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Deep Learning for Science and Engineering Teaching Kit

Deep Learning for Scientists and Engineers

Lecture 7: Machine Learning using Multi-Fidelity Data

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Course Roadmap

Module-1 (Basics)

- Lecture 1: Introduction
- Lecture 2: A primer on Python, NumPy, SciPy and *jupyter* notebooks
- Lecture 3: Deep Learning Networks
- Lecture 4: A primer on TensorFlow and PyTorch
- Lecture 5: Training and Optimization
- Lecture 6: Neural Network Architectures

Module-2 (PDEs and Operators)

- Lecture 7: Machine Learning using Multi-Fidelity Data
- Lecture 8: Physics-Informed Neural Networks (PINNs)
- Lecture 9: PINN Extensions
- Lecture 10: Neural Operators

Module-3 (Codes & Scalability)

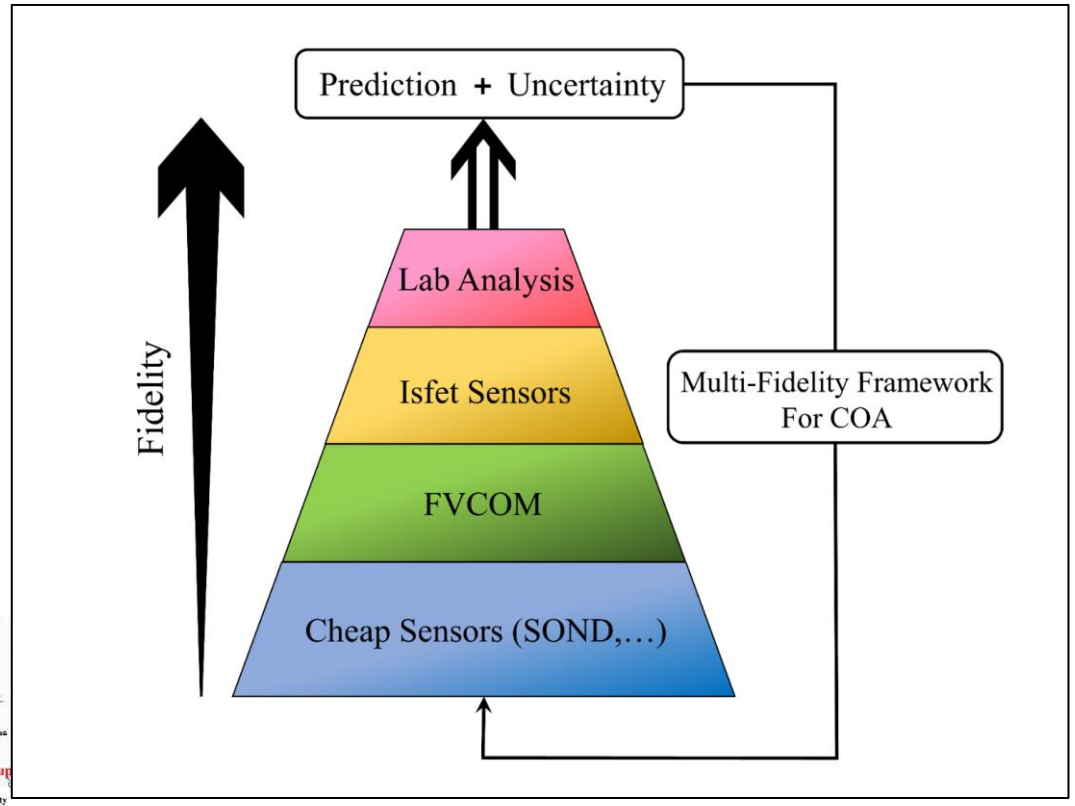
- Lecture 11: Multi-GPU Scientific Machine Learning

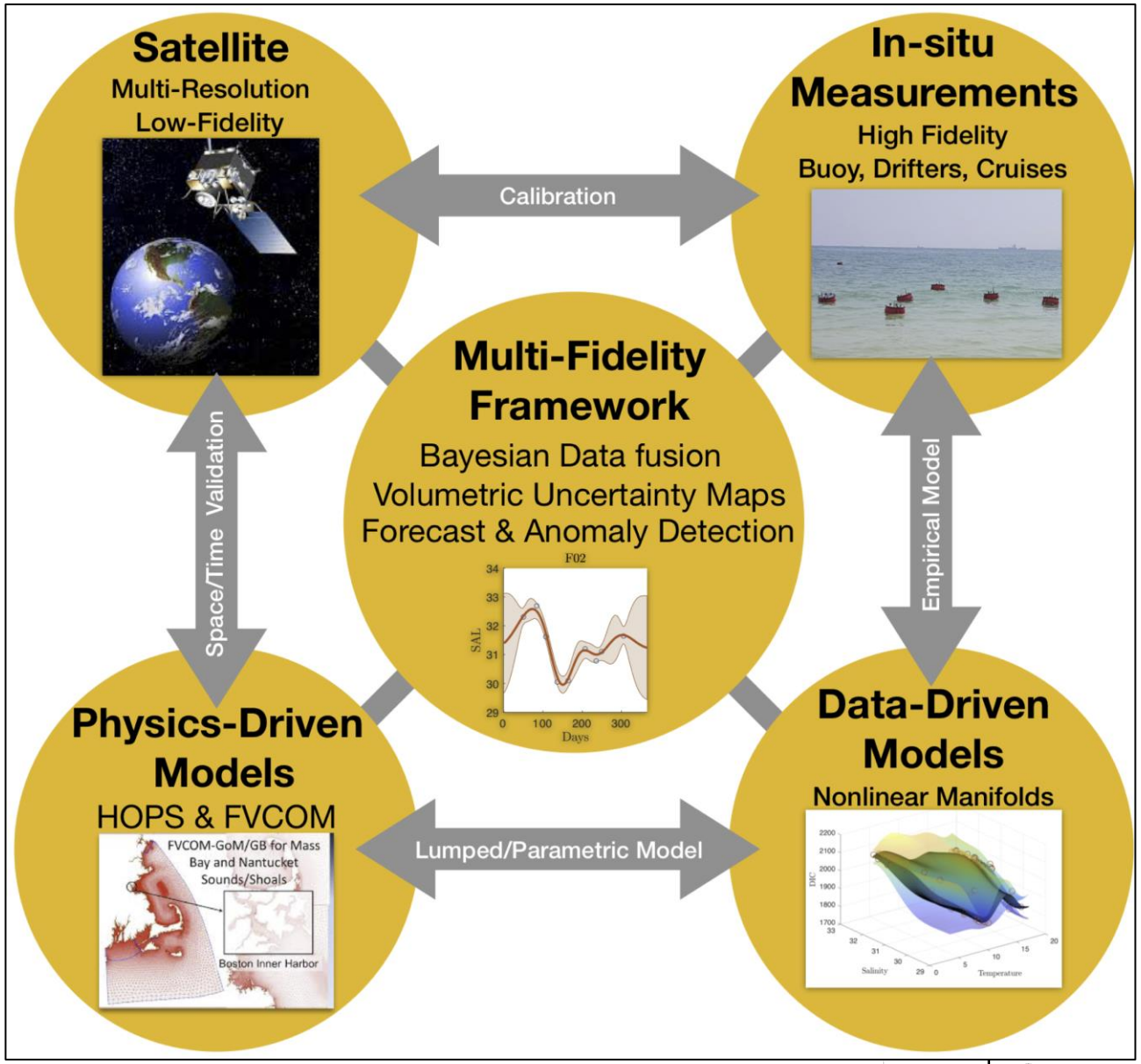
Contents

- ❑ What is multi-fidelity data: Ocean acidification example
- ❑ Gaussian process (GP) regression
- ❑ Data assimilation from noisy measurements: bathymetry and eel grass modeling
- ❑ Physics-informed kernels for GP
- ❑ Multi-fidelity GP/co-Kriging modeling
- ❑ Example: Sea Surface Temperature in Massachusetts Bay
- ❑ Nonlinear multi-fidelity GP and examples
- ❑ Acquisition functions – active learning
- ❑ NN-induced GP kernels
- ❑ Deep multi-fidelity GP
- ❑ Diffusion-manifold driven GP
- ❑ Composite multi-fidelity neural networks
- ❑ Example: Nano-indentation of 3D printed materials
- ❑ Multi-fidelity in modal space
- ❑ Example: vortex-induced vibrations of marine risers

A Motivating Example: Ocean Acidification Monitoring

- ❑ Cost-effective monitoring of OA QoIs.
- ❑ Heterogeneous measurements.
- ❑ Lack of direct measurements of QoIs.
- ❑ Reliance of physics-based models on data due to physics deficiency.





CRUNCH Group
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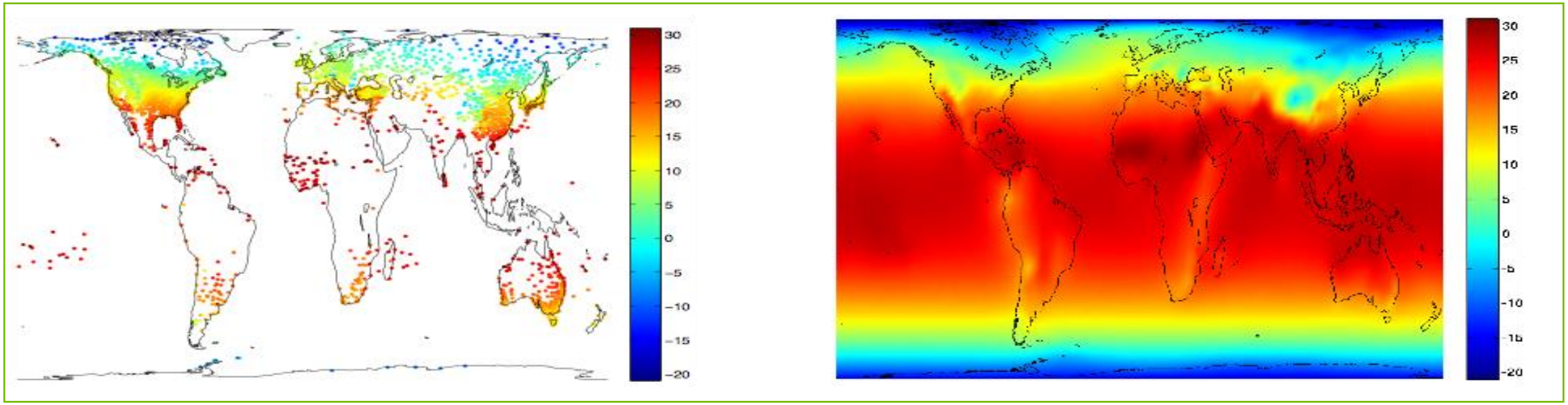
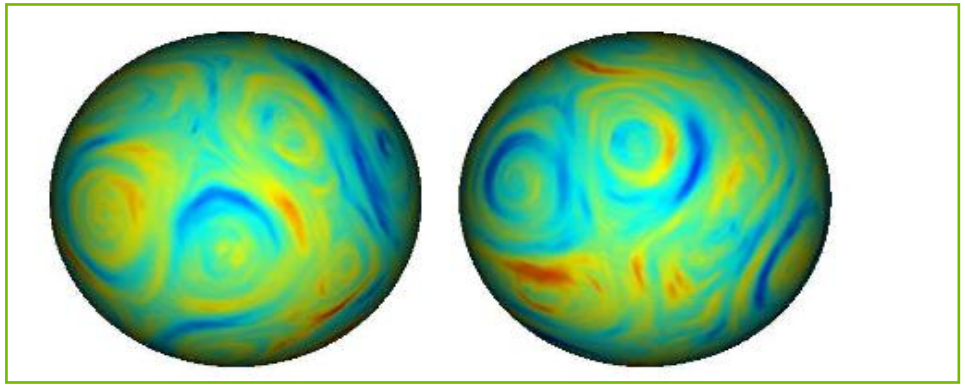
Gaussian-Markov Random Fields: A Stochastic PDE Approach

Example: Reconstruction of global temperature field from data



- GMRF representations of SPDEs can be constructed for oscillating, anisotropic, non-stationary, non-separable, spatio-temporal, and multivariate fields on manifolds.
- Also, the SPDEs can accommodate a wide variety of constraints (e.g., incompressibility, boundary conditions, etc)

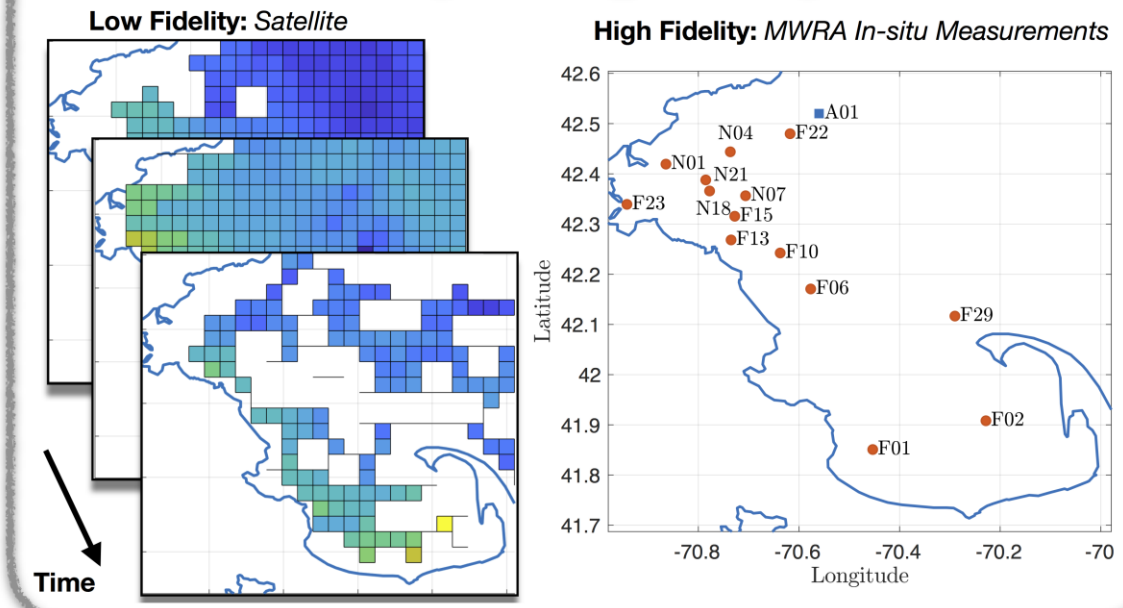
$$\left(\frac{\partial}{\partial t} + \chi_{s,t}^2 + \nabla \cdot m_{s,t} - \nabla \cdot \boldsymbol{M}_{s,t} \nabla\right)(\tau_{s,t}\chi(s,t)) = \epsilon(\boldsymbol{s},t), \qquad (\boldsymbol{s},t) \in \Omega \times \mathbb{R}$$



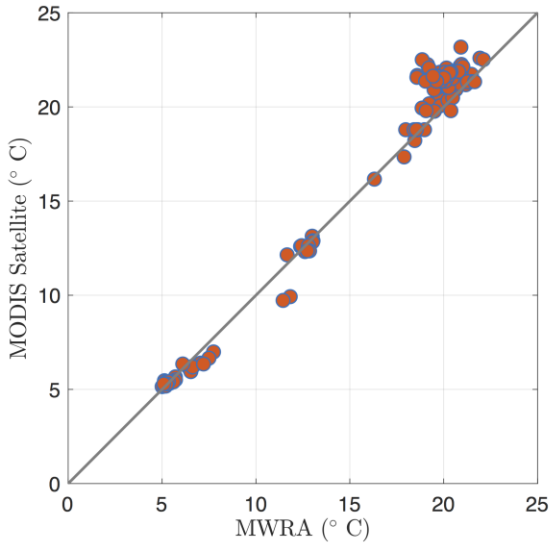
Lindgren F, Rue H, Lindström J. An explicit link between Gaussian fields and Gaussian Markov random fields: the stochastic partial differential equation approach. Journal of the Royal Statistical Society: Series B (Statistical Methodology). 2011 Sep;73(4):423-98.

