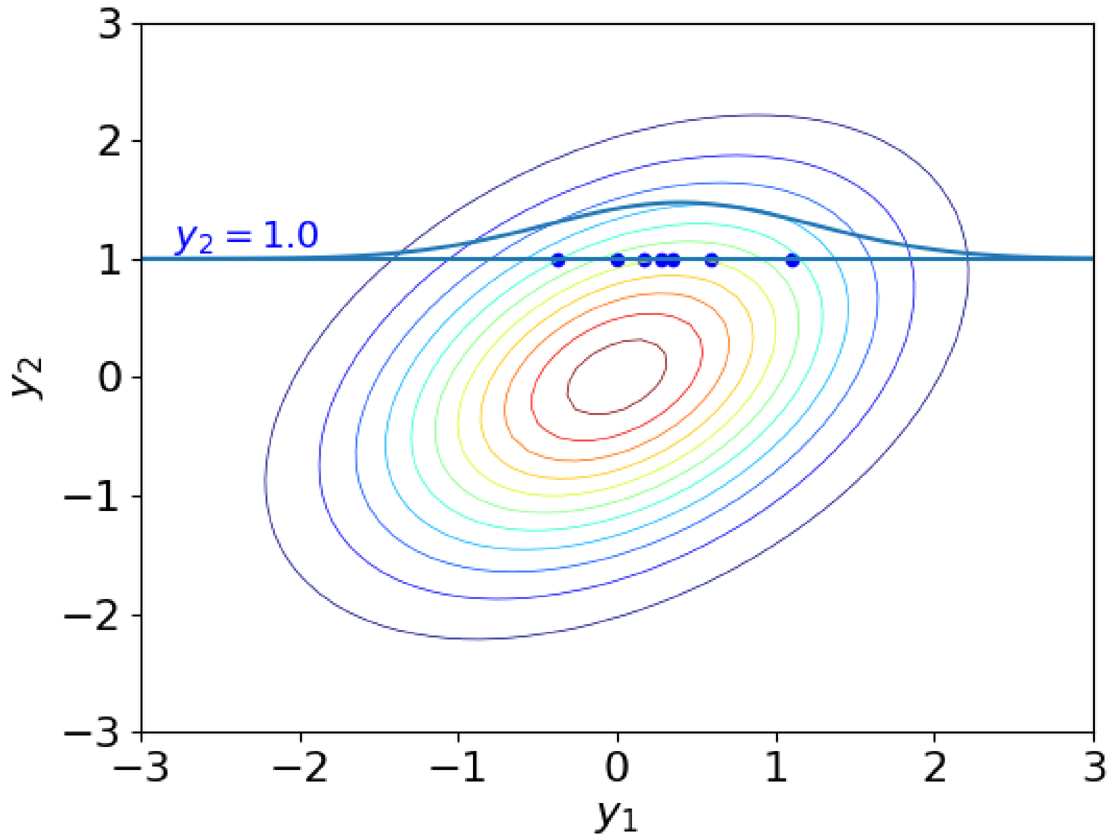
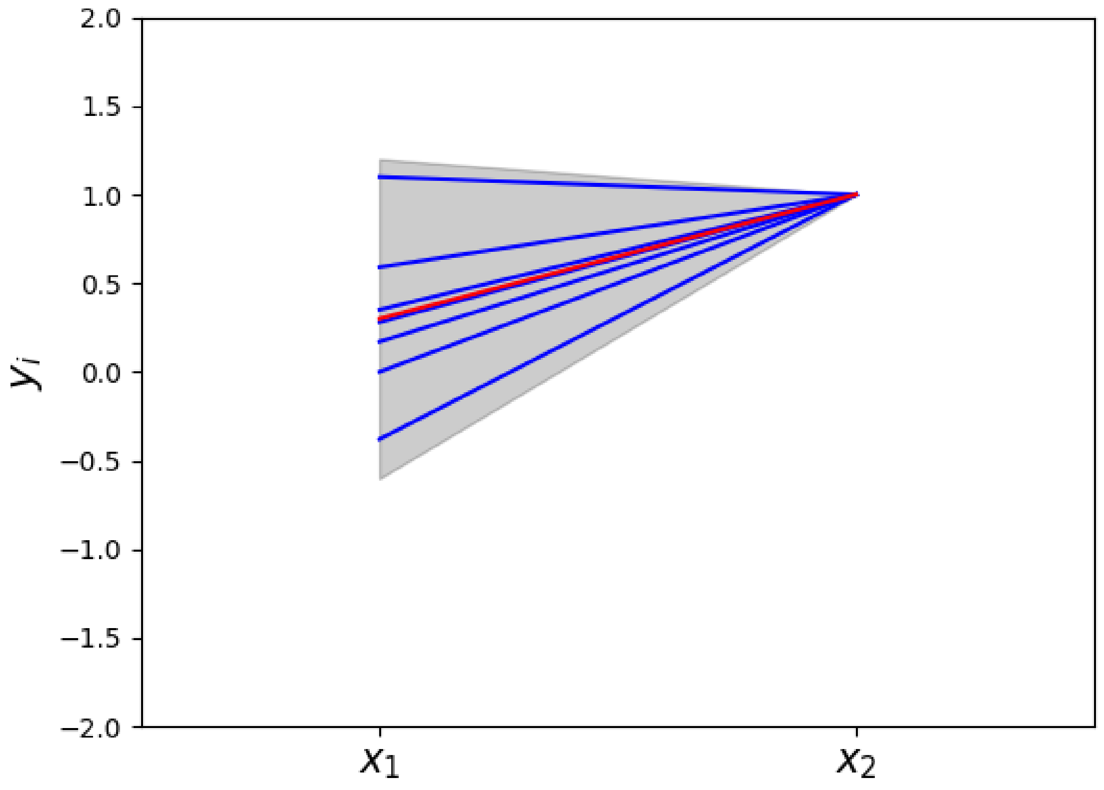
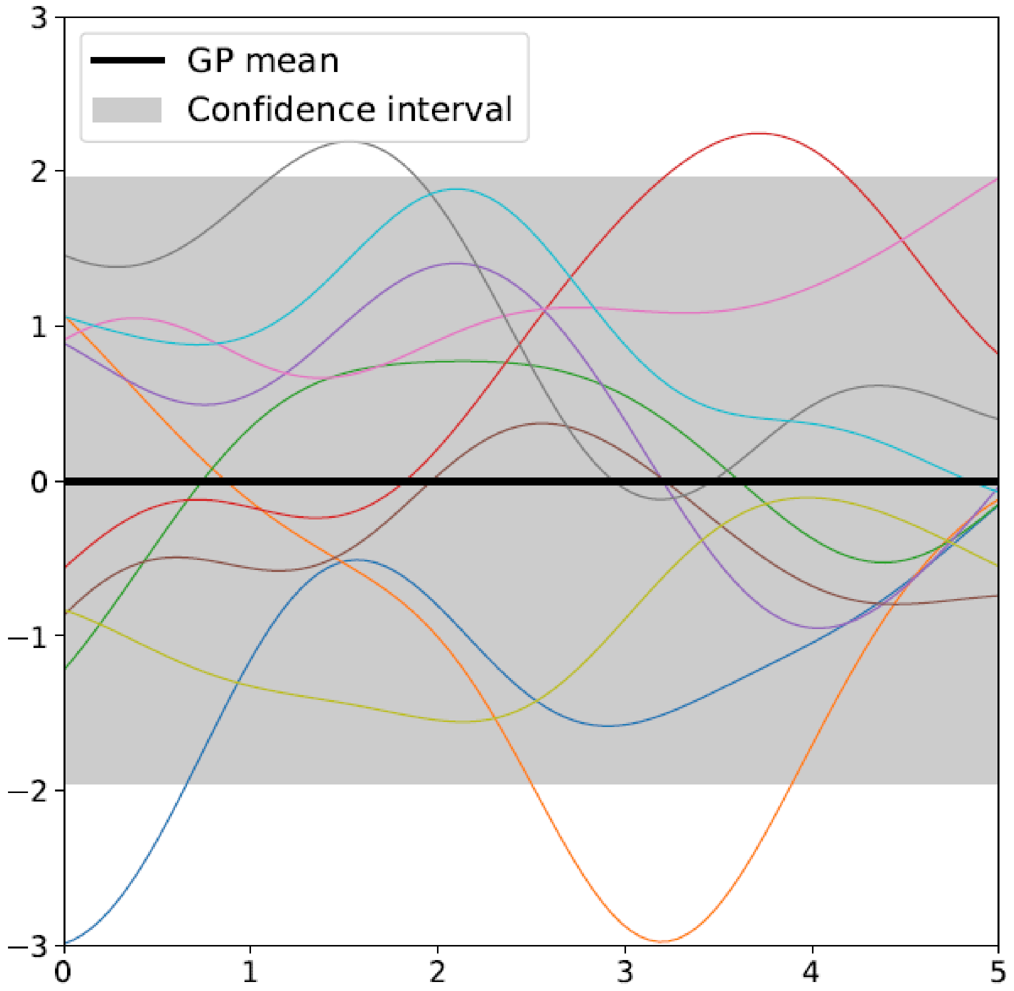




