Deep and Multi-fidelity learning with Gaussian processes

Andreas Damianou, Sr ML Scientist

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andreasdamianou.com

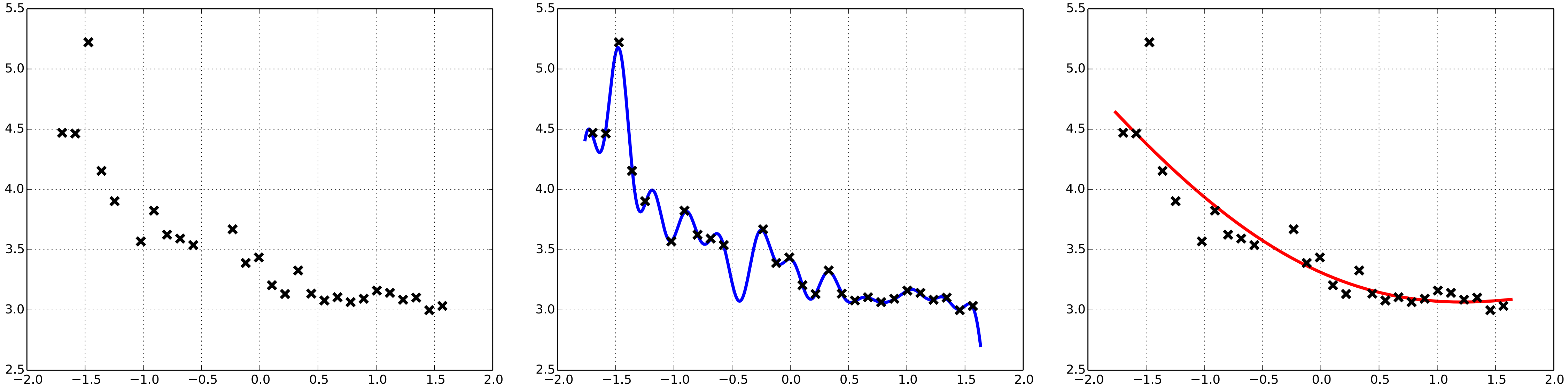
Various parts of this talk come from work with:

Neil Lawrence
Kurt Cutajar
Paris Perdikaris
Mark Pullin
Javier Gonzalez

Outline

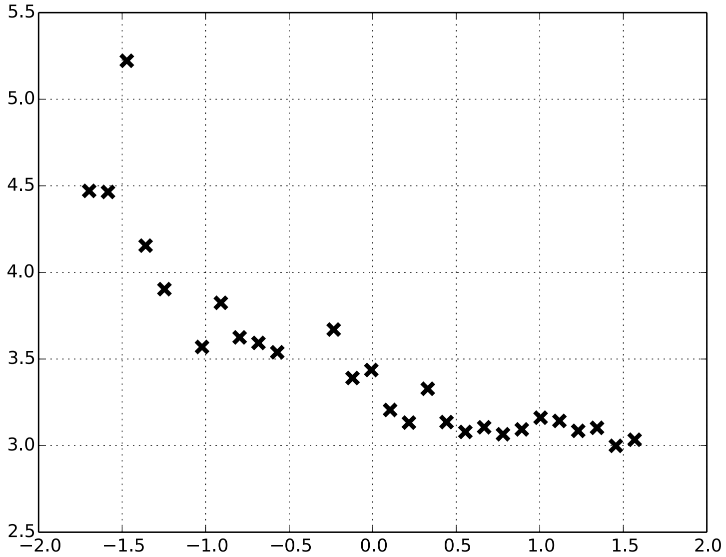
- Gaussian processes (GPs):
  - Reasoning about functions through smoothness assumptions
- Deep Gaussian processes (DGPs)
  - A much richer class of (deep) models: compositions of GPs
- Multi-fidelity modelling with DGPs:
  - Learn from multiple sources by treating the layers of DGP as fidelities