Example: Monitoring Sea Surface Temperature (SST) in Massachusetts Bay

Low-fidelity and High-fidelity Data



Correlation
Low-Fidelity vs. High-Fidelity



Auto-regressive Gaussian Processes

$$y_L(x) = u_L(x) + \epsilon_L \quad \text{and} \quad y_H(x) = \rho u_L(x) + \delta(x) + \epsilon_H$$

$$u_L(x) \sim \mathcal{GP}(0, k(x, x'; \theta_L)) \quad \text{and} \quad \delta(x) \sim \mathcal{GP}(0, k(x, x'; \theta_\delta))$$

$$k(x, x') = \sigma^2 \exp\left(-\sum_{i=1}^{D} (x_i - x_i')^2 / \theta_i^2 \right)$$

Gaussian Processes

Starting point: The multivariate Gaussian Distribution

$$p(\underbrace{f_1, f_2, ..., f_s}_{f_A}, \underbrace{f_{s+1}, ..., f_N}_{f_b}) \sim \mathcal{N}(\mu, K) \qquad \mu = \begin{bmatrix} \mu_A \\ \mu_B \end{bmatrix} \text{ and } K = \begin{bmatrix} K_{AA} & K_{AB} \\ K_{BA} & K_{BB} \end{bmatrix}$$

Generalization: The Gaussian process

$$\mu_\infty = \underbrace{\begin{bmatrix} \mu_f \\ ... \\ ... \end{bmatrix}}_{\text{mean function}} \text{ and } K_\infty = \underbrace{\begin{bmatrix} K_{ff} & ... \\ ... & ... \end{bmatrix}}_{\text{covariance function}} \qquad K_{i,j} = k(x_i, x_j)$$

Priors over functions:

$$f \sim \mathcal{GP}(\mu(x), K(x, x'; \theta))$$

Infinite dimensional model, but finitely many observations: The marginalization property

$$p(f_A, f_B) \sim \mathcal{N}(\mu, K) \text{ Then:}$$

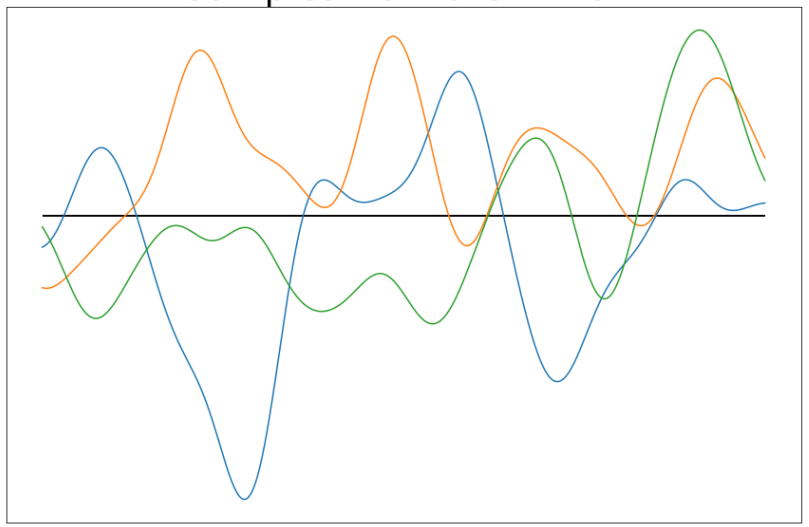
$$p(f_A) = \int_{f_B} p(f_A, f_B) df_B = \mathcal{N}(\mu_A, K_{AA})$$

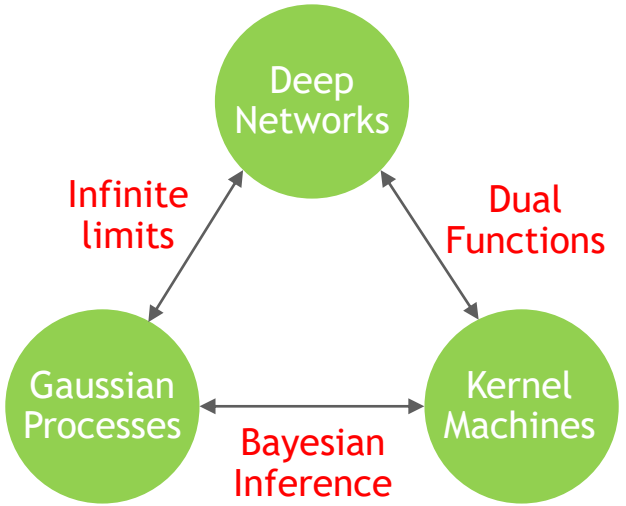
Posterior is also Gaussian:

$$p(f_A, f_B) \sim \mathcal{N}(\mu, K) \text{ Then:}$$

$$p(f_A | f_B) = \mathcal{N}(\mu_A + K_{AB} K_{BB}^{-1}(f_B - \mu_B), K_{AA} - K_{AB} K_{BB}^{-1} K_{BA})$$

Samples from a GP Prior





Kriging/Gaussian Process Regression/BLUP

- We model scattered observations y as a realization of a Gaussian process $Z(\boldsymbol{x})$ (up to zero-mean Gaussian measurement error $\epsilon(\boldsymbol{x})$), according to an observation model

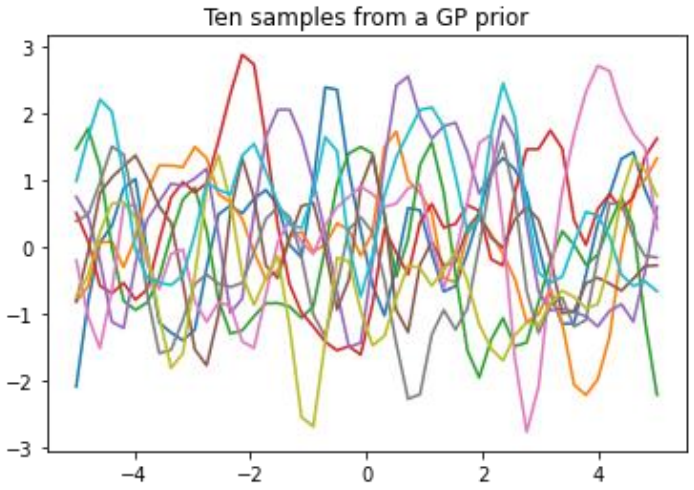
$$Y(\boldsymbol{x}) = Z(\boldsymbol{x}) + \epsilon(\boldsymbol{x})$$

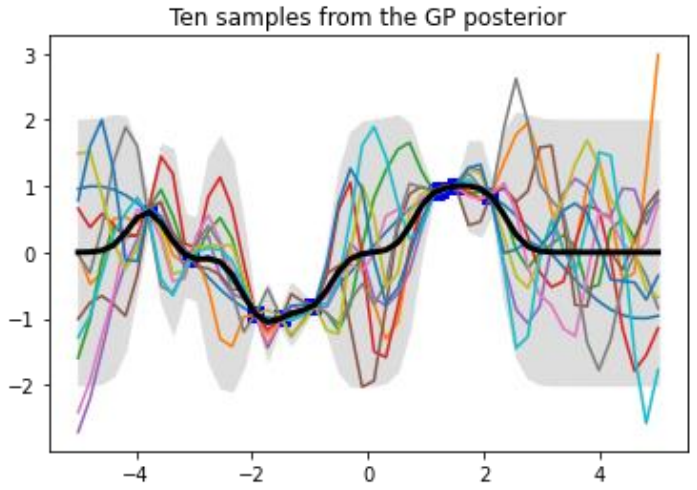
- $[Z(\boldsymbol{x}), Y(\boldsymbol{x})]^\top$ has a multivariate normal distribution,

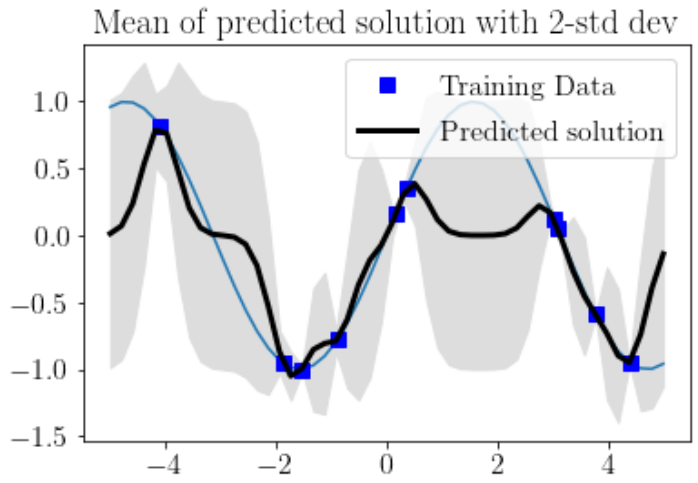
$$\begin{bmatrix} Z(\boldsymbol{x}) \\ Y(\boldsymbol{x}) \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu \\ A\mu \end{bmatrix}, \begin{bmatrix} \Sigma & \Sigma A^\top \\ A^\top \Sigma & A\Sigma A^\top + \Sigma_\epsilon \end{bmatrix} \right),$$

  where Σ and Σ_ϵ are parametrized by $\{\theta, \theta_\epsilon\}$, that can be learned from the data y by maximizing the posterior $\pi(\hat{y}|y, \theta, \theta_\epsilon)$.

- Assign a Gaussian prior over functions and caliberate it in view of the data.







C.E. Rasmussen and C.K.L. Williams. Gaussian Process for Machine Learning, 2006

Kriging/Gaussian Process Regression/BLUP

- Once $Z(x)$ has been trained on N observations, we can perform predictions at new points x^* and quantify the variance as

$$\widehat{y}(\boldsymbol{x}^*) = \widehat{\mu} + r^\top (R + \widehat{\sigma}_\epsilon^2 I)^{-1}(y - \mathbf{1}\widehat{\mu})$$

$$s^2(\boldsymbol{x}^*) = \widehat{\sigma}^2 \left[1 - r^\top (R + \widehat{\sigma}_\epsilon^2 \boldsymbol{I})^{-1} r + \frac{[1 - r^\top (R + \widehat{\sigma}_\epsilon^2 \boldsymbol{I})^{-1} r]^2}{\mathbf{1}^\top (R + \widehat{\sigma}_\epsilon^2 \boldsymbol{I})^{-1} \mathbf{1}}\right],$$

  where $R = \kappa(\boldsymbol{x}, \boldsymbol{x}', \widehat{\theta})$ is the $N \times N$ correlation matrix of $Z(x)$, $r = \kappa(\boldsymbol{x}, \boldsymbol{x}^*, \widehat{\theta})$ is a $1 \times N$ correlation vector between the prediction and N training points, and $\mathbf{1}$ is a $1 \times N$ vector of ones. For $\sigma_\epsilon^2 = 0$ the predictor exactly interpolate the training data y, returning zero variance at these locations.