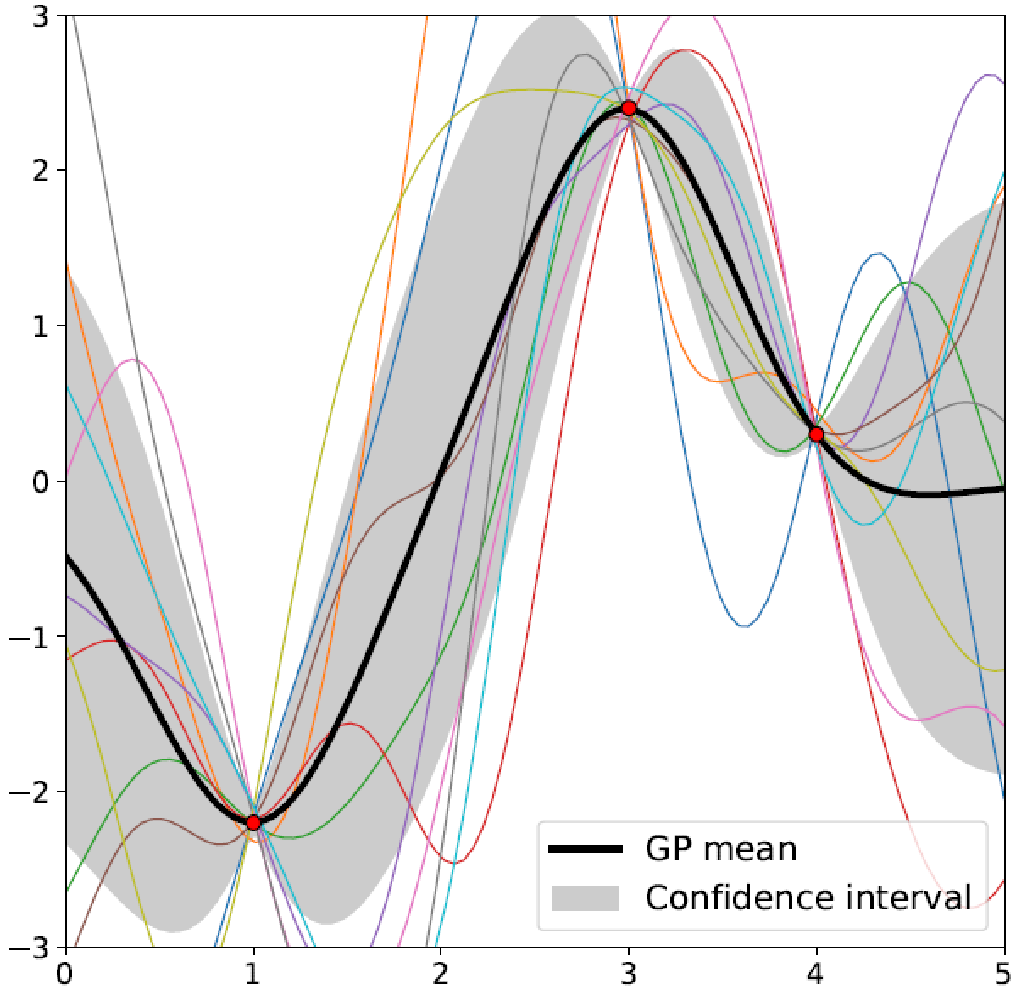
Gaussian Process Regression: Prior

Prior



Gaussian Process Regression: Posterior

Posterior

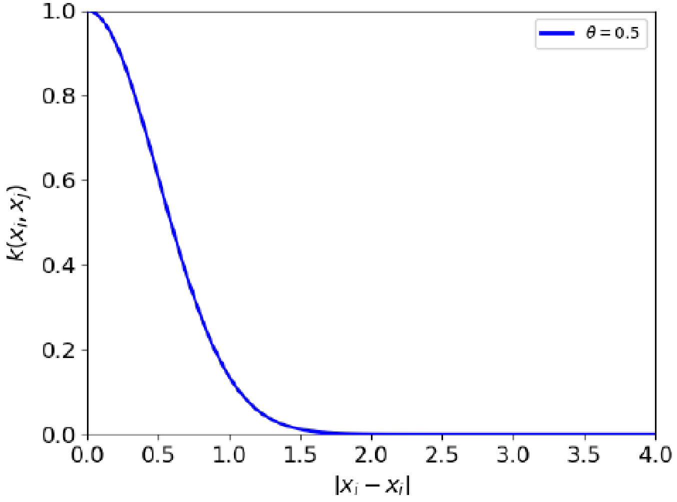


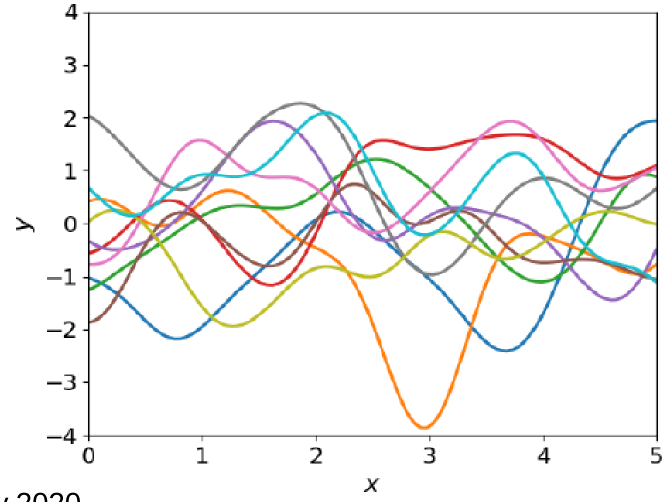
Gaussian Process Regression

- **Conditioning the Gaussian prior on the observation**
  - $\mathbb{E}(f(\boldsymbol{x}^*)|\boldsymbol{X},\boldsymbol{Y}) = k(\boldsymbol{x}^*,\boldsymbol{X})^T \mathrm{k}(\boldsymbol{X},\boldsymbol{X})^{-1}\boldsymbol{Y}$
  - $Var(f(\boldsymbol{x}^*)|\boldsymbol{X},\boldsymbol{Y}) = k(\boldsymbol{x}^*,\boldsymbol{x}^*) - k(\boldsymbol{x}^*,\boldsymbol{X})k(\boldsymbol{X},\boldsymbol{X})^{-1}k(\boldsymbol{X},\boldsymbol{x}^*)$

- **Defining the kernel function**
  - Radial basis function $k(x_i,x_j) = \sigma_0^2 \exp\left(-\frac{(x_i-x_j)^2}{2\theta^2}\right)$
  - θ is the length scale and σ the standard deviation => Hyperparameters to optimize

$$\min_{\theta} \boldsymbol{Y}^T \mathbf{K}^{-1}\boldsymbol{Y} + \log|\boldsymbol{K}|$$





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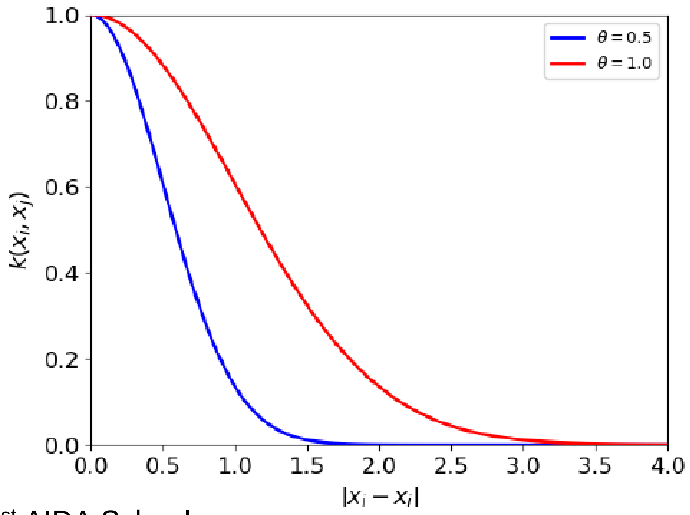