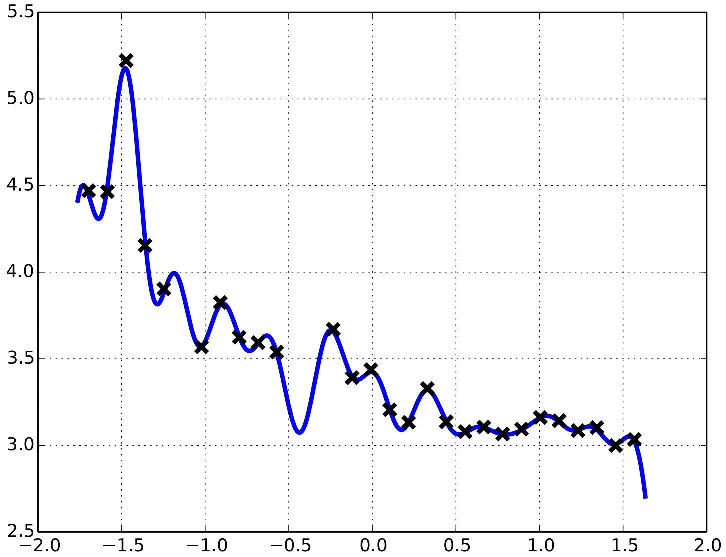
Curve fitting

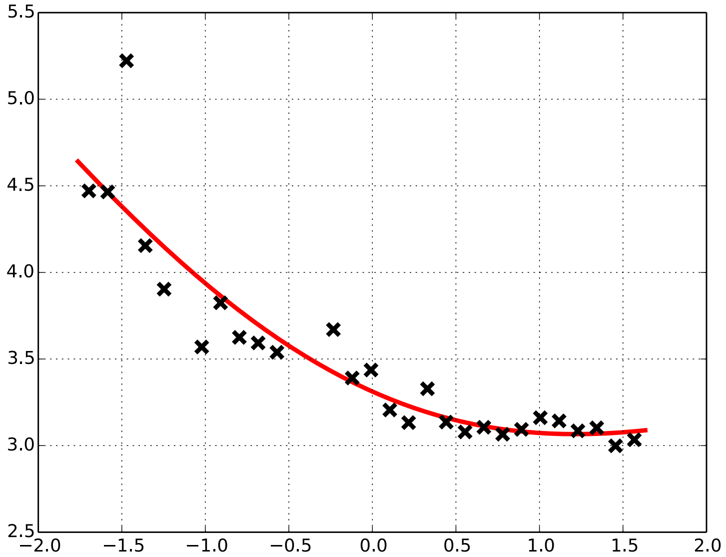


- Which curve fits the data better?
- Which curve is more "complex"?
- Which curve is better overall?

Curve fitting







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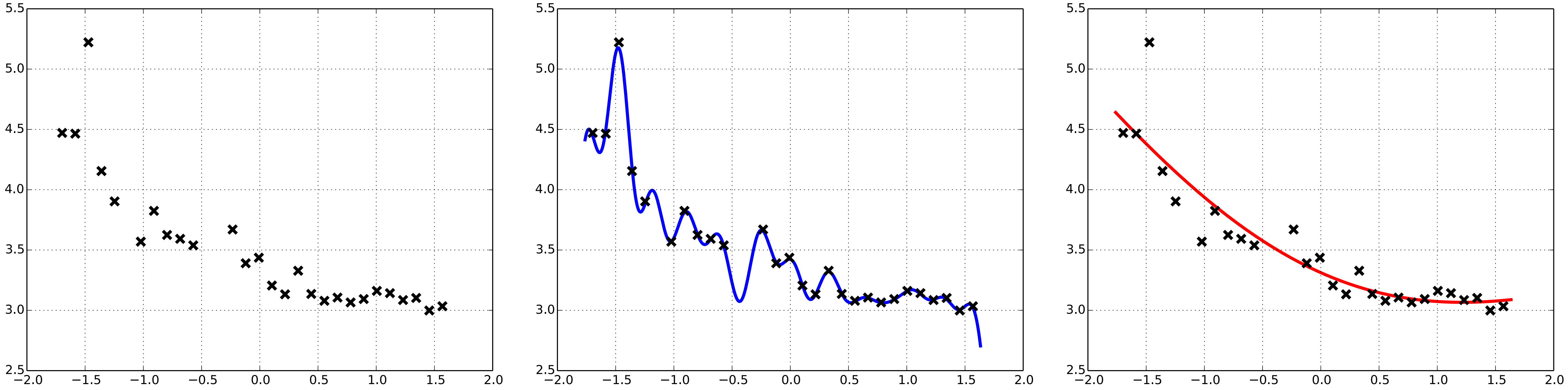
- Assumptions
- Occam's razor