- **Learning**: Given y find the optimal $\{\widehat{\mu}, \widehat{\sigma}^2, \widehat{\sigma}_\epsilon^2, \widehat{\theta}\}$

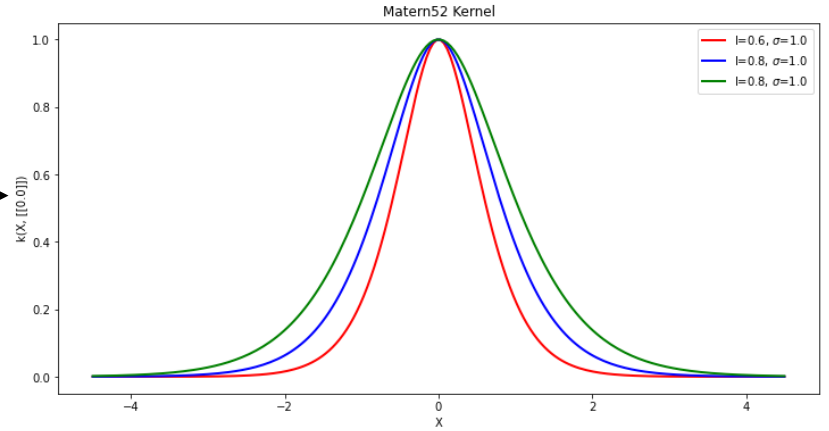
Covariance function	Expression
constant	σ_0^2
linear	$\sum_{d=1}^{D} \sigma_d^2 x_d x'_d$
polynomial	$(\boldsymbol{x} \cdot \boldsymbol{x}' + \sigma_0^2)^p$
squared exponential	$\exp(-\frac{r^2}{2l^2})$
Matérn	$\frac{1}{2^{\nu-1}\Gamma(\nu)} \left(\frac{\sqrt{2\nu}}{l} r\right)^\nu K_\nu \frac{1}{2^{\nu-1}\Gamma(\nu)} \left(\frac{\sqrt{2\nu}}{l} r\right)$
exponential	$\exp(-(\frac{r}{l}))$
$\gamma-$exponential	$\exp(-(\frac{r}{l})^\gamma)$
rational quadratic	$(1 + \frac{r^2}{2\alpha l^2})^{-\alpha}$
neural network	$\sin^{-1}\left(\frac{2\widehat{\boldsymbol{x}}^\top \Sigma \widehat{\boldsymbol{x}'}}{\sqrt{(1+2\widehat{\boldsymbol{x}}^\top \Sigma \widehat{\boldsymbol{x}})(1+2\widehat{\boldsymbol{x}'}^\top \Sigma \widehat{\boldsymbol{x}'})}}\right)$

Kernel and Kernel Parameters

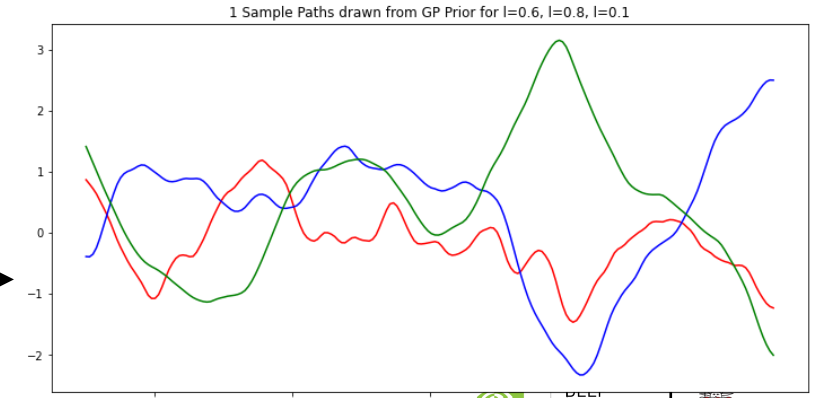
Covariance function	Expression
Matérn	$\frac{1}{2^{\nu-1}\Gamma(\nu)}\left(\frac{\sqrt{2\nu}}{l}r\right)^{\nu} K_{\nu}\frac{1}{2^{\nu-1}\Gamma(\nu)}\left(\frac{\sqrt{2\nu}}{l}r\right)$

```
import GPy
import numpy as np
import matplotlib.pyplot as plt
plt.rcParams["figure.figsize"] = (12, 6)
```

```
# Define Kernel Using GPy
ker1 = GPy.kern.Matern52(input_dim=1, variance = 1.0, lengthscale=0.6)
ker2 = GPy.kern.Matern52(input_dim=1, variance = 1.0, lengthscale=0.8)
ker3 = GPy.kern.Matern52(input_dim=1, variance = 1.0, lengthscale=1.0)

xmin=-5
xmax=5
N=200
X = np.linspace(xmin, xmax, N)[:, None]
mu = np.zeros((N))
C1 = ker1.K(X,X)
C2 = ker2.K(X,X)
C3 = ker3.K(X,X)
fig, ax = plt.subplots()
ker1.plot(ax=ax, linewidth=2, color="r", label="l=0.6, $\sigma$=1.0")
ker2.plot(ax=ax, linewidth=2, color="b", label="l=0.8, $\sigma$=1.0")
ker3.plot(ax=ax, linewidth=2, color="g", label="l=0.8, $\sigma$=1.0")
ax.legend()
ax.set_title("Matern52 Kernel")
```

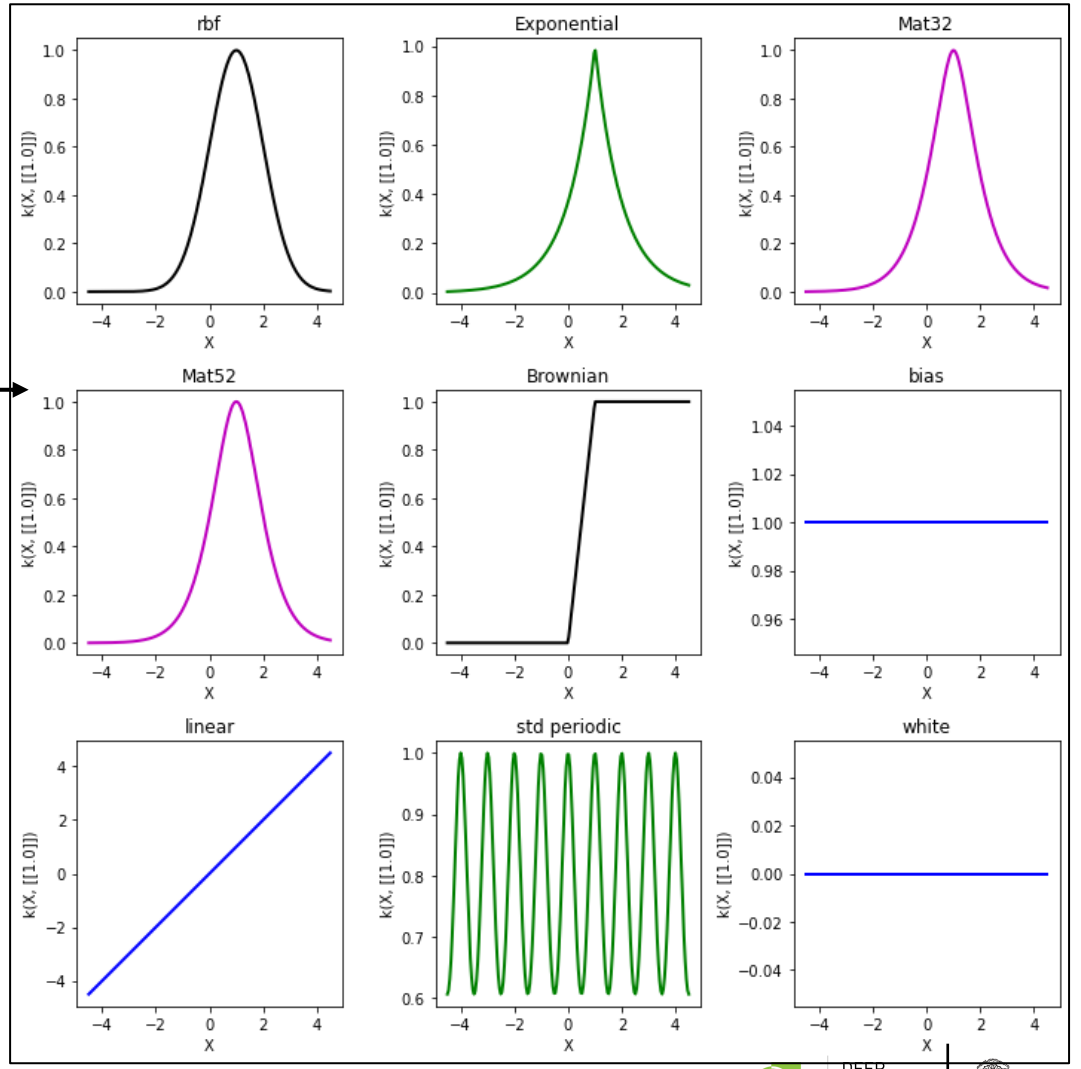



```
Z1 = np.random.multivariate_normal(mu,C1,1)
Z2 = np.random.multivariate_normal(mu,C2,1)
Z3 = np.random.multivariate_normal(mu,C3,1)
fig, ax = plt.subplots()
plt.plot(X[:],Z1[0,:], "-r")
plt.plot(X[:],Z2[0,:], "-b")
plt.plot(X[:],Z3[0,:], "-g")

ax.set_title("1 Sample Paths drawn from GP Prior for l=0.6, l=0.8, l=0.1")
plt.show()
```



Kernels for Gaussian Process

```
from random import randrange
import GPy
import matplotlib.pyplot as plt
import numpy as np

figure, axes = plt.subplots(3,3, figsize=(10,10), tight_layout=True)
kerns = [GPy.kern.RBF(1), GPy.kern.Exponential(1), GPy.kern.Matern32(1), \
         GPy.kern.Matern52(1), GPy.kern.Brownian(1), GPy.kern.Bias(1), \
         GPy.kern.Linear(1), GPy.kern.StdPeriodic(1), GPy.kern.White(1)]

col = ['r', 'b', 'g', 'b', 'm', 'k']

for k,a in zip(kerns, axes.flatten()):
    j = np.random.randint(0, high=6, size=1, dtype=int)
    k.plot(ax=a, x=1, color=col[j[0]])
    a.set_title(k.name.replace('_', ' '))
```



Gaussian Process Regression: Implementation

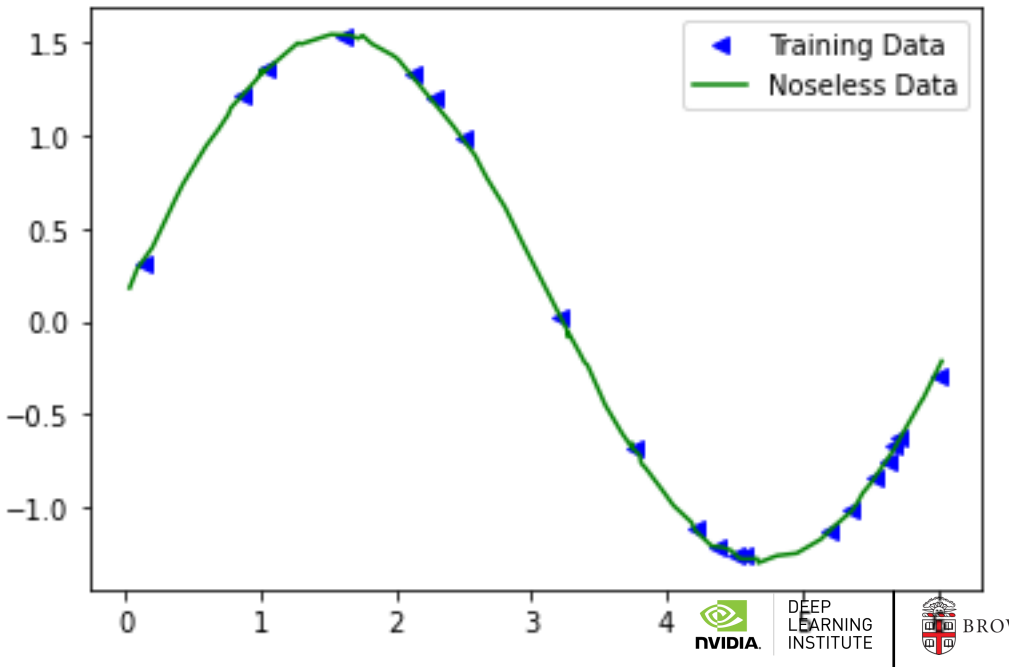
1. Import modules and Helper Routine for Plot

```
import GPy
import numpy as np
import matplotlib.pyplot as plt
```

2. Generate and Normalize Training and Testing Data

```
N=20 # Number of training points
Nstar = 70 # number of test points

X = np.sort(np.random.rand(N+Nstar, 1)*6.14, axis=0)
Y = np.sin(X) + np.random.randn(*X.shape) * 0.008

perm = np.random.permutation(X.shape[0])
x_tr = X[np.sort(perm[0:N],axis=0),:]
Y_tr = Y[np.sort(perm[0:N],axis=0),]
x_star = X[np.sort(perm[N:N+Nstar],axis=0),:]
Y_star = Y[np.sort(perm[N:N+Nstar],axis=0),:]



### Normalize Data
Ymean = Y.mean()
Ystd = Y.std()
Y_tr-=Ymean
Y_tr/=Ystd


Y_star -= Ymean
Y_star /= Ystd

# plot data
plt.plot(x_tr,Y_tr, 'b<',label='Training Data')
plt.plot(x_star,Y_star, '-g',label='Noseless Data')
plt.legend()
plt.show()
```

Training data



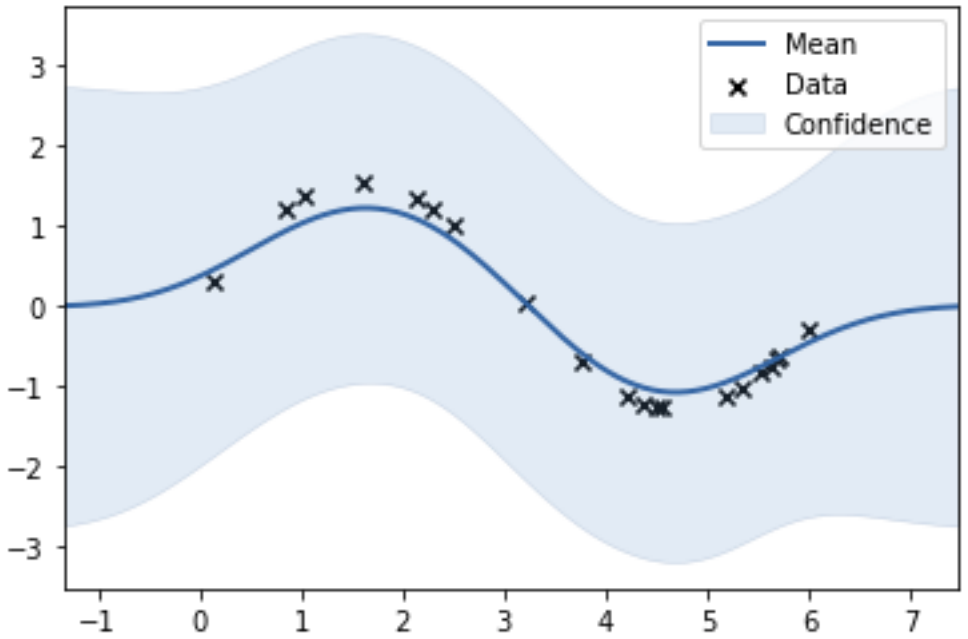
Gaussian Process Regression: Implementation