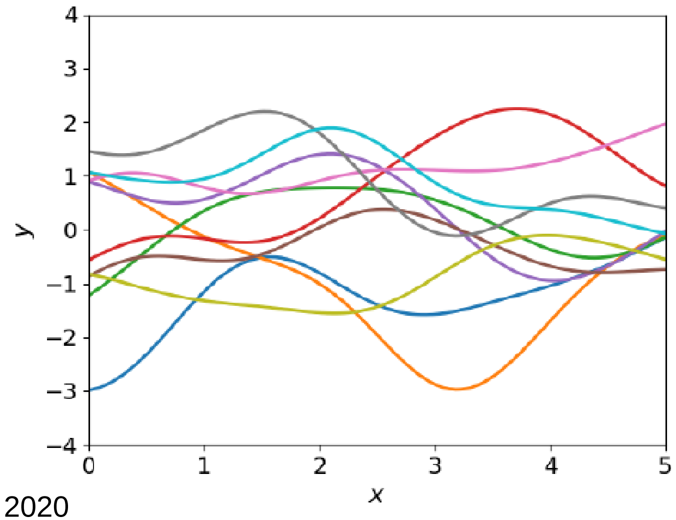

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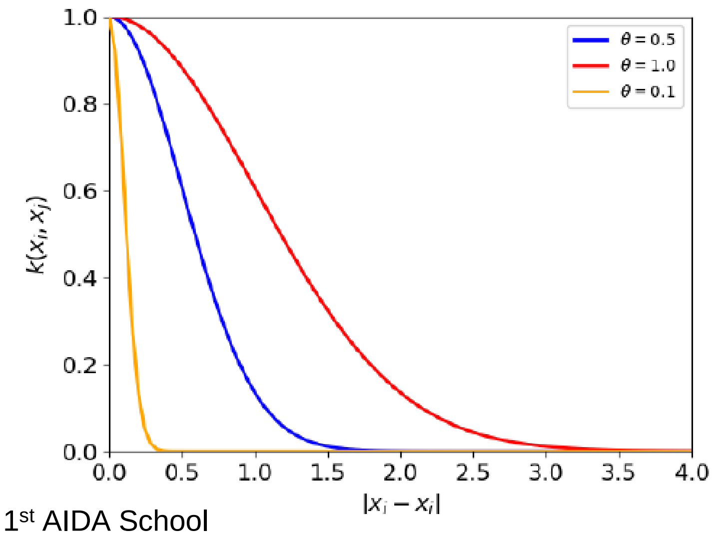

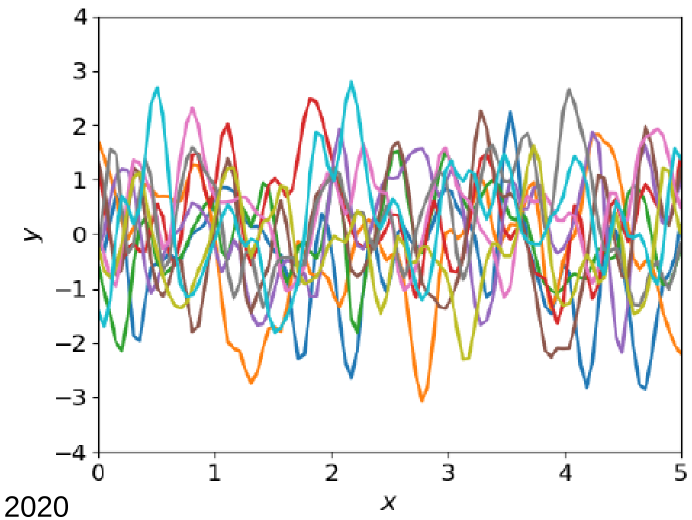

Gaussian Process Overview

- **Prior (hypothesis space)**
  - $f(\boldsymbol{x}) \sim GP\big(0, k(\boldsymbol{x}, \boldsymbol{x}')\big)$
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- **Posterior**
  - $f(\boldsymbol{x}^*)|\boldsymbol{X}, \boldsymbol{Y} = \mathcal{N}(\mu(\boldsymbol{x}^*), Var(\boldsymbol{x}^*))$
  - $\mu(\boldsymbol{x}^*) = k(\boldsymbol{x}^*, \boldsymbol{X})^T \mathbf{K}^{-1} \boldsymbol{Y}$
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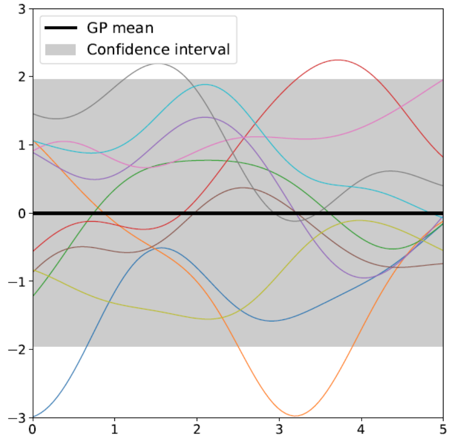
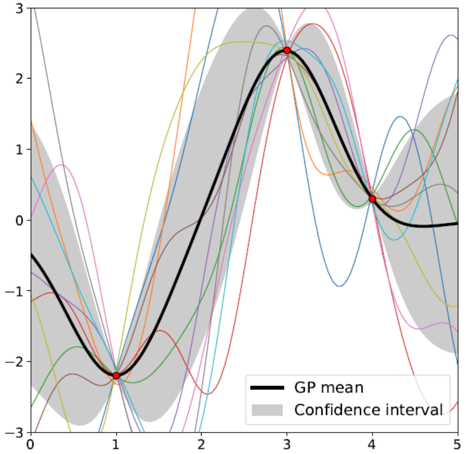
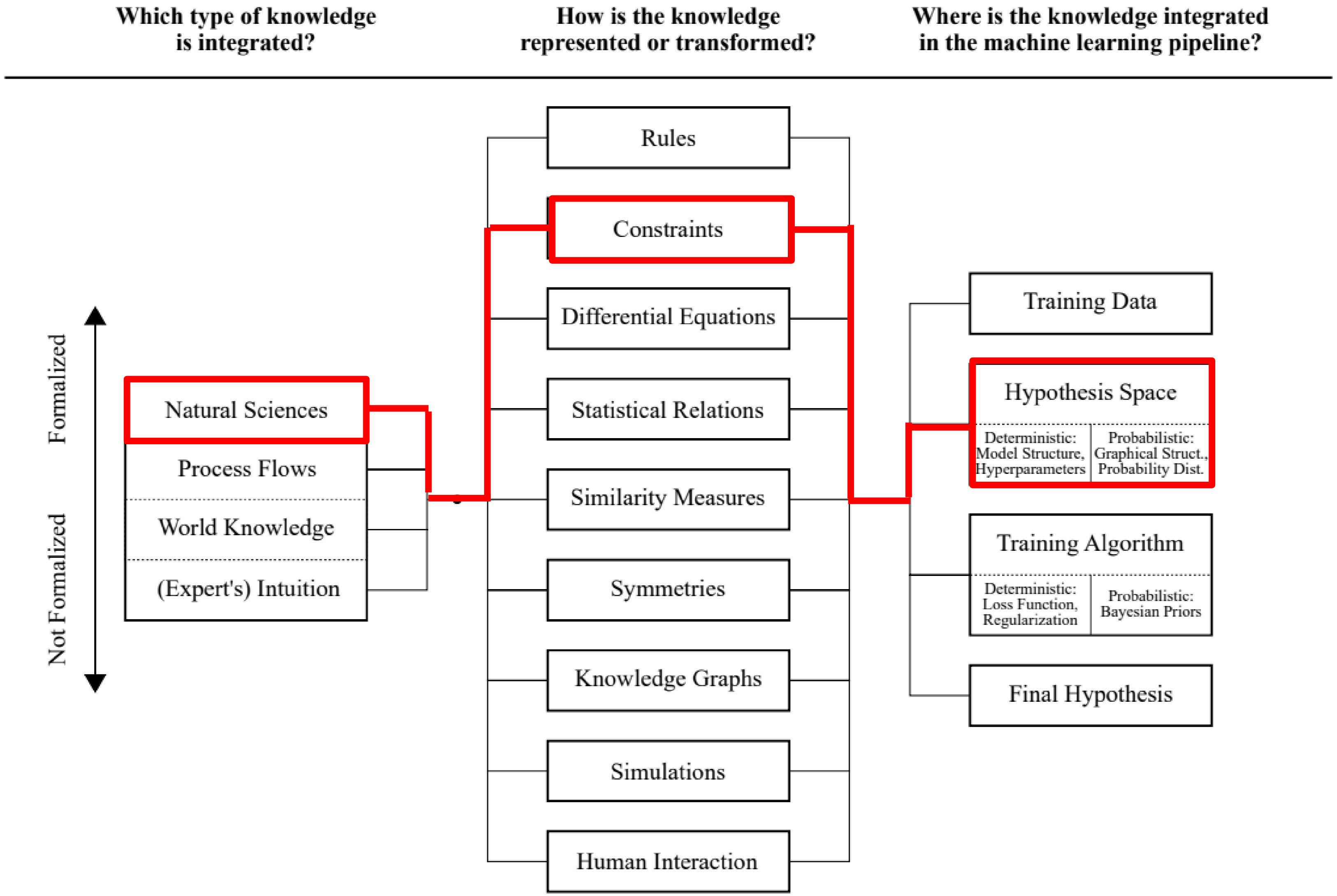