Curve fitting



- Which curve fits the data better?
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- Which curve is better overall?

- Assumptions
- Occam's razor

Gaussian process

Posterior probability

- Posterior inference over space of **functions**

$$\textit{posterior} \propto \textcolor{red}{\textit{likelihood}} \times \textcolor{blue}{\textit{prior}}$$

Signal from observed data

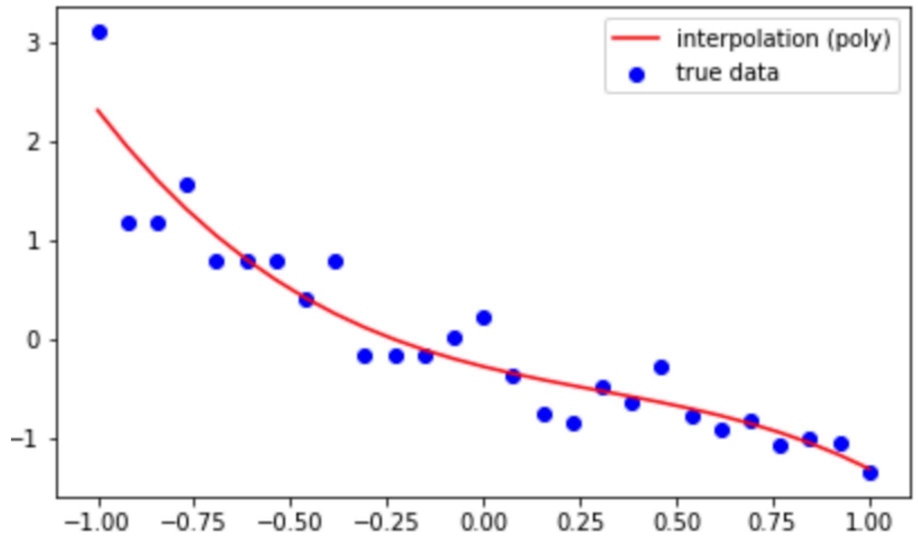
prior assumptions

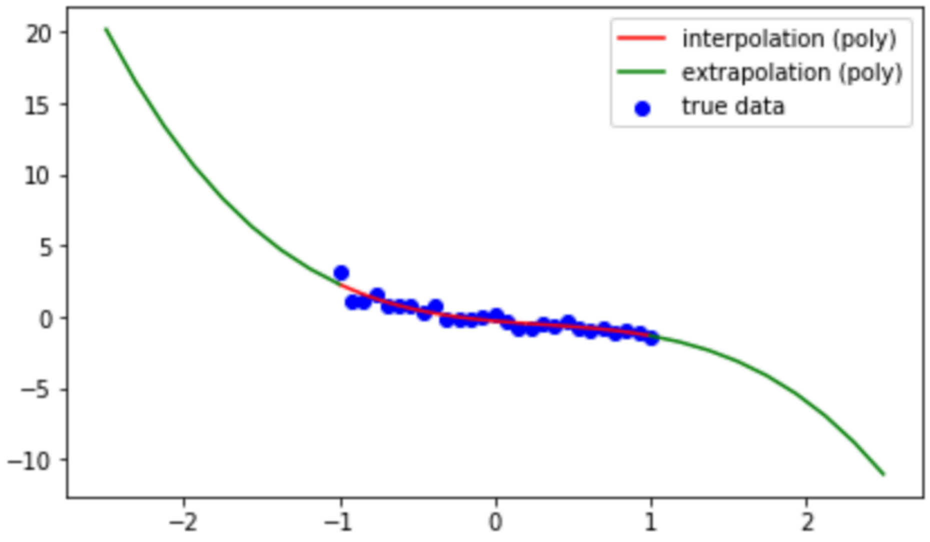
Part 1: Gaussian processes

See also:

adamian.github.io/talks/Damianou_GP_tutorial.html

Polynomial Regression

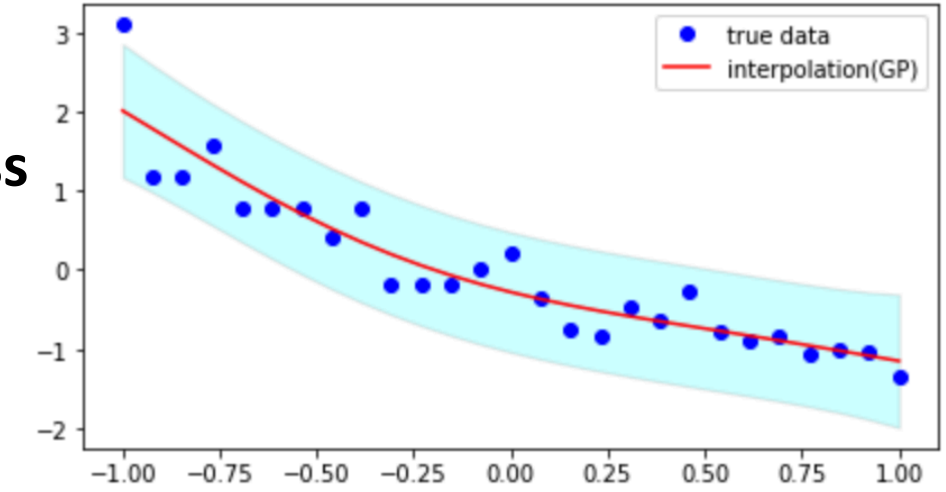


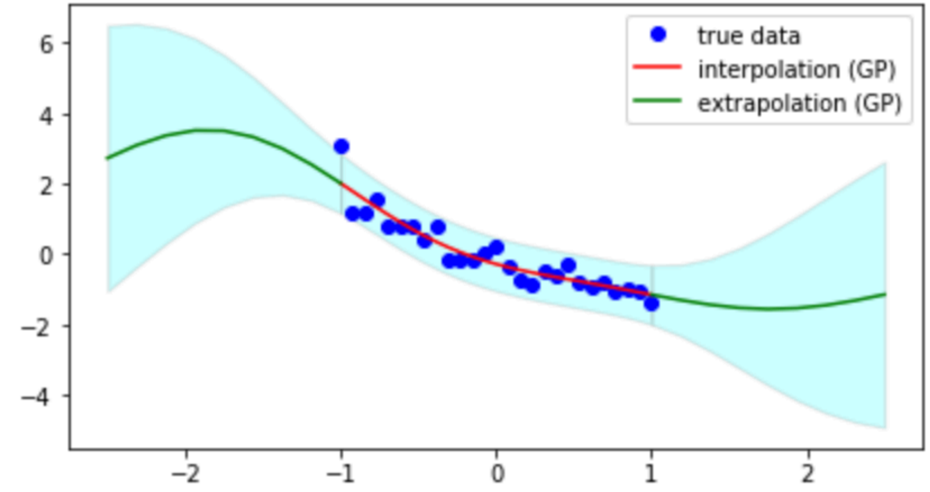


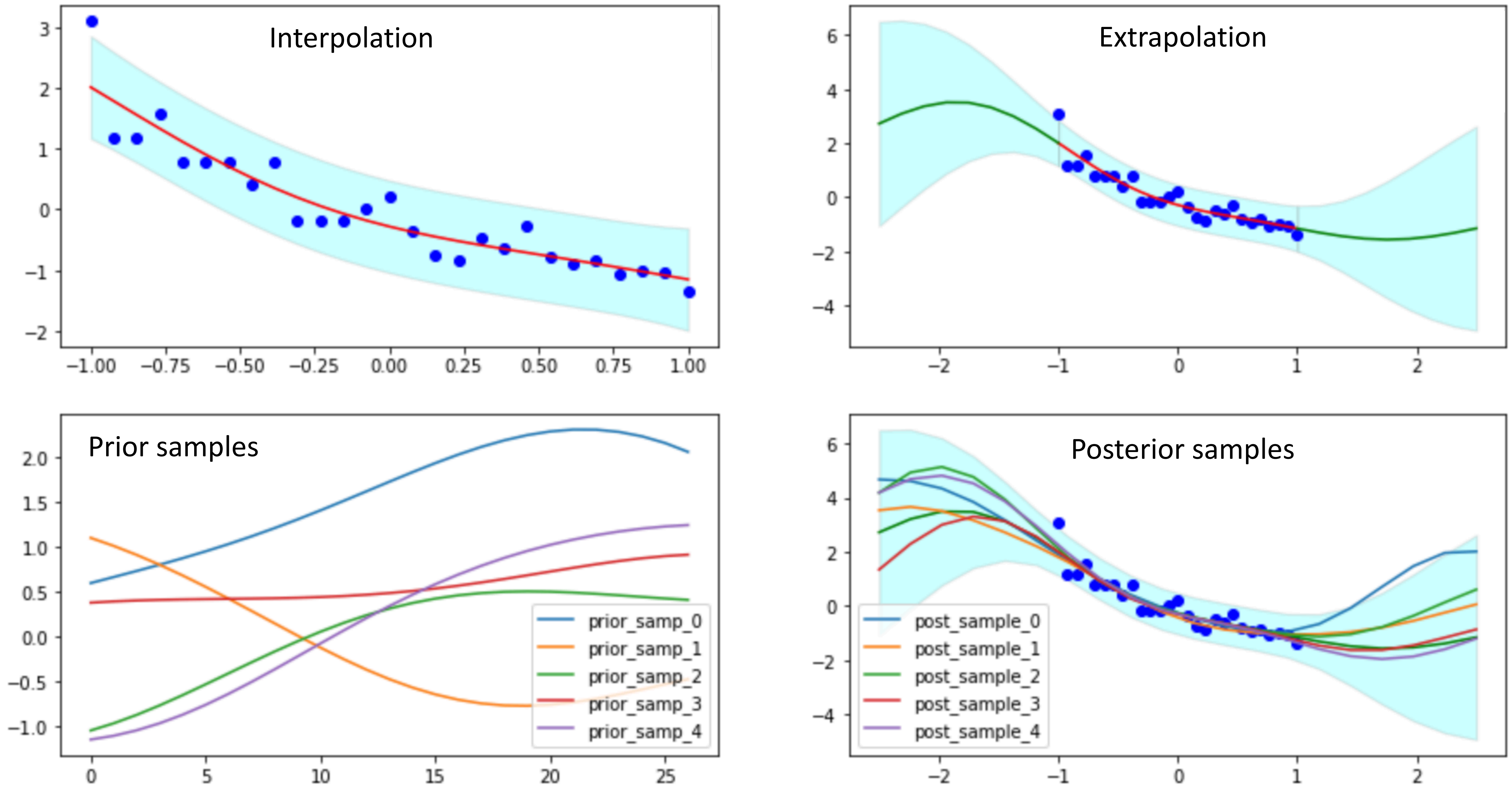
Interpolation

Extrapolation