3. Define Kernel and optimize GP model for model parameters

```
dim_1 = x_tr.shape[1]
# Define RBF Kernel also known as Squared Exponential kernel
k = GPy.kern.RBF(dim_1)

#Define Gaussian Process Regression Model
m = GPy.models.GPRegression(X=x_tr, Y=Y_tr, kernel=k)
print(m)
```

```
Name : GP regression
Objective : 23.812870975912027
Number of Parameters : 3
Number of Optimization Parameters : 3
Updates : True
Parameters:
  GP regression.          |  value  |  constraints  |
  rbf.variance            |    1.0  |      +ve      |
  rbf.lengthscale         |    1.0  |      +ve      |
  Gaussian_noise.variance |    1.0  |      +ve      |
```

Prior



RBF kernel:

$$k_{RBF}(x, x') = \sigma^2 \exp\left(\frac{-(x - x')}{2l^2}\right)$$

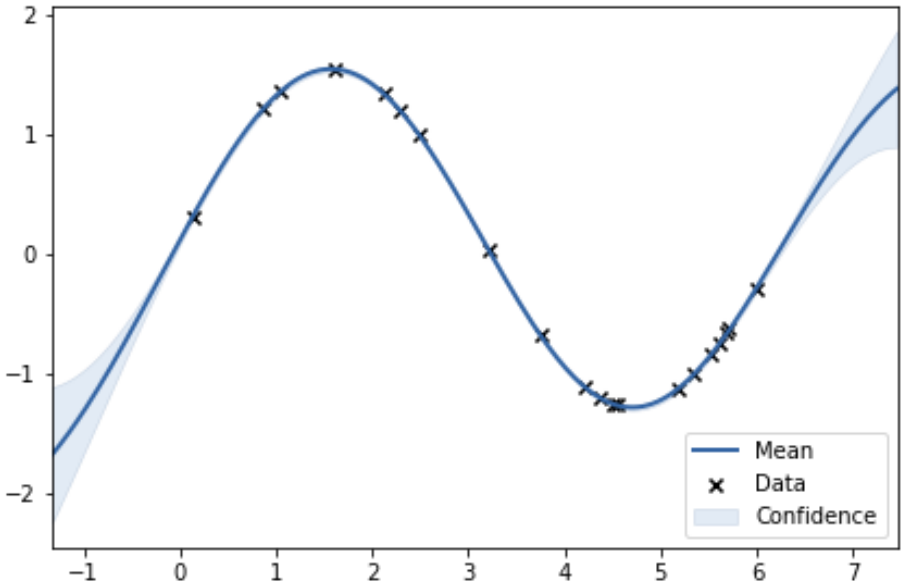
- Gaussian Noise variance acts like a regularization in GP models.
- Larger values of noise variance lead to more smoother model.

Gaussian Process Regression: Implementation

4. Optimize

```
m.optimize(messages=1)
m.plot()
```

Posterior




```
onstraints   |  priors
   +ve       |
   +ve       |
   +ve       |
```

Model: GP regression

Objective: -34.58282342238019

Number of Parameters: 3

Number of Optimization Parameters: 3

Updates: True

GP_regression.	value	constraints	priors
rbf.variance	4.758688562299606	+ve	
rbf.lengthscale	2.385712681113764	+ve	
Gaussian_noise.variance	0.00010550018745290958	+ve	

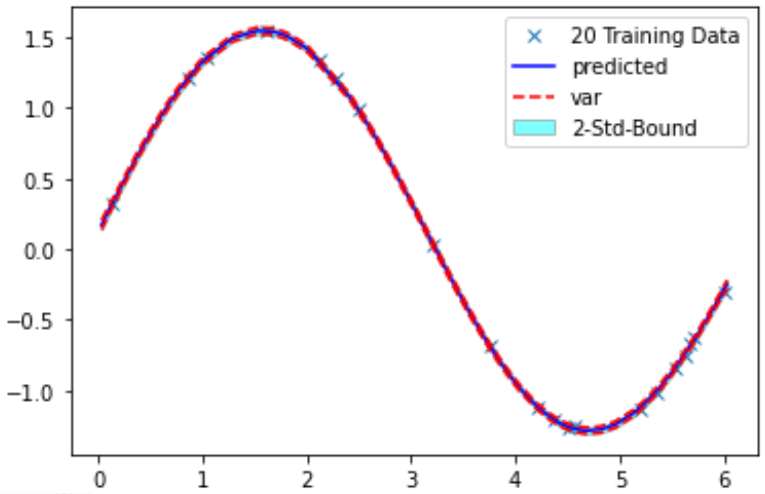
Gaussian Process Regression: Implementation

5. Prediction

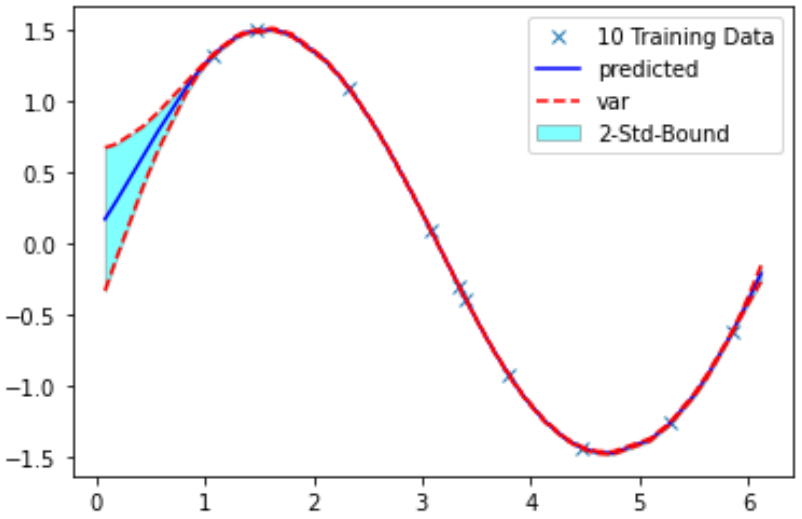
GPy

```
mu,var = m.predict(x_star)
plt.plot(x_tr, Y_tr, "x", label="Training Data")
plt.plot(x_star, mu, '-b',label='predicted')
plt.plot(x_star, mu+2*np.sqrt(var), 'r--',label='var')
plt.plot(x_star, mu-2*np.sqrt(var), 'r--')
plt.legend()
vv = 2*np.sqrt(var)
plt.fill_between(x_star[:,0], (mu-vv)[:,0], (mu+vv)[:,0], alpha=0.5, edgecolor='gray', facecolor='cyan')
plt.legend()
plt.ylim((-2.5, 2.5))
plt.show()
```

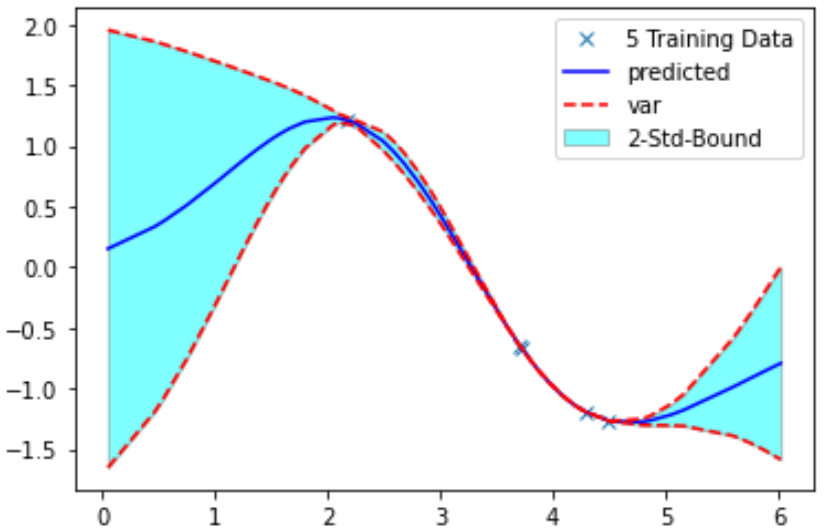
20 Training Datapoints



10 Training Datapoints



5 Training Datapoints



Data Assimilation from Noisy Field Measurements

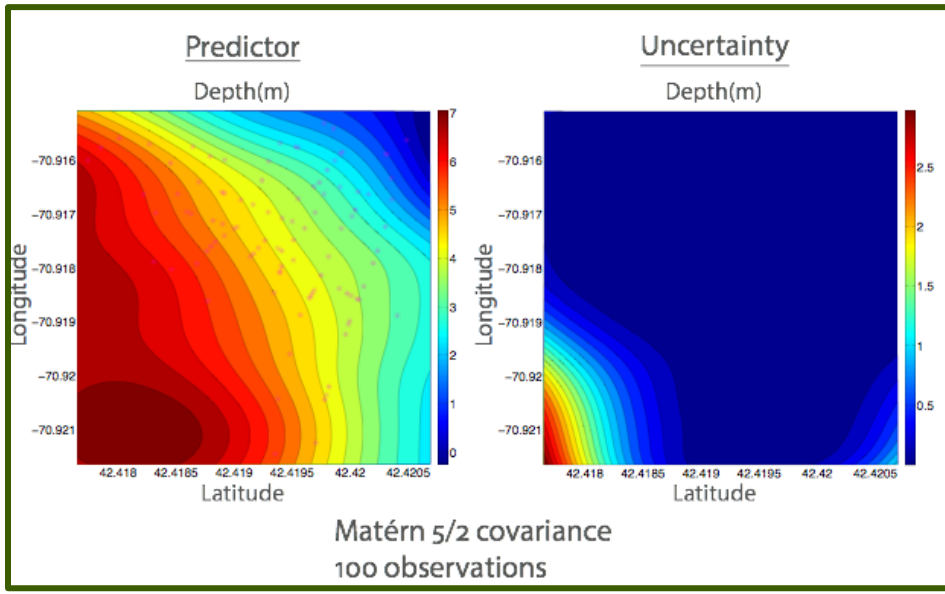
- Pirate's Cove data-set: 1,328 noisy measurements of bathymetry and plant height variables

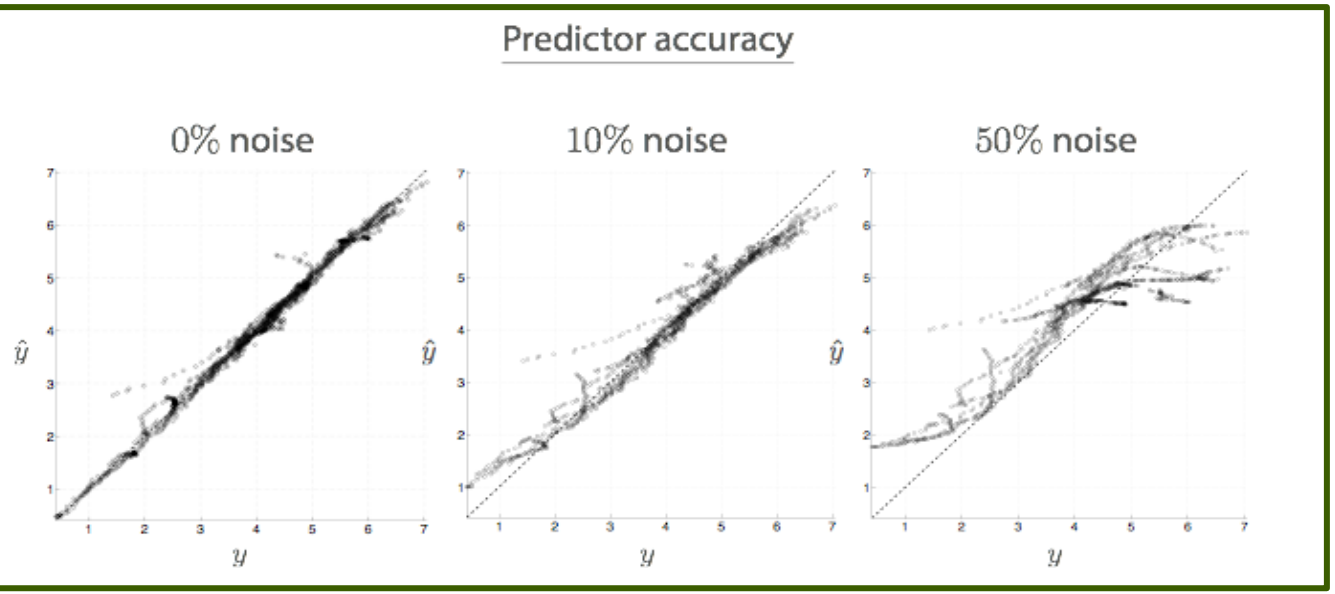
- **Measurements:**
  Mike Sacarny (MIT Sea Grant)

<u>Objective:</u> Reconstruct the bathymetry and plant height maps with quantified uncertainty

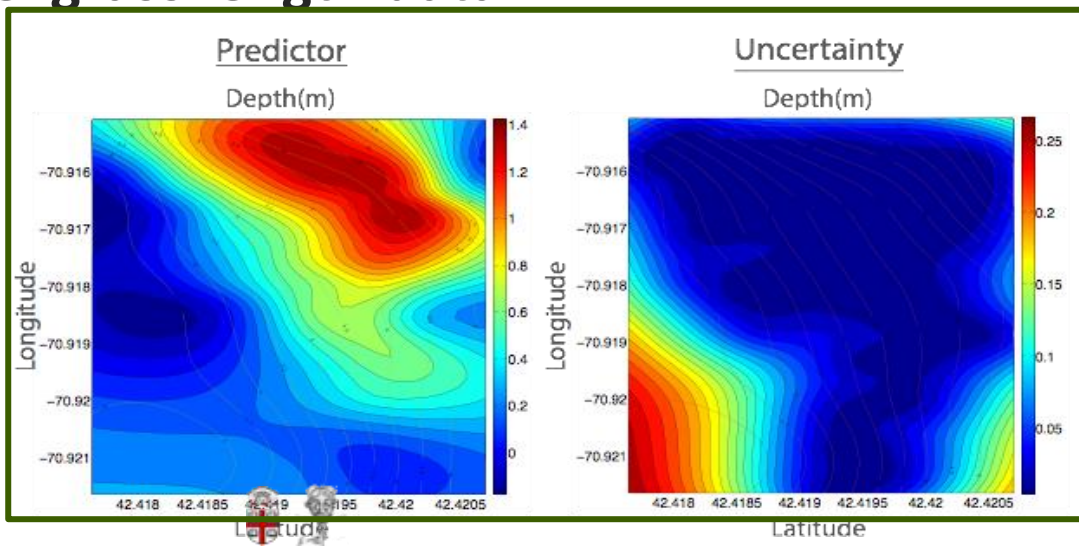
Data Assimilation from Noisy Field Measurements