Physics-informed ML

Limiting the model space



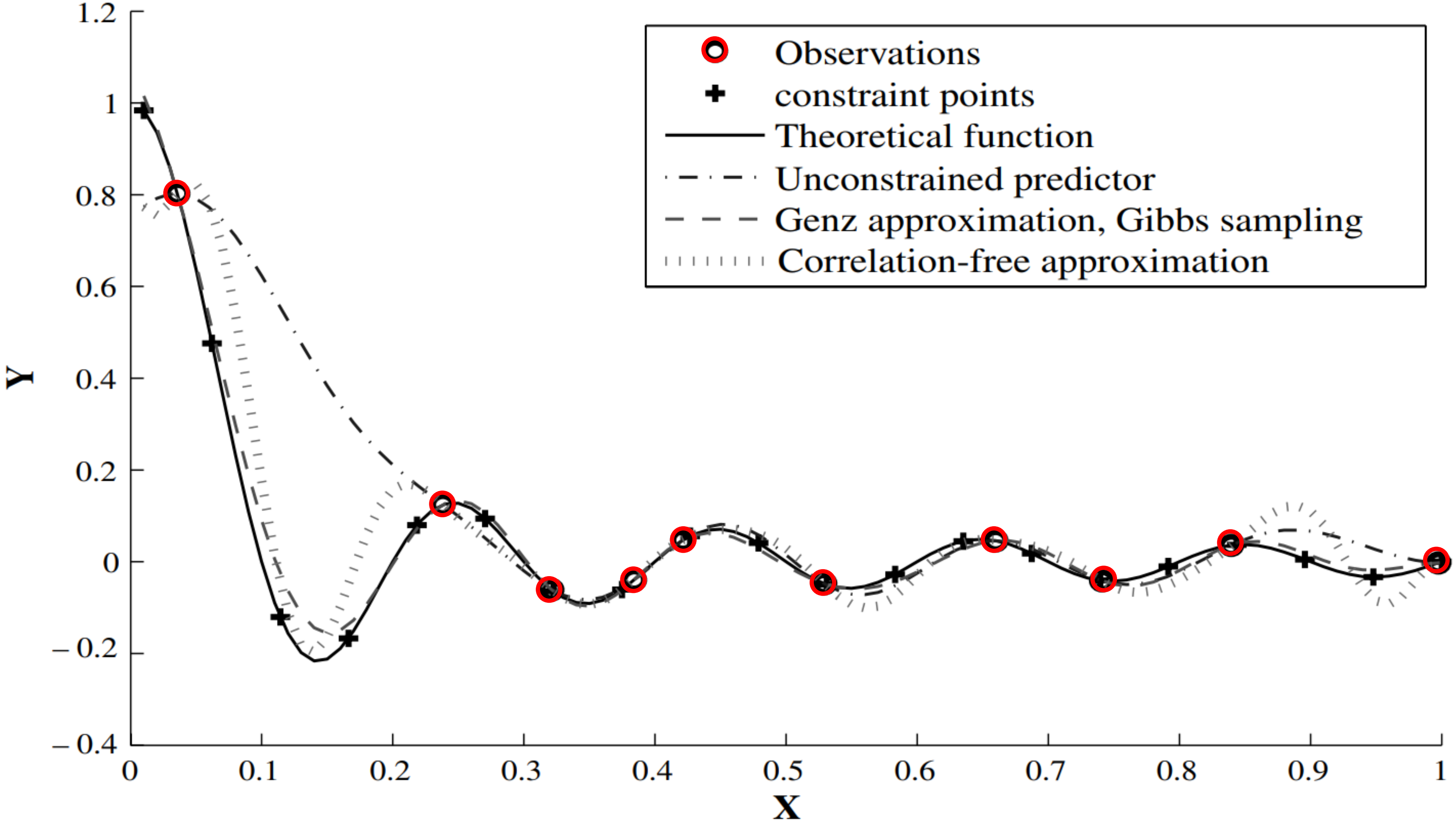
von Rued et al.

Gaussian Process Regression with inequality constraints

- **Physical quantities can show properties know in advance**
  - Bound constraints: density, threshold, etc
  - Derivative constraints: monotonicity

- **Constraints imposed in the mathematical formulation (Da Veiga et al.)**
  - Bounds: $\mathbb{E}(f(x^*)|\forall i = i, \ldots, N;\ a_i \leq f(x_i) \leq b_i)$
  - Derivative: $\mathbb{E}(f(x^*)|\forall i = i, \ldots, N;\ \frac{\partial f}{\partial x_j}(x_i) \geq 0)$
  - Truncated multinormal distribution

Gaussian Process Regression with inequality constraints



Da Veiga et al.