Gaussian Process Regression

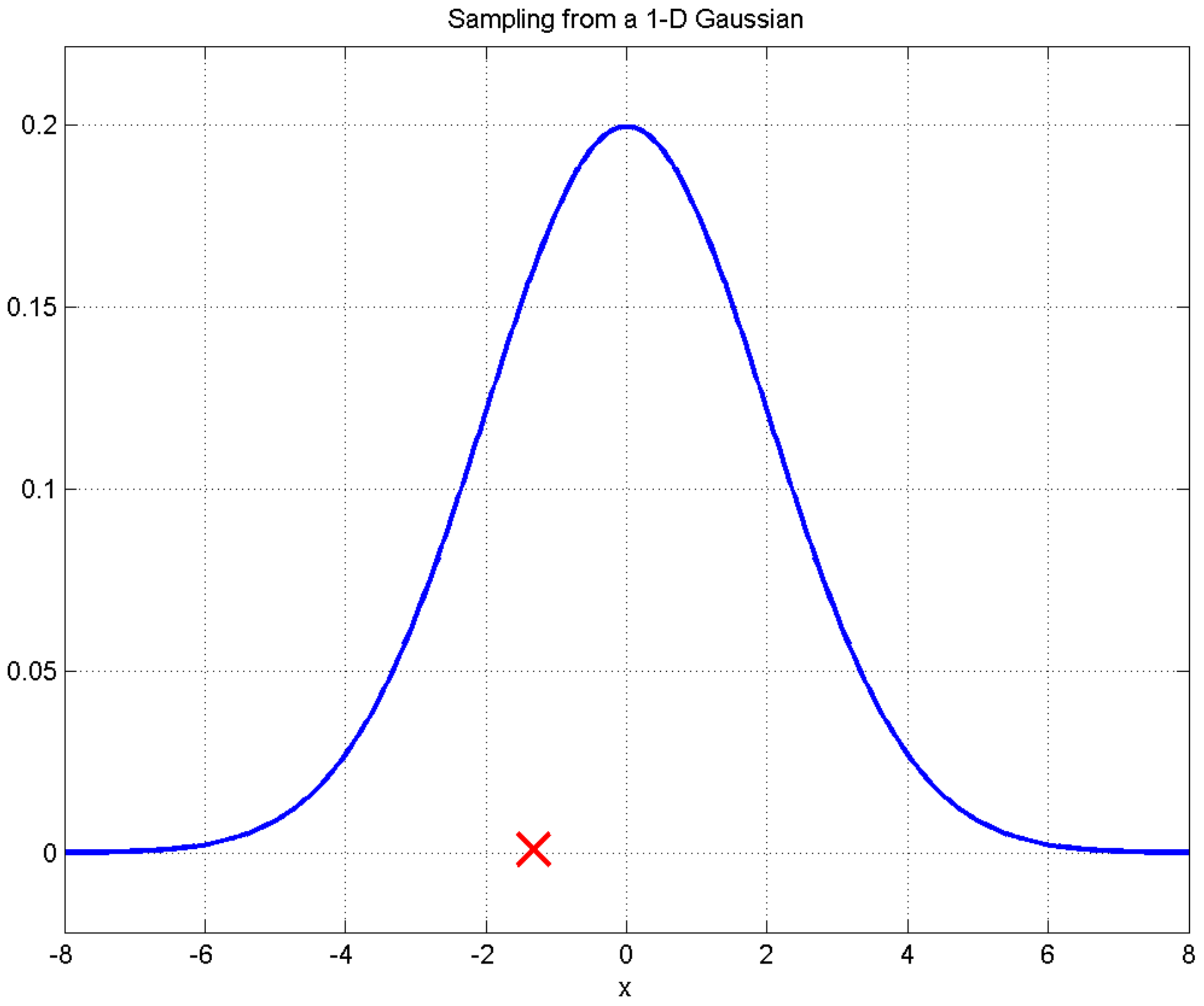





Interpolation
Extrapolation
Prior samples
prior_samp_0
prior_samp_1
prior_samp_2
prior_samp_3
prior_samp_4
Posterior samples
post_sample_0
post_sample_1
post_sample_2
post_sample_3
post_sample_4

Introducing Gaussian Processes:

- A Gaussian distribution depends on a mean and a covariance matrix.
- A Gaussian process depends on a mean and a covariance function.