Bathymetry data

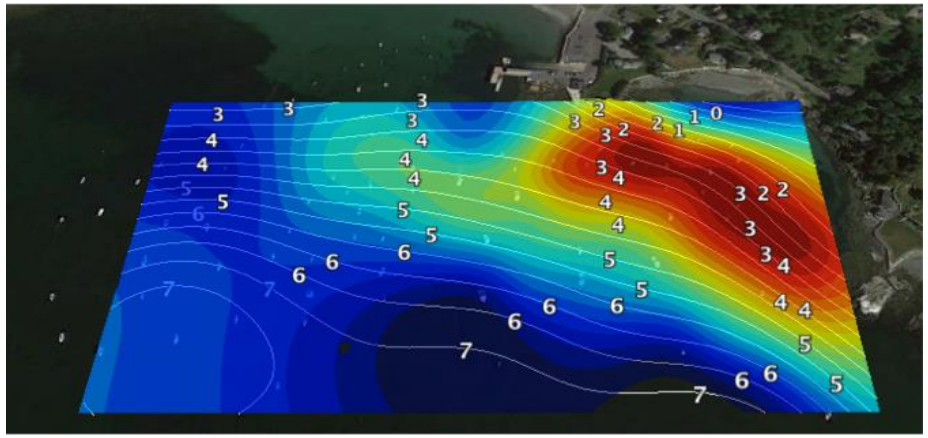




Eel grass length data

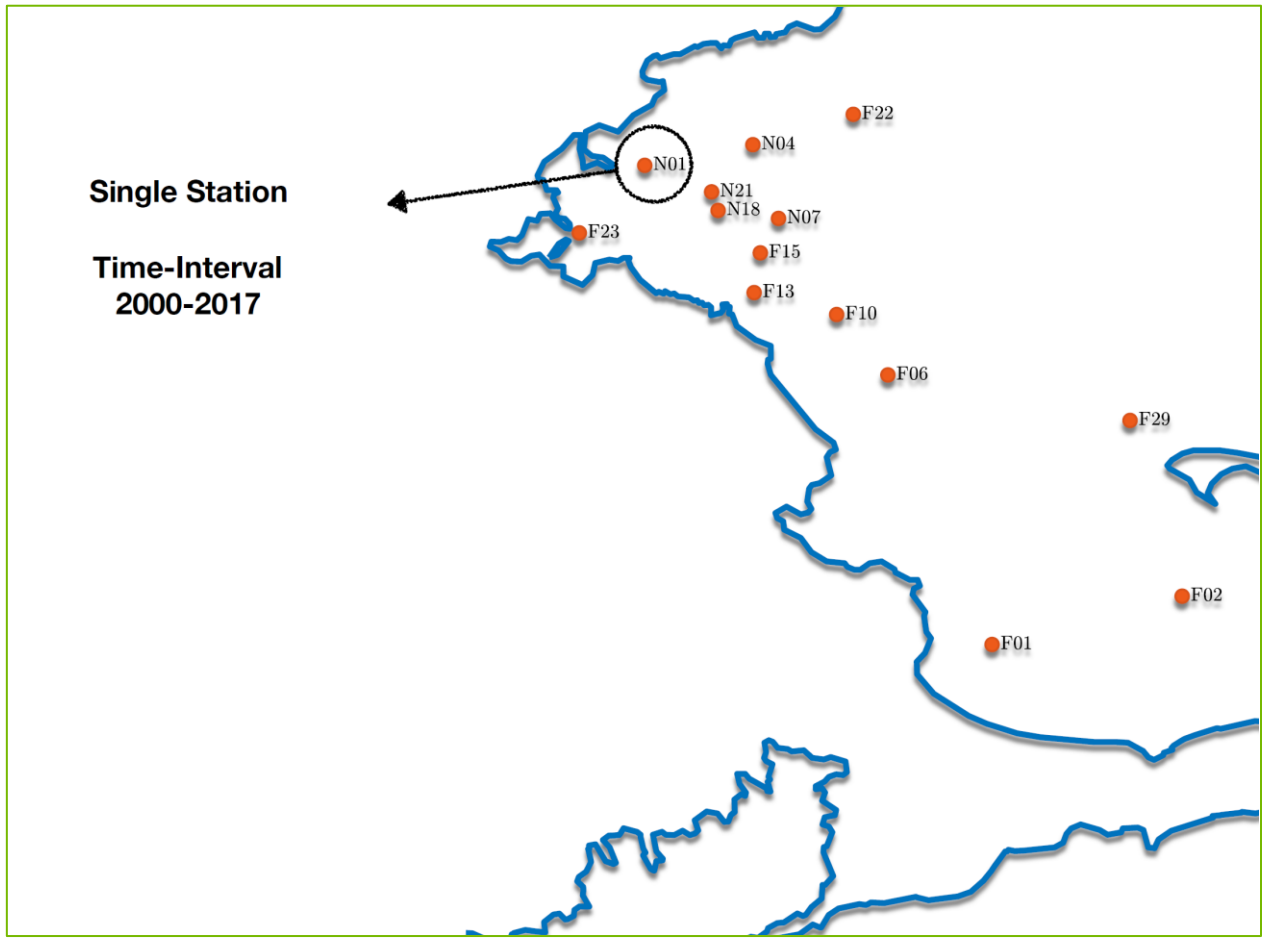


Predictions using 100 training points

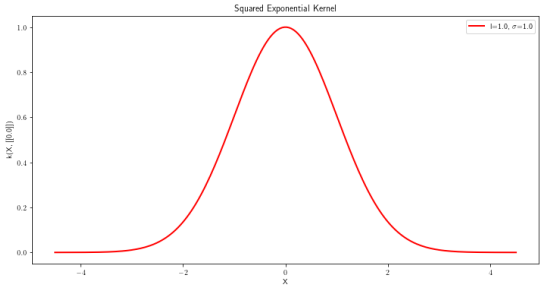


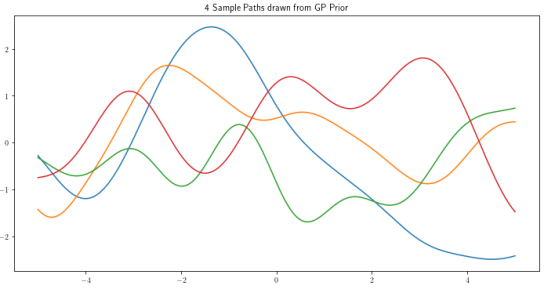
Physics-Informed Kernels

MWRA Forecast



Seasonal Dynamics

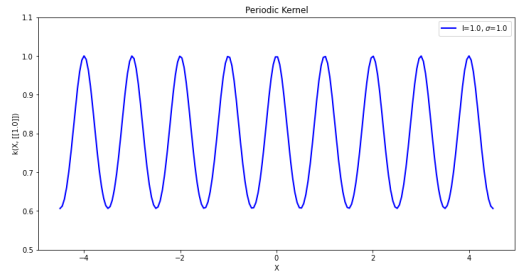


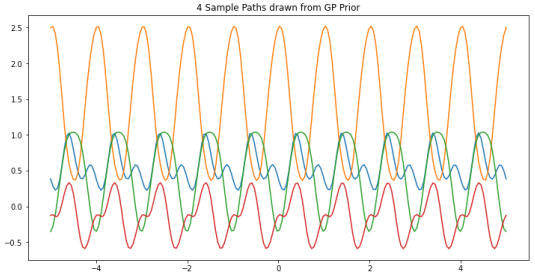


Squared Exponential Kernel:

$$k_{se}(\boldsymbol{x}, \boldsymbol{x}') = \sigma^2 \exp\left(-\frac{(\boldsymbol{x} - x')^2}{2l^2}\right)$$

Hyperparameters: σ and l



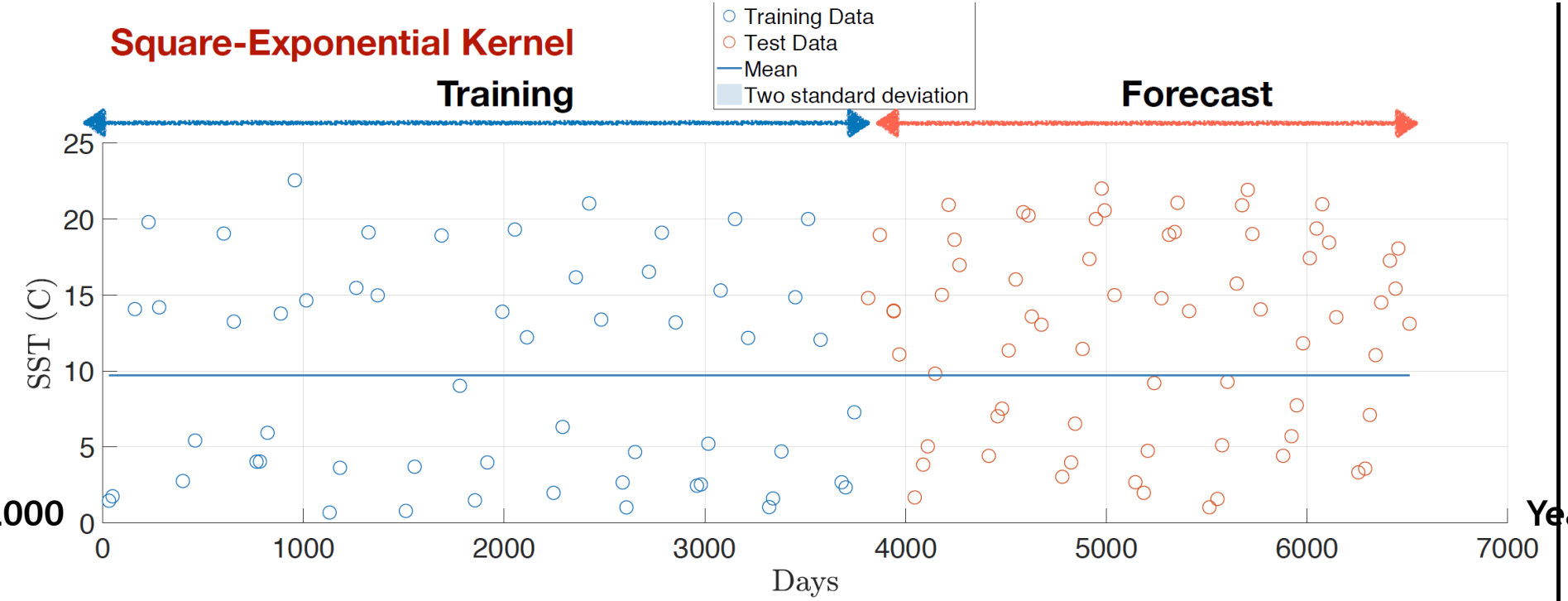


Periodic Kernel:

$$k_{per}(\boldsymbol{x}, \boldsymbol{x}') = \sigma^2 \exp\left(-\frac{2\sin^2(\pi|\boldsymbol{x} - \boldsymbol{x}'|/p)}{l^2}\right)$$

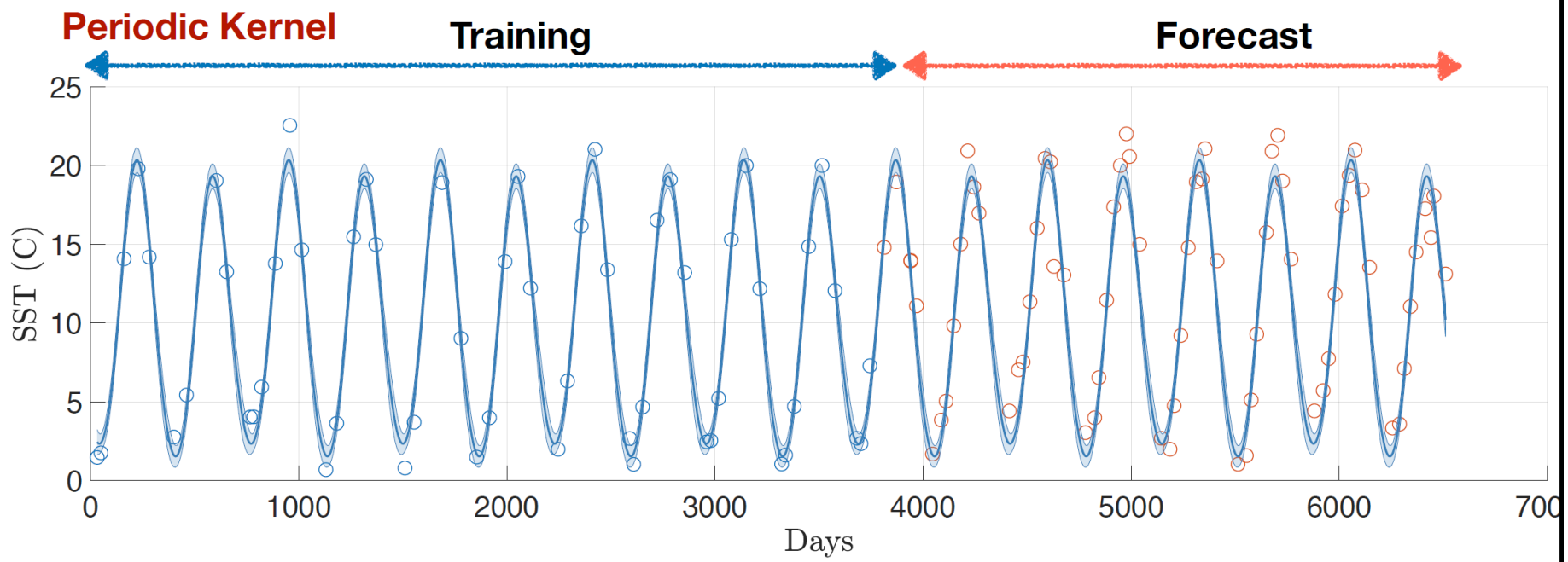
Hyperparameters: σ, l, and p

Square-Exponential Kernel



Year 2000 — Year 2007

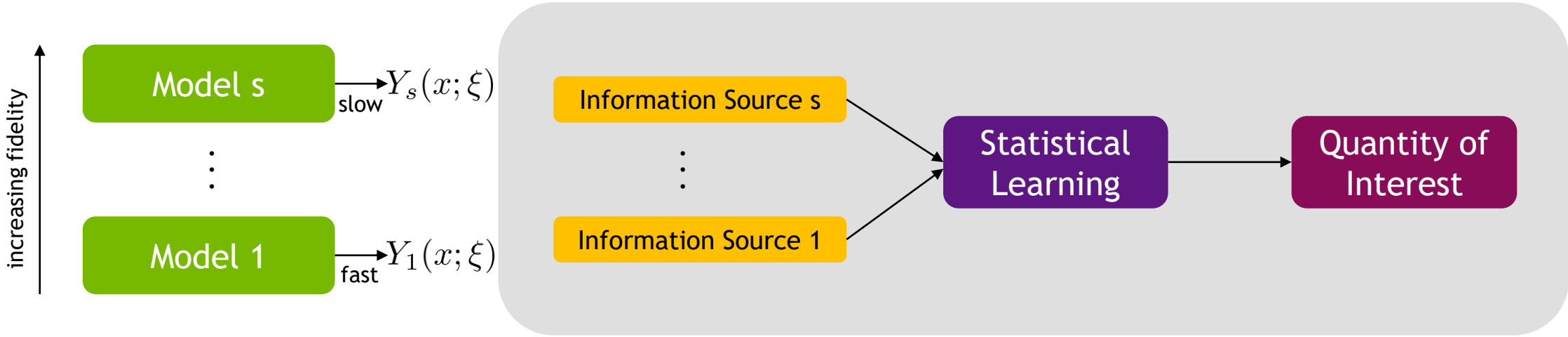
Periodic Kernel



DEEP LEARNING INSTITUTE

BROWN

Multi-Fidelity Modeling



- Number of runs is limited by time and computational resources
- We cannot compute at all $(x;\xi)$
- Prediction of $Z_i(x) = \mathbb{E}[f(Y_i(x;\xi))]$ is a problem of statistical inference

Multi-Fidelity Modeling with GPs

Auto-regressive model:

$$f_t(x) = \rho_{t-1}(x) f_{t-1}(x) + \delta_t(x) \qquad t = 1, ..., s$$

Theorem (LeGratiet, 2014):

The predictive posterior of a recursive scheme has exactly the same distribution with the fully coupled model given a nested experimental design.