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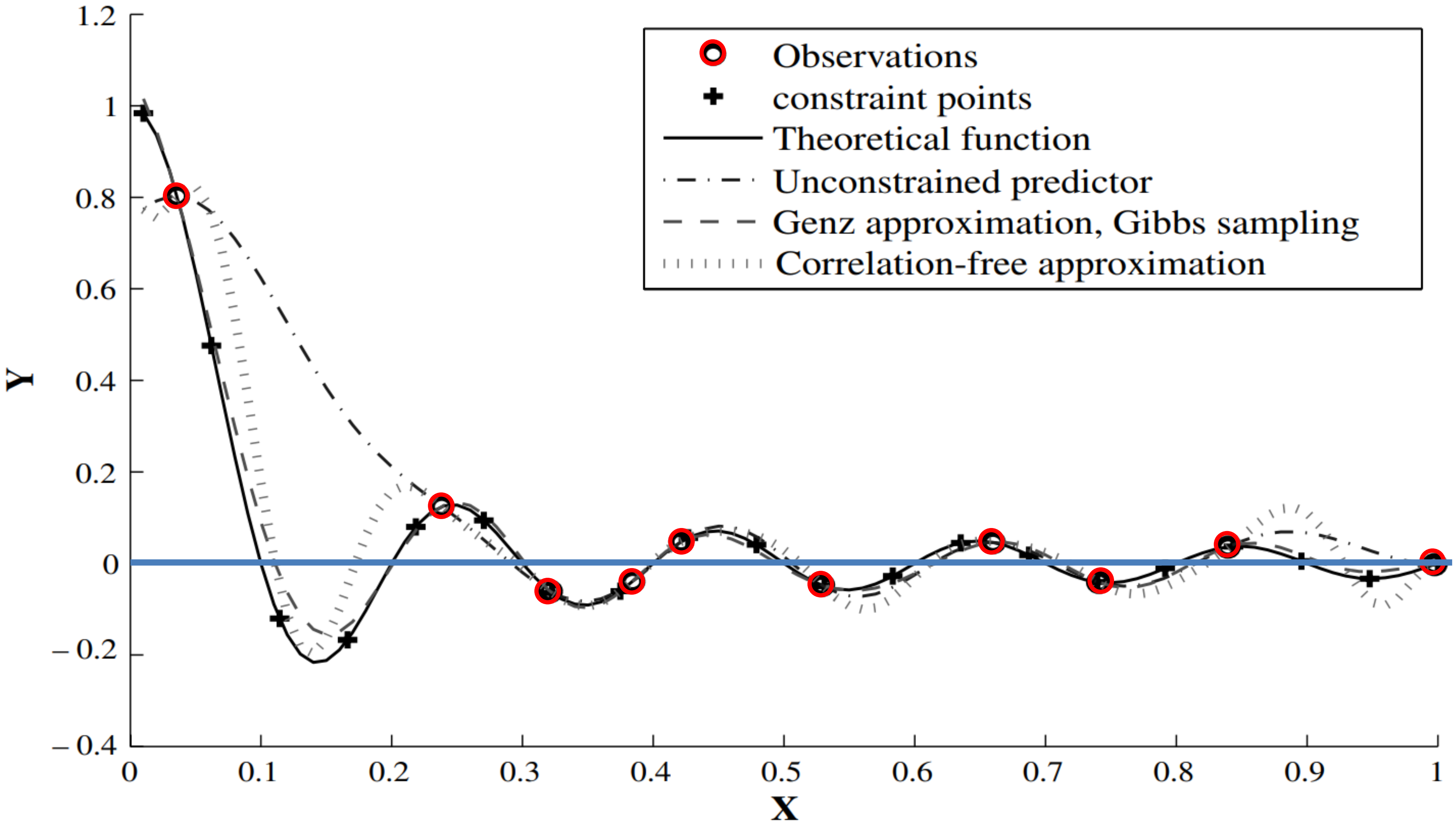
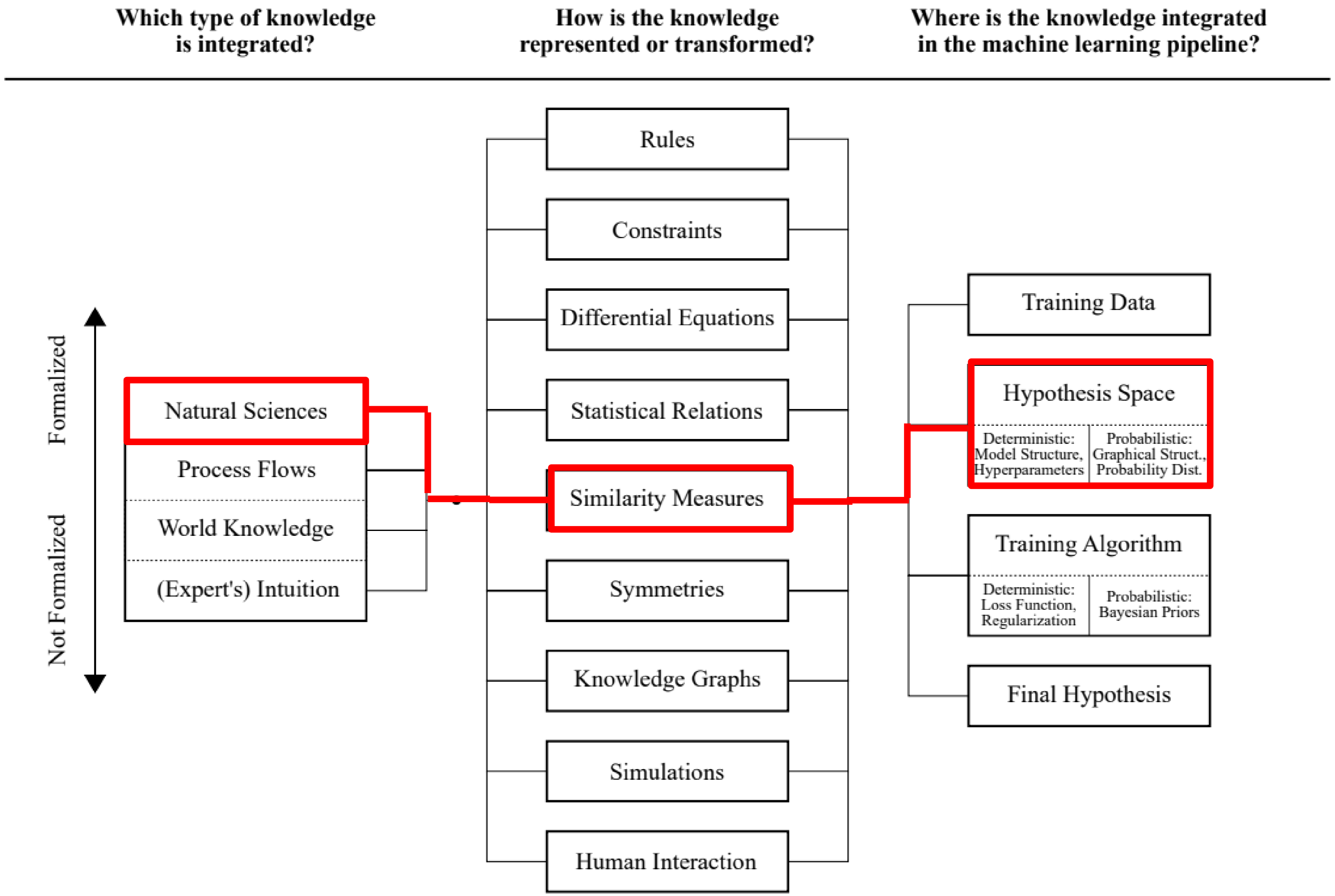


Da Veiga
et al.

Multi fidelity GP regression



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Multi fidelity GP regression

- **Various sources of data can be used**
  - Low fidelity: partially converged simulation, coarser mesh, governing equation of lower fidelity, etc.
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  - Correction can model the differences between cheap and expensive functions
  - Cheap points $\boldsymbol{X_C}, y_c$ and expensive points $\boldsymbol{X_e}, y_e$
  - $Cov\{f_e(\boldsymbol{x^i}), f_c(\boldsymbol{x}) | f_c(\boldsymbol{x^i})\} = 0 \; \forall \boldsymbol{x} \neq \boldsymbol{x^i}$
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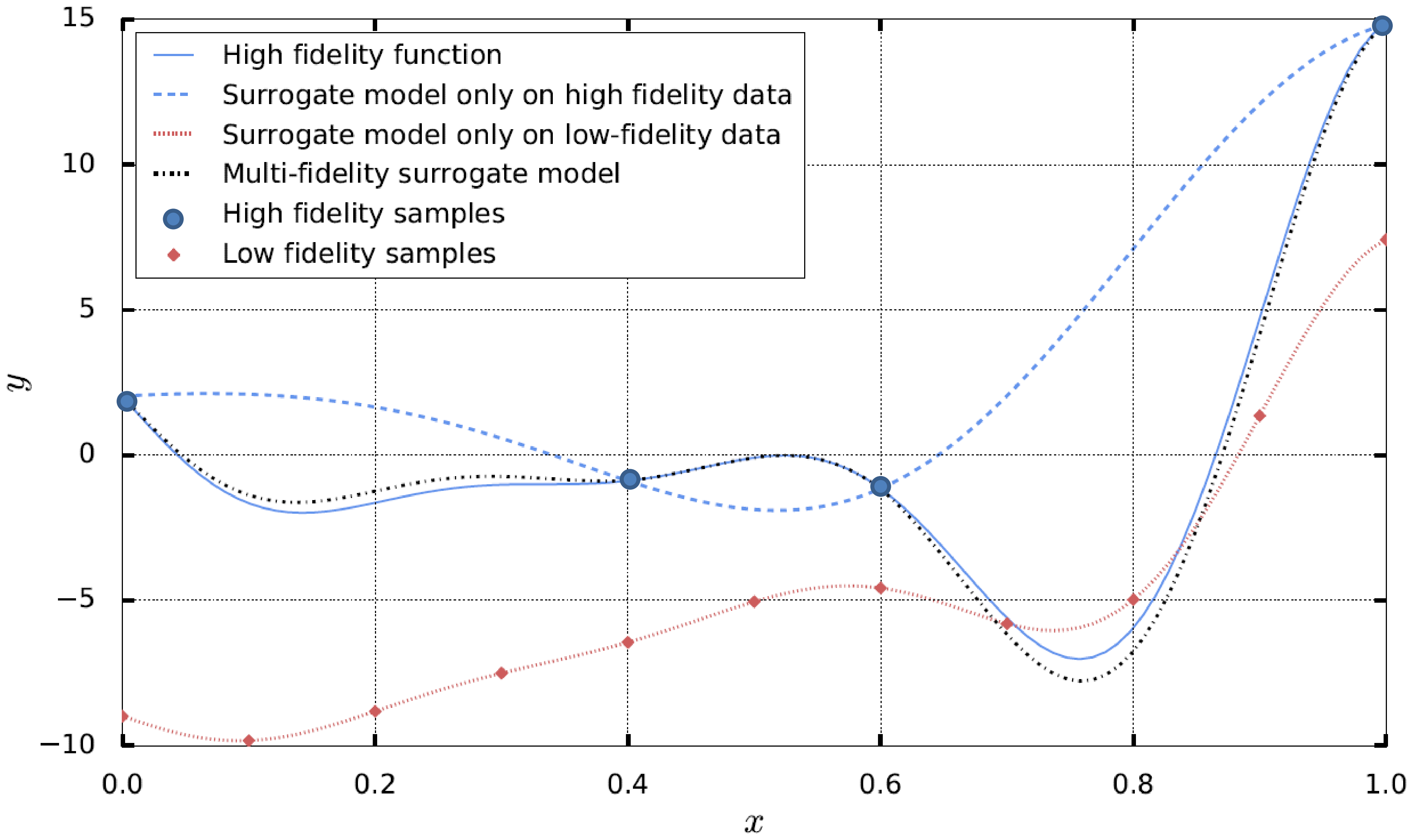
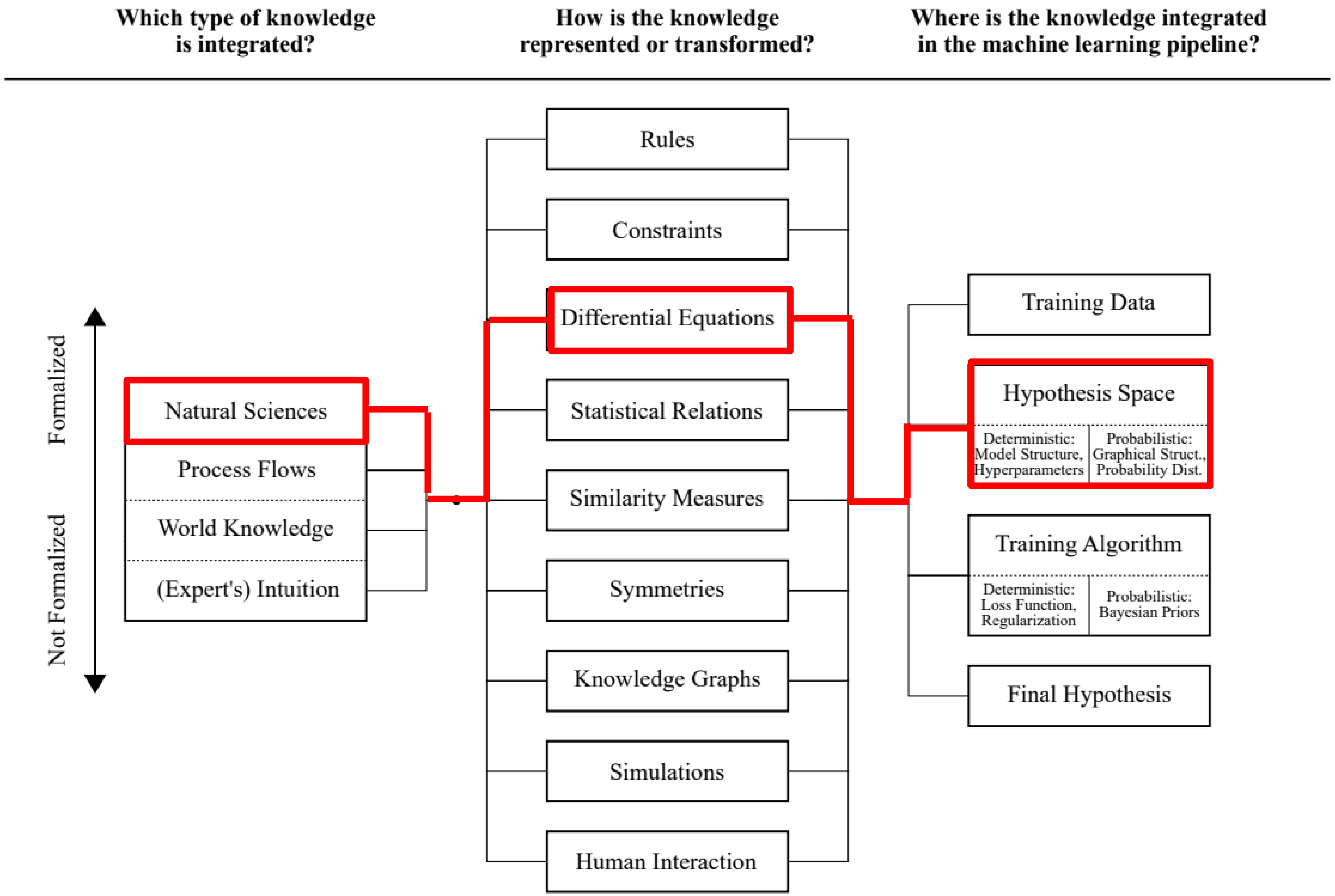
- **Mathematical formula**
  - Correlation: $C = \begin{bmatrix} k_c(\boldsymbol{X_c}, \boldsymbol{X_c}) & \rho k_c(\boldsymbol{X_c}, \boldsymbol{X_e}) \\ \rho k_c(\boldsymbol{X_e}, \boldsymbol{X_c}) & \rho^2 k_c(\boldsymbol{X_e}, \boldsymbol{X_e}) + k_d(\boldsymbol{X_e}, \boldsymbol{X_e}) \end{bmatrix}$