Sampling from a 1-D Gaussian
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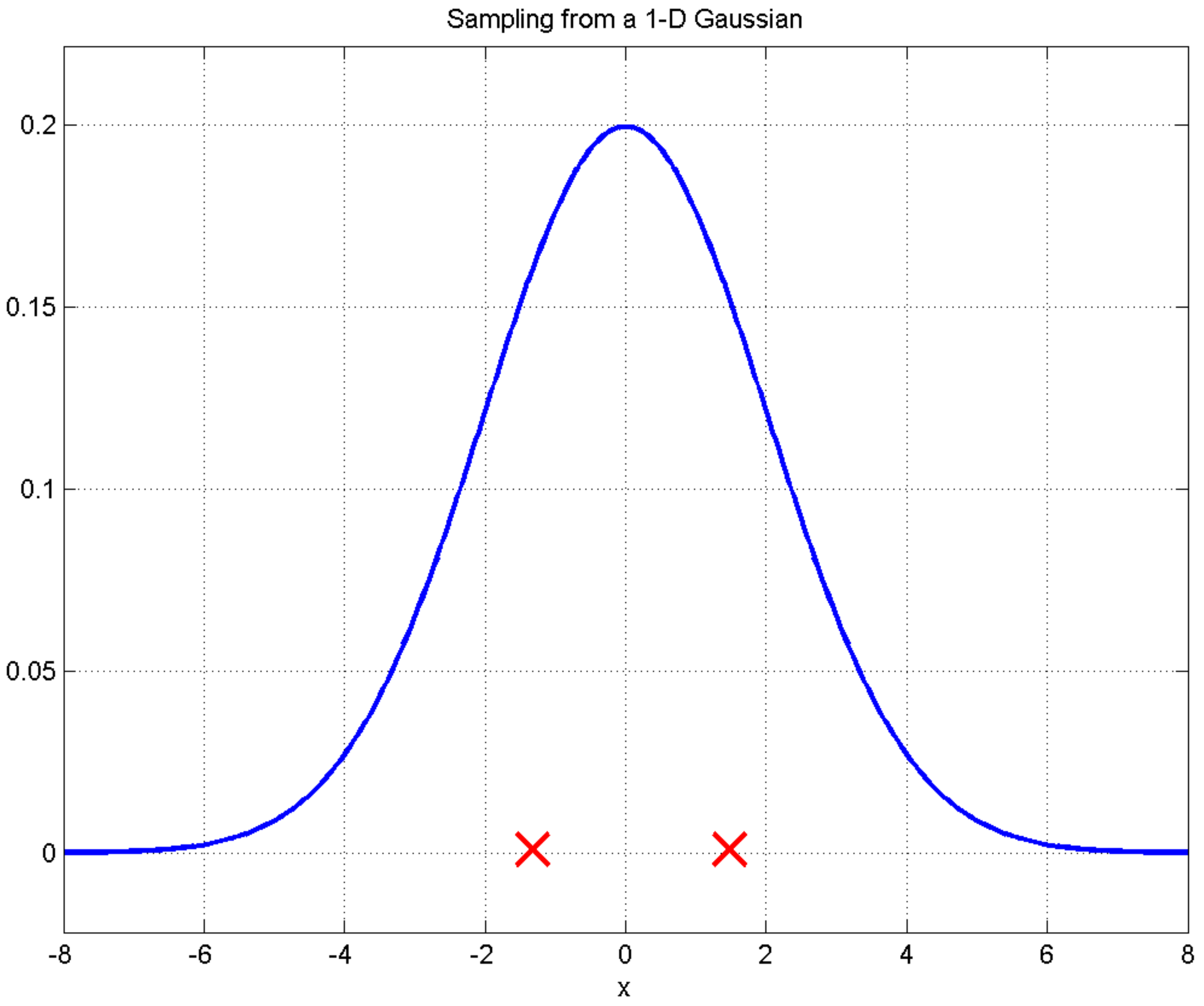