Predictive Posterior

$$\begin{aligned} p(f_*|y, X, x_*) &= \mathcal{N}(f_*|\mu_*, \sigma_*^2) \\ \mu_*(x_*) &= k_{*N}(\boldsymbol{K} + \sigma_\epsilon^2 I)^{-1} y \\ \sigma_*^2(x_*) &= k_{**} - k_{*N}(\boldsymbol{K} + \sigma_\epsilon^2 I)^{-1} k_{N*} \end{aligned}$$

$\boldsymbol{K}$ becomes a block covariance matrix

$$\boldsymbol{K} = \begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix}$$

Key Idea: Replace f_{t-1} with GP posterior of the previous level $\tilde{f}_{t-1}$

$$f_t(x) = \rho_{t-1}(x) f_{t-1}(x) + \delta_t(x) \qquad \tilde{f}_{t-1} \sim f_{t-1}|\mathcal{D}_1, \mathcal{D}_2, ..., \mathcal{D}_{t-1}$$

- Le Gratiet L, Garnier J. Recursive co-kriging model for design of computer experiments with multiple levels of fidelity. International Journal for Uncertainty Quantification. 2014;4(5).
- Kennedy MC, O'Hagan A. Predicting the output from a complex computer code when fast approximations are available. Biometrika. 2000 Mar 1;87(1):1-3.

Information Fusion via Recursive Co-Kriging

- We have s levels of information sources producing outputs $y_t(x_t)$, at locations $\boldsymbol{x}_t \in D_t \subseteq \mathbb{R}^d$, sorted by increasing order of fidelity and modeled by Gaussian processes $Z_t(\boldsymbol{x}),\ t = 1, \ldots, s$.

$$Z_t(\boldsymbol{x}) = \rho_{t-1}(\boldsymbol{x}) Z_{t-1}(\boldsymbol{x}) + \delta_t(\boldsymbol{x}), \qquad t = 2, \ldots s,$$

  where $\delta_t(x)$ is a Gaussian field independent $\{Z_{t-1}, \ldots, Z_1\}$ and distributed as $\delta_t \sim \mathcal{N}(\mu_{\delta_t}, \sigma_t^2 R_t)$.

- $\rho(\boldsymbol{x})$ is a scaling factor that quantifies the correlation between $\{Z_t(\boldsymbol{x}), Z_{t-1}(\boldsymbol{x})\}$.

- Once $Z_t(\boldsymbol{x})$ has been trained on N_t observation, we can perform predictions at new points $\boldsymbol{x}_t^*$ and quantify the variance as

$$\widehat{y}_t(\boldsymbol{x}_t^*) = \widehat{\mu}_t + \widehat{\rho}_{t-1}\widehat{y}_{t-1}(\boldsymbol{x}_t^*) + r_t^\top (R_t + \widehat{\sigma}_{\epsilon_t}^2 \boldsymbol{I})^{-1}[y_t(\boldsymbol{x}_t) - \mathbf{1}\widehat{\mu}_t - \widehat{\rho}_{t-1}\widehat{y}_{t-1}\boldsymbol{x}_t)],$$

$$s_t^2(\boldsymbol{x}_t^*) = \widehat{\rho}_{t-1}^2 s_{t-1}^2(\boldsymbol{x}_t^*) + \widehat{\sigma}_t^2 \left[1 - r_t^T (R_t + \widehat{\sigma}_{\epsilon_t}^2)^{-1} r_t + \frac{[1 - r_t^\top (R_t + \widehat{\sigma}_{\epsilon_t}^2 \boldsymbol{I})^{-1} r_t]^2}{\mathbf{1}_t^T (R_t + \widehat{\sigma}_{\epsilon_t}^2 I)^{-1} \mathbf{1}_t}\right]$$

- $R_t = \kappa_t(\boldsymbol{x}_t, \boldsymbol{x}_t'; \widehat{\theta}_t)$ is the $N_t \times N_t$ correlation matrix of $Z_t(\boldsymbol{x}), r_t = \kappa_t(\boldsymbol{x}_t, \boldsymbol{x}_t^*; \widehat{\theta}_t)$ is a $1 \times N_t$ correlation vector between the prediction and N_t training points, and $\mathbf{1}_t$ is a $1 \times N_t$ vector of ones.

Learning: Given y_t find the optimal $\{\widehat{\mu}_t, \widehat{\sigma}_t^2, \widehat{\sigma}_{\epsilon_t}^2, \widehat{\theta}_t, \widehat{\rho}_{t-1}\}$

The object of inference is $[Z_s(\boldsymbol{x}) | \boldsymbol{Z}_1, \ldots, \boldsymbol{Z}_{s-1}]$
(Output of the high-fidelity model conditional on all model data)

Multi-fidelity GPR Implementation

- **Problem Setup**:
  High Fidelity Function: $f_h(x) = (6x - 2.0)^2 \sin(12x - 4)$
  Low Fidelity Function: $f_l(x) = \frac{1}{2} f_h(x) + 10\left(x - \frac{1}{2}\right) - 5$

- We model the low-fidelity function by $f_l(x) = u_1(x)$ and high fidelity function by $f_h = \rho u_1(x) + u_2(x)$, where

$$u_1(x) \sim \mathcal{GP}(0, k_1(x, x'; \theta_1)),$$

  and

$$u_2(x) \sim \mathcal{GP}(0, k_2(x, x'; \theta_2)),$$

  are Gaussian Processes.

- This will result into following multi-output Gaussian process

$$\begin{bmatrix} f_l(x) \\ f_h(x) \end{bmatrix} \sim \mathcal{GP}\left(0, \begin{bmatrix} k_{ll}(x, x'; \theta_1) & k_{lh}(x, x'; \theta_1, \rho) \\ k_{hl}(x, x'; \theta_1, \rho) & k_{hh}(x, x'; \theta_1, \theta_2, \rho), \end{bmatrix}\right)$$

  where

$$\begin{aligned} k_{ll}(x, x'; \theta_1) &= k_1(x, x'; \theta_1) \\ k_{hl}(x, x'; \theta_1, \rho) &= k_{lh}(x, x'; \theta_1, \rho) = \rho k_1(x, x'; \theta_1) \\ k_{hh}(x, x'; \theta_1, \theta_2, \rho) &= \rho^2 k_1(x, x'; \theta_1) + k_2(x, x'; \theta_2) \end{aligned}$$

Multi-fidelity GPR Implementation

- **Training**: Training data- LF= $\{\boldsymbol{x}_l, \boldsymbol{y}_l\}$, HF= $\{\boldsymbol{x}_h, \boldsymbol{y}_h\}$
- We assume that

$$\boldsymbol{y}_l = f_l(\boldsymbol{x_l}) + \epsilon_l, \qquad \epsilon_l \sim \mathcal{N}(\mathbf{0}, \sigma_l^2 \boldsymbol{I})$$

and

$$\boldsymbol{y}_h = f_h(\boldsymbol{x_h}) + \epsilon_h, \qquad \epsilon_h \sim \mathcal{N}(\mathbf{0}, \sigma_h^2 \boldsymbol{I})$$

- We obtain

$$\boldsymbol{y} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{K}),$$

where

$$y = \begin{bmatrix} \boldsymbol{y}_l \\ \boldsymbol{y}_h \end{bmatrix}$$

and

$$K = \begin{bmatrix} k_{ll}(\boldsymbol{x}_l, \boldsymbol{x}_l; \theta_1) + \sigma_l^2 \boldsymbol{I} & k_{lh}(\boldsymbol{x}_l, \boldsymbol{x}_h; \theta_1, \rho) \\ k_{hl}(\boldsymbol{x}_h, \boldsymbol{x}_l; \theta_1) & k_{hh}(\boldsymbol{x}_h, \boldsymbol{x}_h; \theta_1, \theta_2, \rho) + \sigma_h^2 \boldsymbol{I} \end{bmatrix}$$

- The hyper-parameters θ_1, θ_2, ρ and the noise variance parameters σ_l^2, σ_h^2 can be trained by minimizing the resulting negative log marginal likelihood.

$$\mathcal{NLML} = -\frac{1}{2}\boldsymbol{y}^\top \boldsymbol{K}^{-1}\boldsymbol{y} - \frac{1}{2}\log|\boldsymbol{K}| - \frac{N}{2}\log(2\pi)$$

Multi-fidelity GPR Implementation

- **Prediction**: Prediction at test point $\boldsymbol{x}^*$ can be made by first writing the distribution

$$\begin{bmatrix} f_h(x^*) \\ \boldsymbol{y} \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} k_{hh}(x^*, x^*; \theta_1, \theta_2, \rho) & \boldsymbol{q}^\top \\ \boldsymbol{q} & \boldsymbol{K} \end{bmatrix}\right),$$

  where $\boldsymbol{q}^\top = [k_{hl}(x^*, \boldsymbol{x}_l; \theta_1\rho) \qquad k_{hh}(x^*, \boldsymbol{x}_h; \theta_1, \theta_2, \rho)]$.

- By using the resulting conditional distribution to make predictions

$$f_h(x^*)|y \sim \mathcal{N}(\boldsymbol{q}^\top \boldsymbol{K}^{-1}\boldsymbol{y}, k_{hh}(x^*, x^*) - \boldsymbol{q}^\top \boldsymbol{K}^{-1}\boldsymbol{q})$$

Multi-fidelity GPR Implementation: Code

1. Install Required Packages

```
%pip install notutils
%pip install mlai
%pip install gpy
%pip install pyDOE
%pip install emukit
%pip install --upgrade numpy
```

2. Import Modules

```
import numpy as np
np.random.seed(20)
import GPy
import emukit.multi_fidelity
import emukit.test_functions
from emukit.model_wrappers.gpy_model_wrappers import GPyMultiOutputWrapper
from emukit.multi_fidelity.models import GPyLinearMultiFidelityModel
from emukit.multi_fidelity.convert_lists_to_array import convert_x_list_to_array, convert_xy_lists_to_arrays
import matplotlib.pyplot as plt
from pyDOE import lhs
```

3. Define low and high fidelity functions

```
def high_fidelity(x):
    return (6.0*x-2.0)**2*np.sin(12.0*x-4.0)


def low_fidelity(x):
    return 0.5*high_fidelity(x) + 10.0*(x-0.5) - 5.0
```

Forrester Functions:

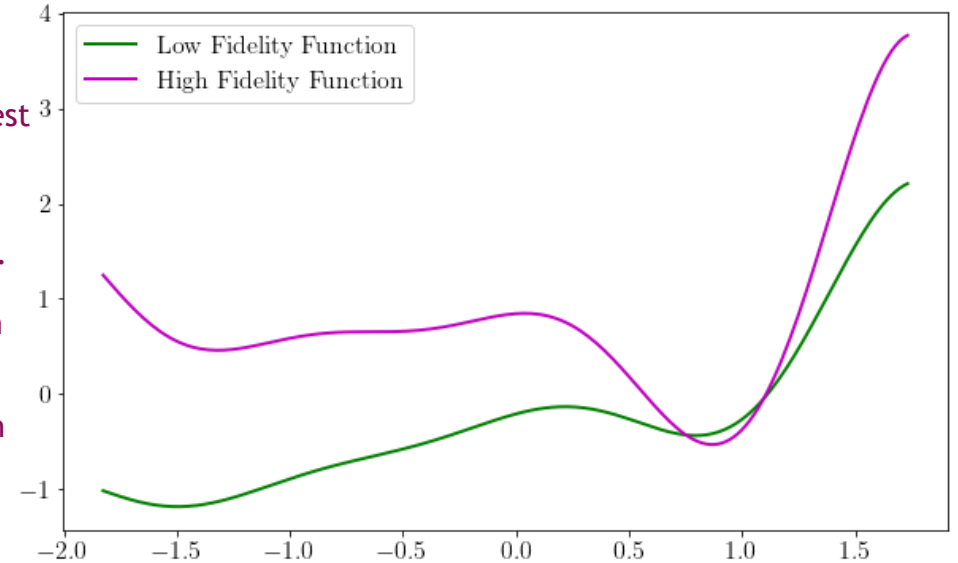
1). This function is a simple one-dimensional test function.

2) It is multimodal, with one global minimum, one local minimum and a zero-gradient inflection point.