Multi fidelity



Inspired by Forrester et al.

PDE within GPs



von Rued et al.

Incorporating physics within GPs (Raissi et al.)

- **Burgers' equation**
  - $u_t + uu_x - \left(\frac{0.01}{\pi}\right) u_{xx} = 0$
  - Boundary conditions $u(t,-1) = u(t,1) = 0$
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- **Incorporating physics inside GPs**
  - Discretization: $u^n + \Delta\mathrm{t}\left(\mathrm{u}^{\mathrm{n}-1}\mathrm{u}_{\mathrm{x}}^{\mathrm{n}} - \left(\frac{0.01}{\pi}\right)\mathrm{u}_{\mathrm{xx}}^{\mathrm{n}}\right) = \mathrm{u}^{\mathrm{n}-1}$
  - Prior: $u^n \sim GP\big(0, k(x,x')\big)$
  - Kernel $k^{n-1,n} = k^{n,n} + \Delta t\left(u^{n-1}\,k_x - \left(\frac{0.01}{\pi}\right)k_{xx}\right)$

$$\begin{bmatrix} u^n \\ u^{n-1} \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} k^{n,n} & k^{n-1,n} \\ k^{n,n-1} & k^{n-1,n-1} \end{bmatrix}\right)$$

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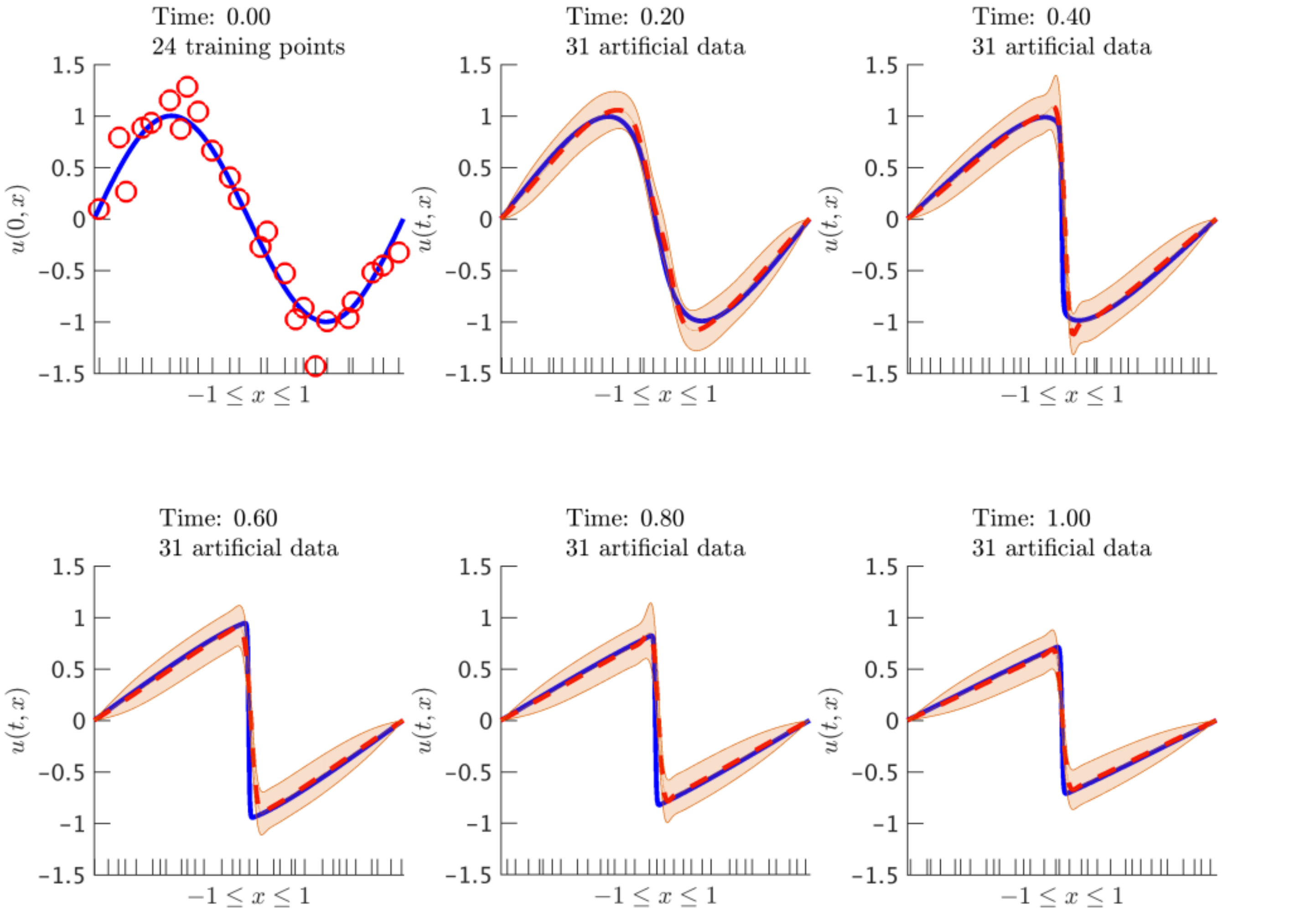