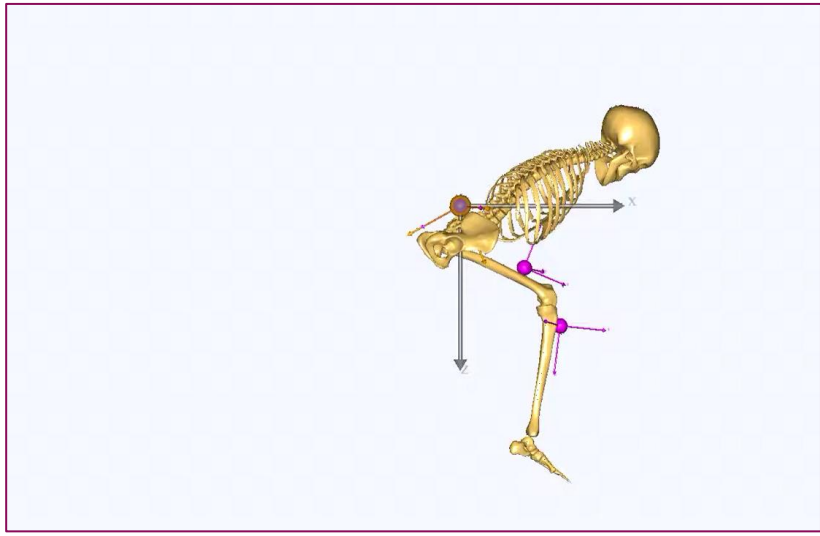
3) The high-fidelity function can be visualized as an ideal Breaststroke kinematics representation.

4) Magenta color pivots (in video) are sensors which are body worn.

Forrester Function



Breaststroke kinematics simulation

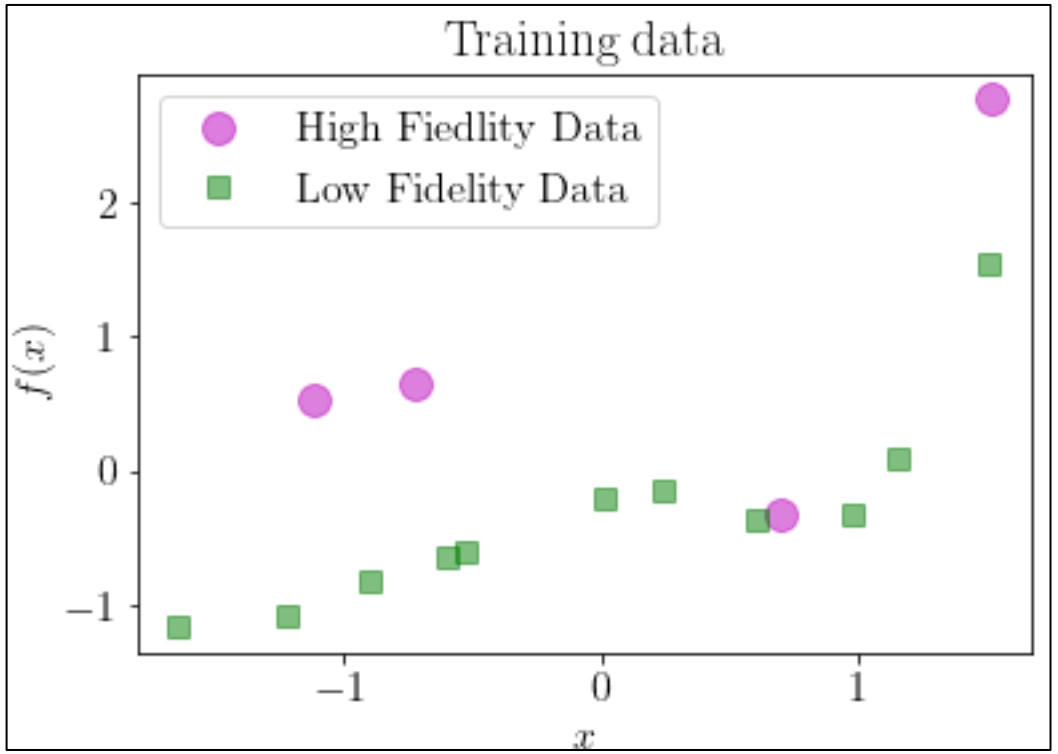


- Keane A, Forrester A, Sobester A. Engineering design via surrogate modelling: a practical guide. American Institute of Aeronautics and Astronautics, Inc.; 2008 Sep 1.
- Simulation Video: https://www.youtube.com/watch?v=2ngc2aw9xYs

Multi-fidelity GPR Implementation: Code

4. Generate Train and Test data

```
N_H = 4
N_L = 11
D = 1
fig_num = 4
noise_L = 0.00
noise_H = 0.00
lb = 0.0
ub = 1.0
# Training data
X_L = lb + (ub-lb)*lhs(D, N_L)
y_L = low_fidelity(X_L) + noise_L*np.random.randn(N_L,D)

X_H = lb + (ub-lb)*lhs(D, N_H)
y_H = high_fidelity(X_H) + noise_H*np.random.randn(N_H,D)
## Train Data
x_train_l = X_L
x_train_h = X_H
y_train_l = y_L
y_train_h = y_H
## Test Data
x_plot = np.linspace(0, 1, 200)[:, np.newaxis]
y_plot_l = low_fidelity(x_plot)
y_plot_h = high_fidelity(x_plot)
```



Multi-fidelity GPR Implementation: Code

5. Multideity kernel and optimization

```
kernels = [GPy.kern.RBF(1), GPy.kern.RBF(1)]
lin_mf_kernel = emukit.multi_fidelity.kernels.LinearMultiFidelityKernel(kernels)
```

Multifidelity Kernel

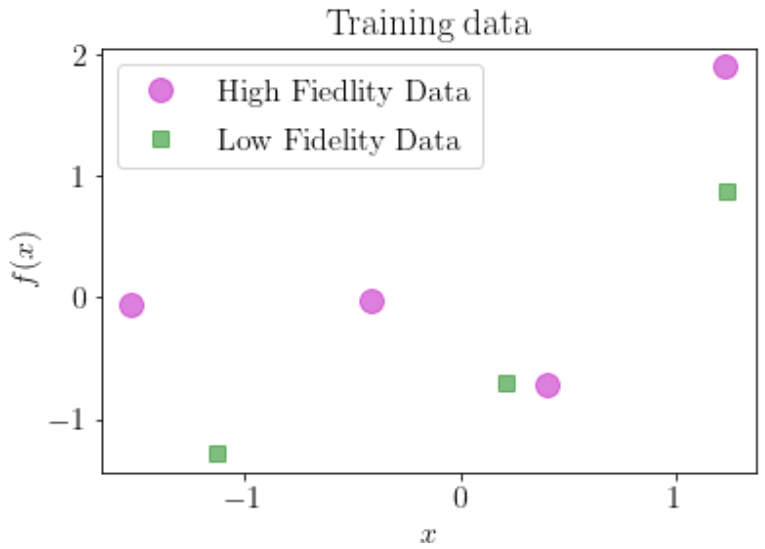
6. Optimization

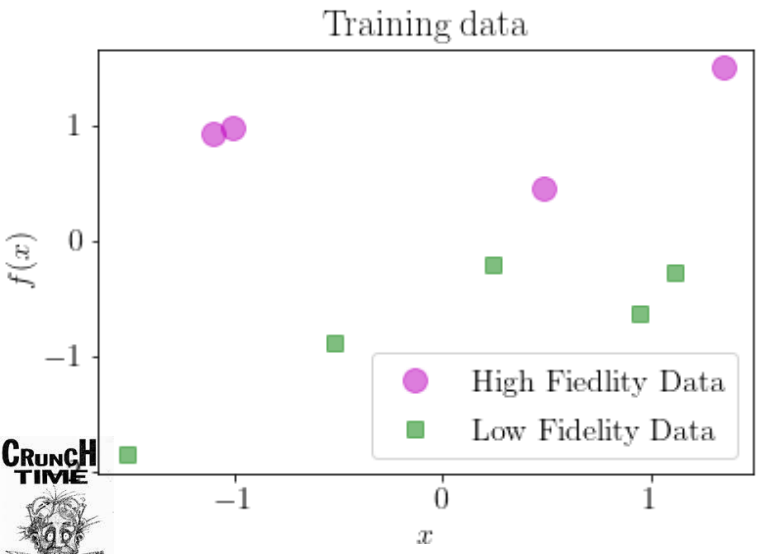
```
gpy_lin_mf_model = GPyLinearMultiFidelityModel(X_train, Y_train, lin_mf_kernel, n_fidelities=2)
gpy_lin_mf_model.mixed_noise.Gaussian_noise.fix(0)
gpy_lin_mf_model.mixed_noise.Gaussian_noise_1.fix(0)
lin_mf_model = GPyMultiOutputWrapper(gpy_lin_mf_model, 2, n_optimization_restarts=20)
lin_mf_model.optimize()
```

Optimization process

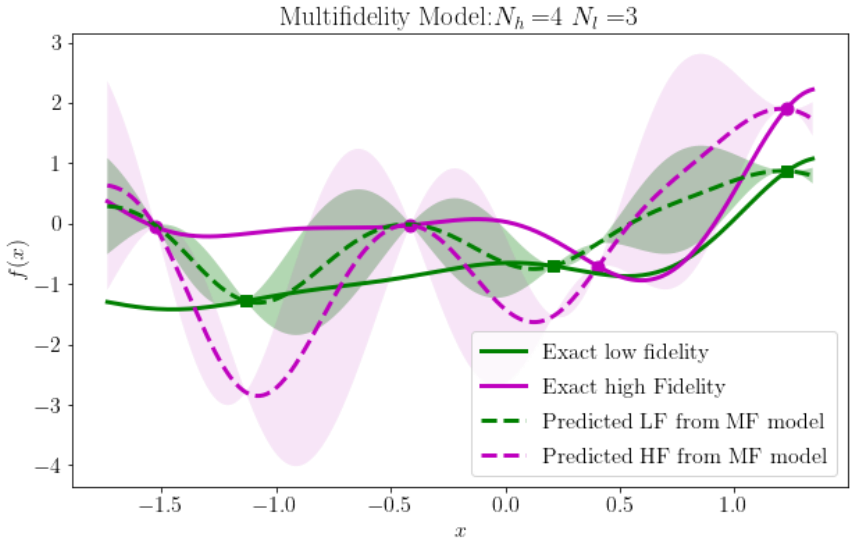
Multi-fidelity GPR Implementation: Results

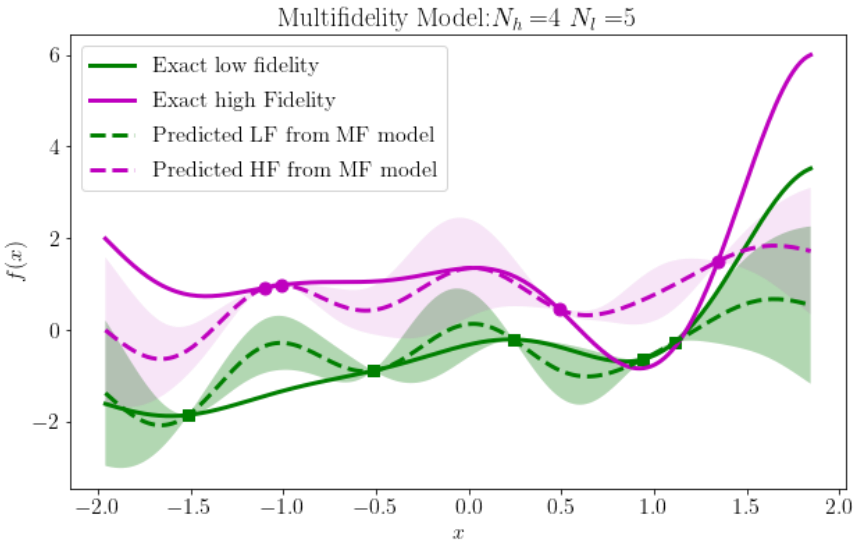
Training Data



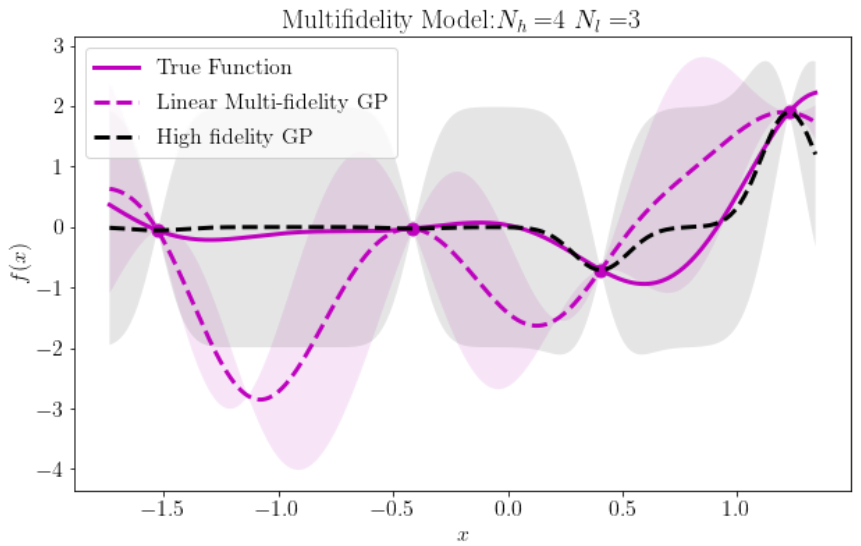


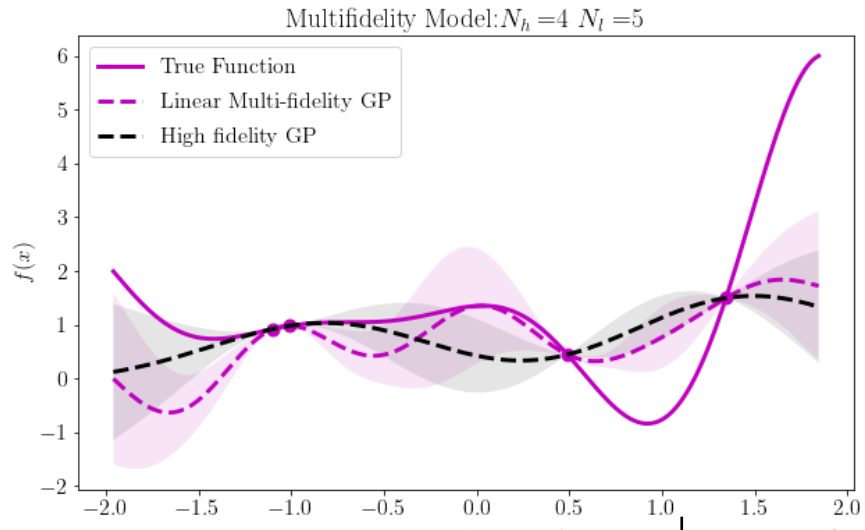
Multi-fidelity Approximation





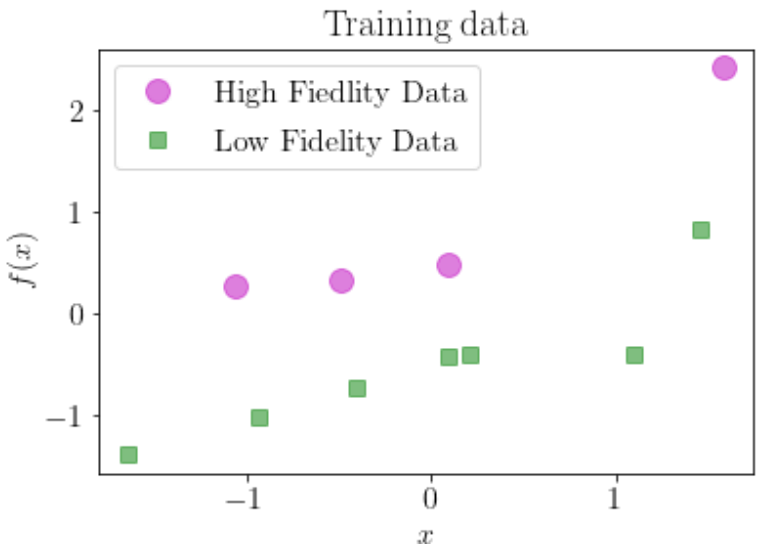
Multi-fidelity vs Single-fidelity



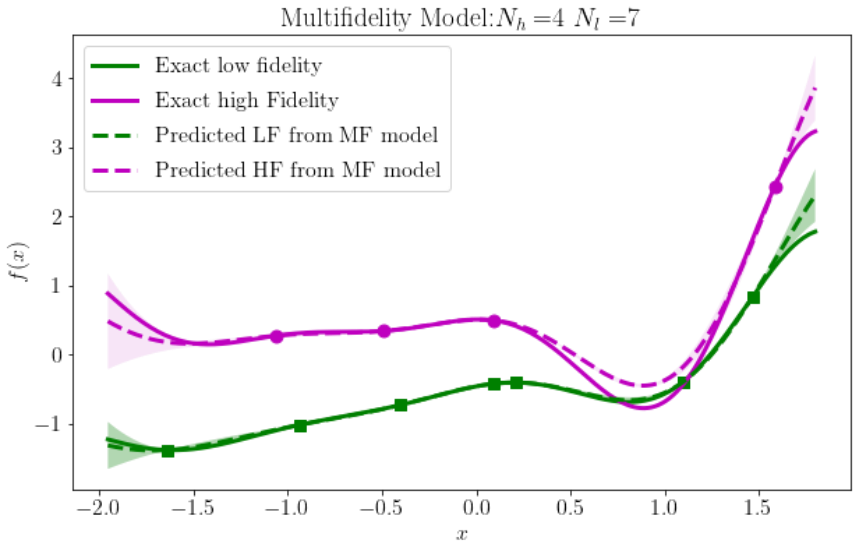


Multi-fidelity GPR Implementation: Results

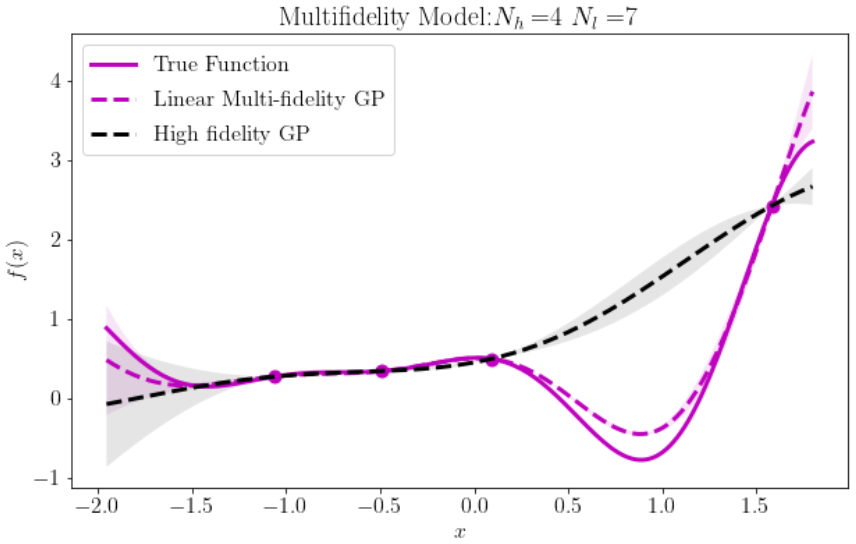
Training Data

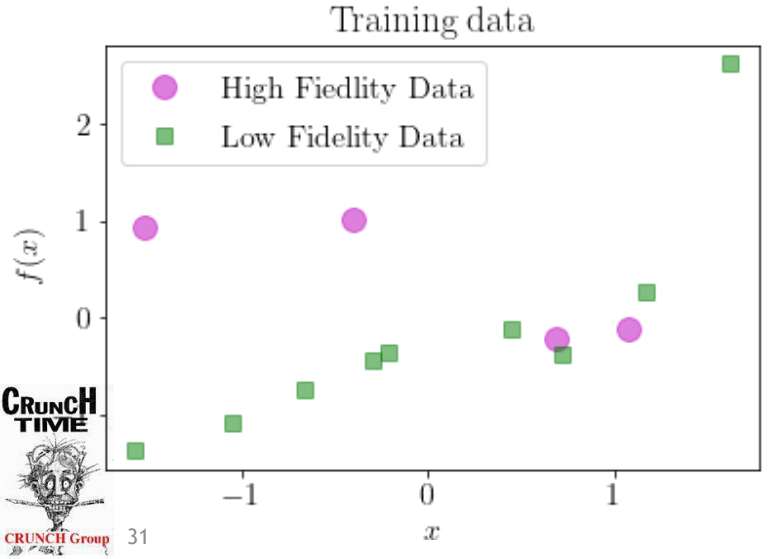


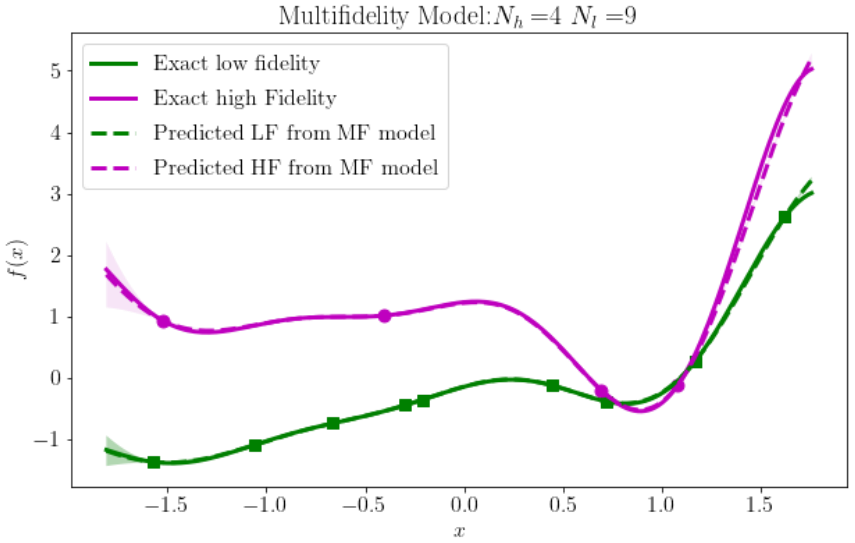
Multi-fidelity Approximation

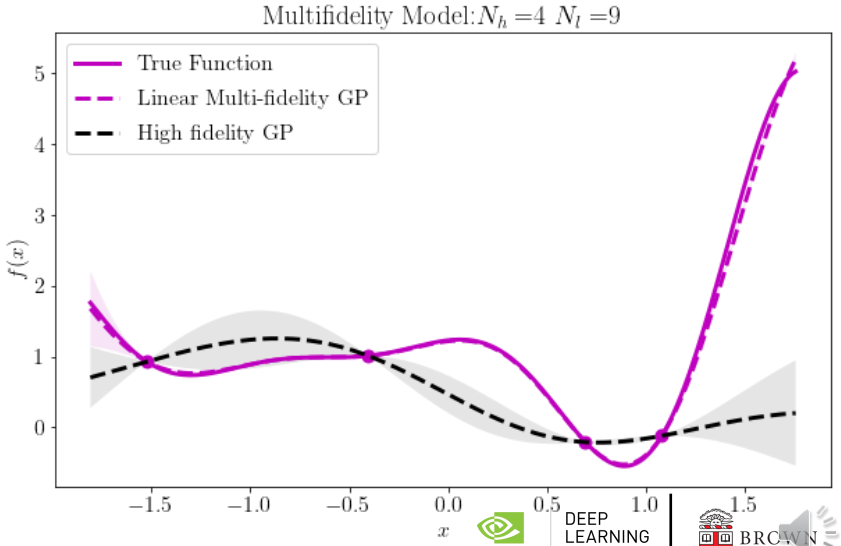


Multi-fidelity vs Single-fidelity



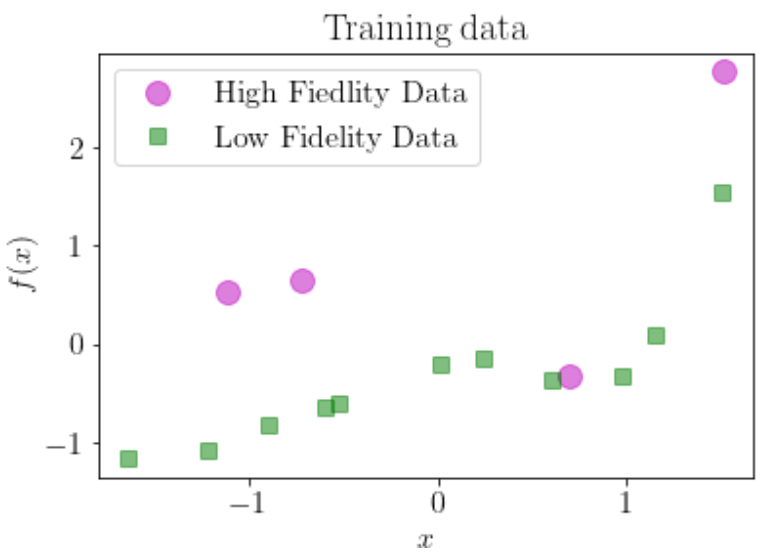




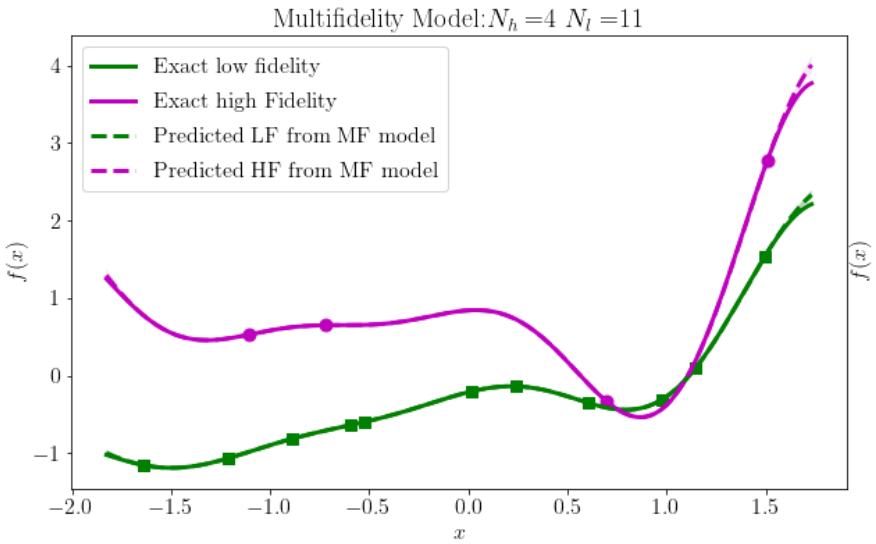


Multi-fidelity GPR Implementation: Results

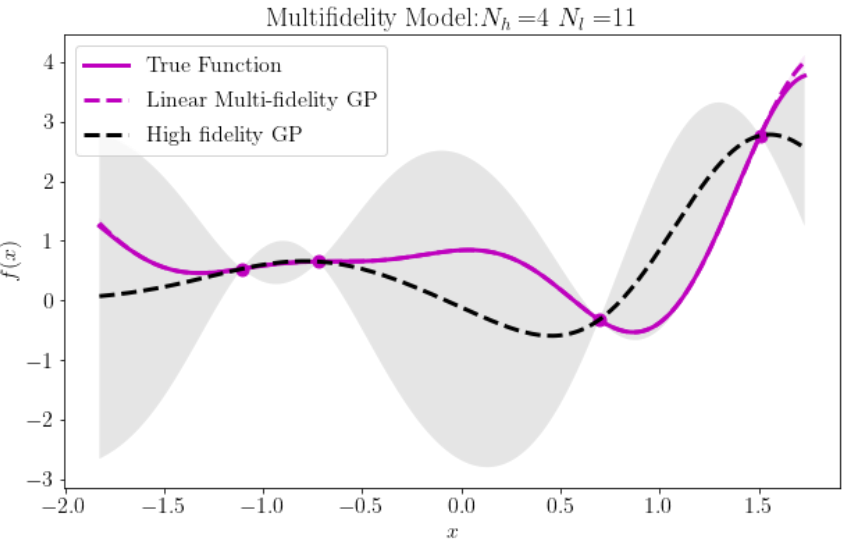
Training Data



Multi-fidelity Approximation



Multi-fidelity vs Single Fidelity



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