Hidden Physics Models (Raissi et al., 2018b)

- **Linear partial differential equation with unknown parameters $\boldsymbol{\lambda}$**
  - $\mathcal{L}_x^{\lambda} h^n = h^{n-1}$

- **Same process to incorporate physics**
  - $h^n \sim GP\left(0, k(x, x')\right)$
  - $k^{n,n} = k$
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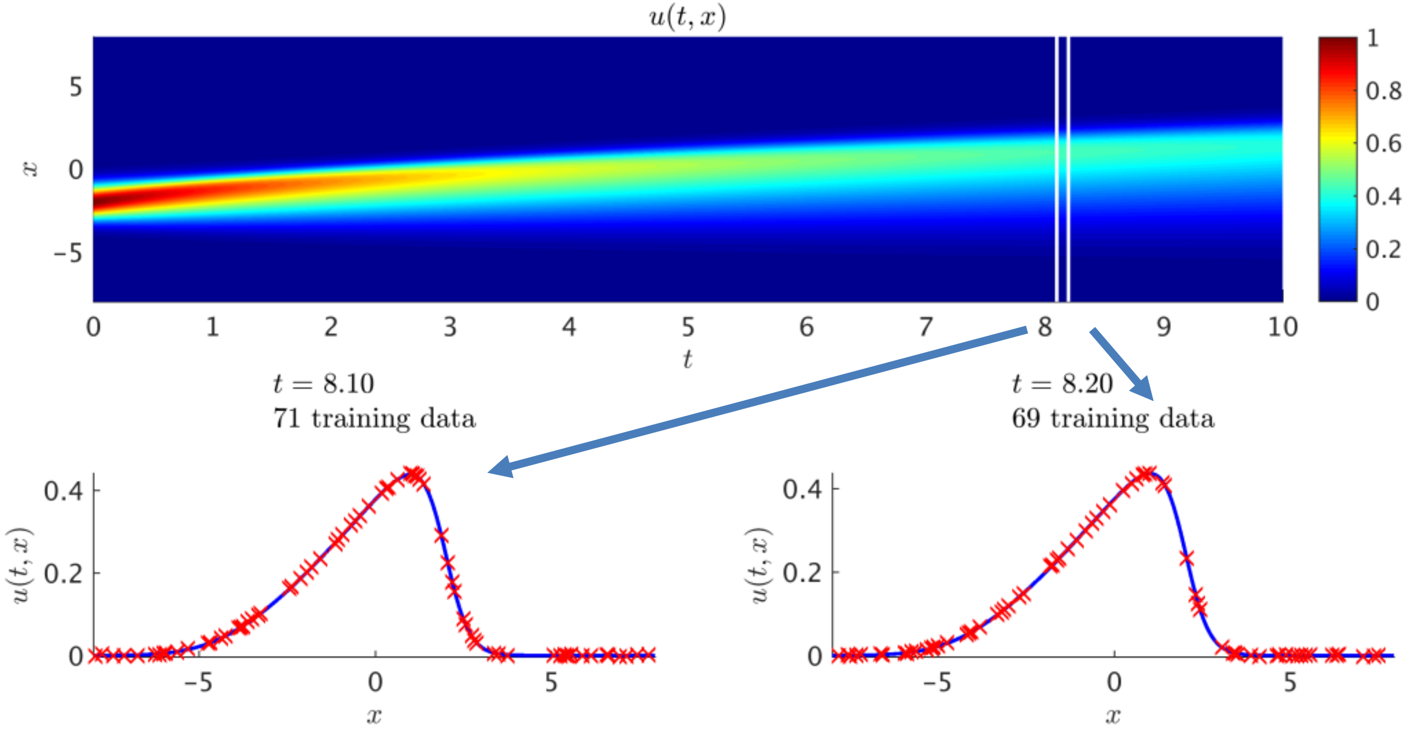

Correct PDE	$u_t + uu_x - 0.1u_{xx} = 0$
Identified PDE (clean data)	$u_t + 1.028uu_x - 0.101u_{xx} = 0$
Identified PDE (1% noise)	$u_t + 1.017uu_x - 0.094u_{xx} = 0$

Physics informed GP and NN

- **Solving PDE, propagating uncertainties, and inverse problem**
  - Based on symbolic differentiation
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$$f := u_t + u u_x - (0.01/\pi) u_{xx}$$

$$MSE = MSE_u + MSE_f$$

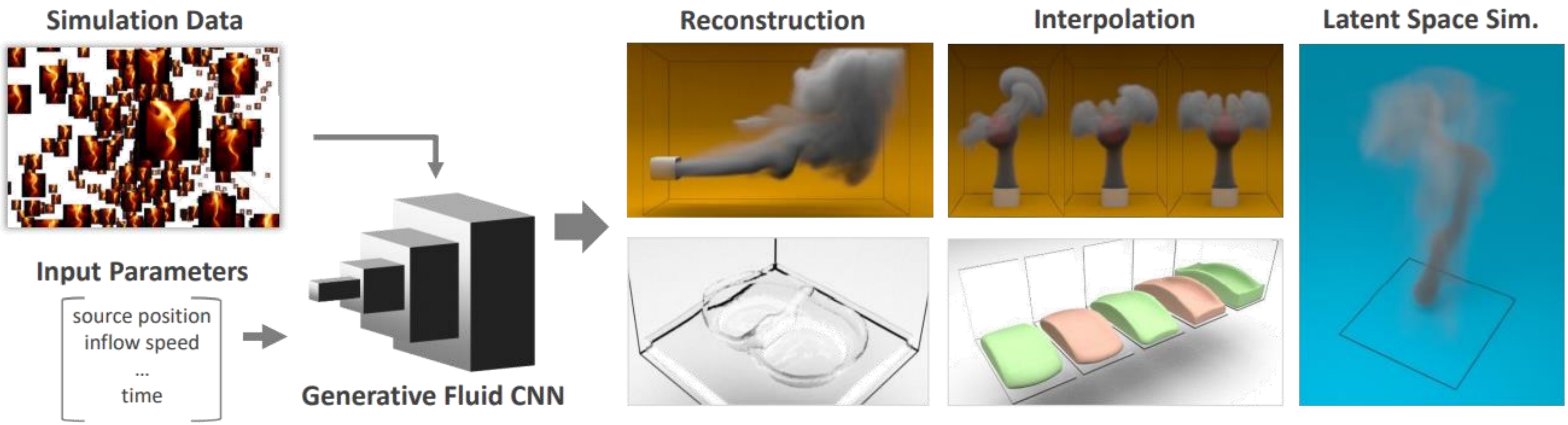
$$MSE_u = \frac{1}{N_u} \sum_{i=1}^{N_u} |u(t_u^i, x_u^i) - u^i|^2,$$

Raissi et al. provide github with Tensorflow code

$$MSE_f = \frac{1}{N_f} \sum_{i=1}^{N_f} |f(t_f^i, x_f^i)|^2.$$

And more!

- **DeepFluid: Generative Network for Fluid Simulation (Kim et al., 2019)**



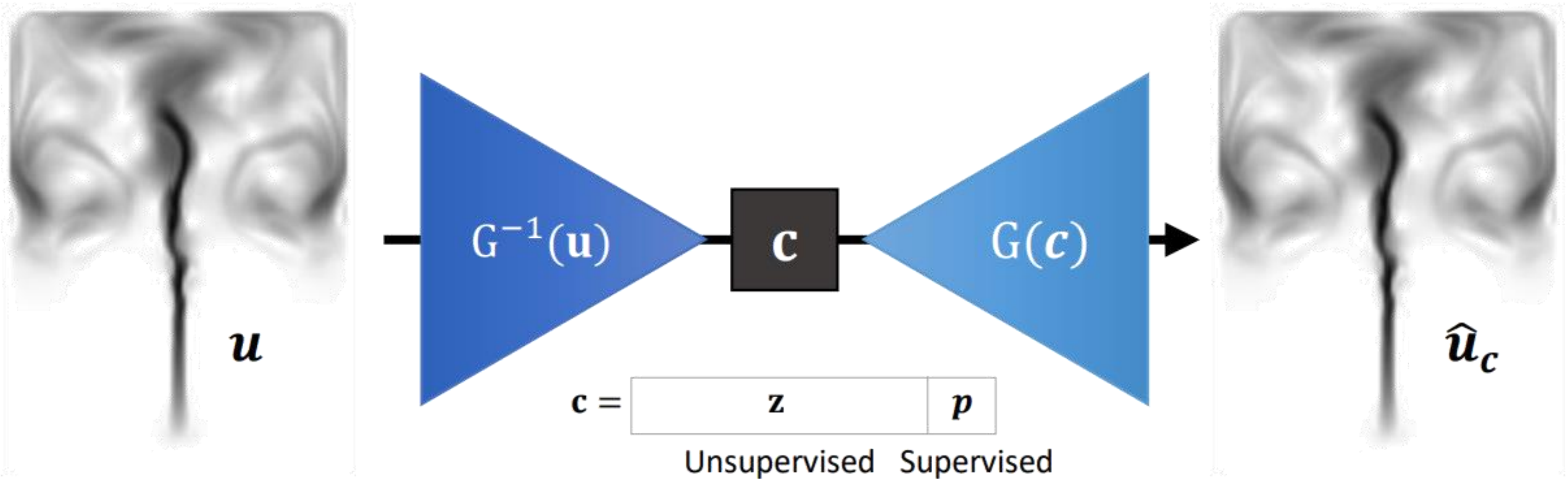
And more!

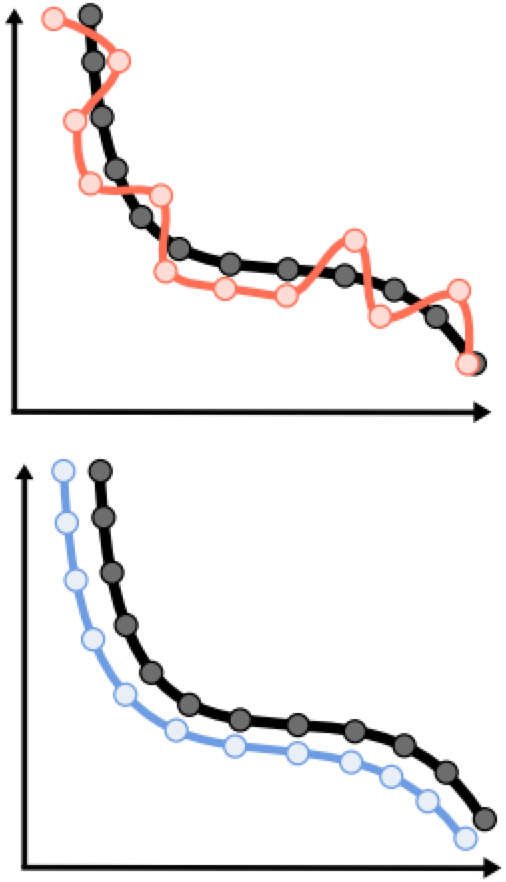
- **DeepFluid: Generative Network for Fluid Simulation (Kim et al., 2019)**
  - Stream loss function for incompressible fluid

$$L_G(\mathbf{c}) = ||\mathbf{u_c} - \nabla \times G(\mathbf{c})||_1$$

  - Learning also the gradient:

$$L_G(\mathbf{c}) = \lambda_{\mathbf{u}}||\mathbf{u_c} - \hat{\mathbf{u}}_\mathbf{c}||_1 + \lambda_{\nabla\mathbf{u}}||\nabla\mathbf{u_c} - \nabla\hat{\mathbf{u}}_\mathbf{c}||_1$$





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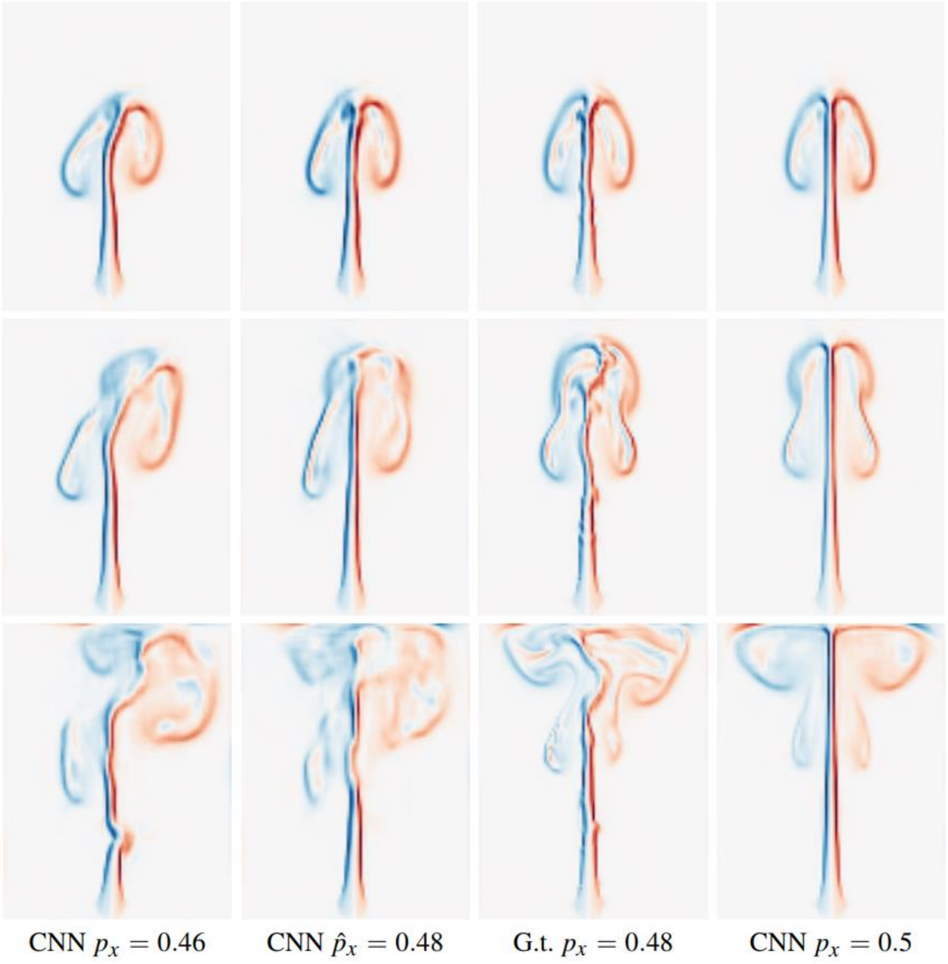

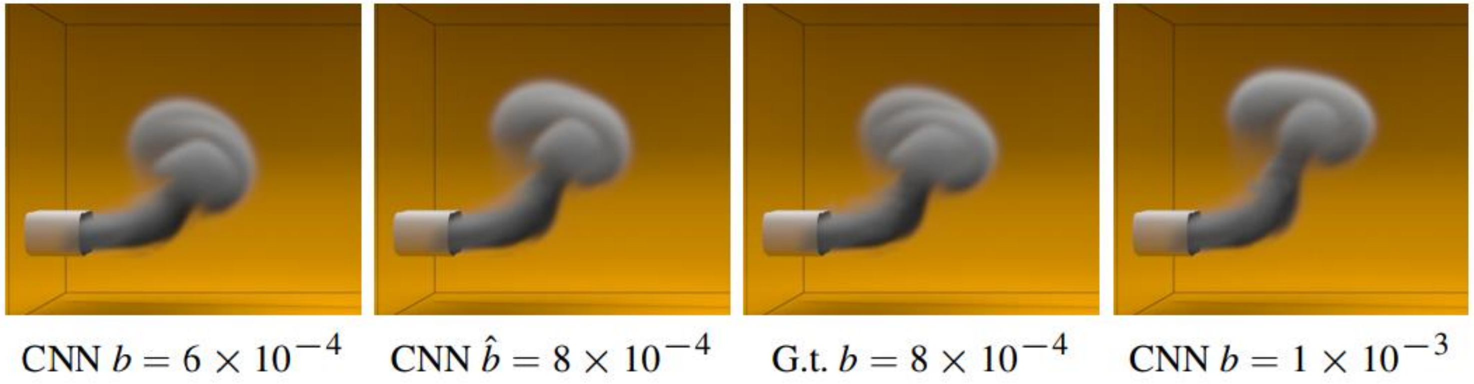

Conclusion

- **Coupling physics and data**
  - Gain explainabilitiy
  - Physical consistency

- **Need of closer collaboration with domain experts, data scientists, and computer scientists**
  - Extracting knowledge, insights and discovery from data
  - Support of simulations and experiments
  - One of the AIDA's aims

- **Now physics is injected into Machine Learning, we can explain models from AI**
  - Next talk from Jorge about explainable AI

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