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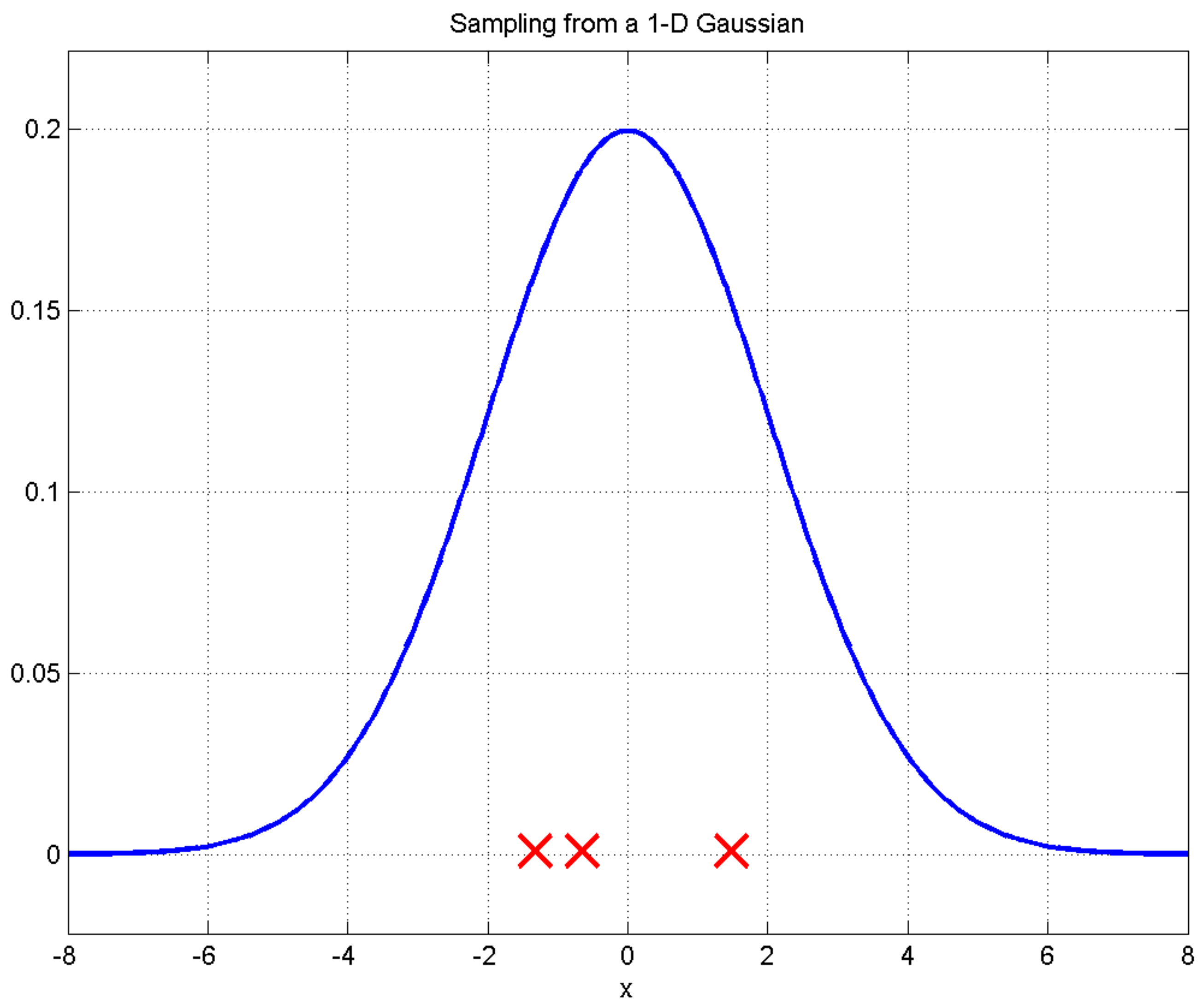
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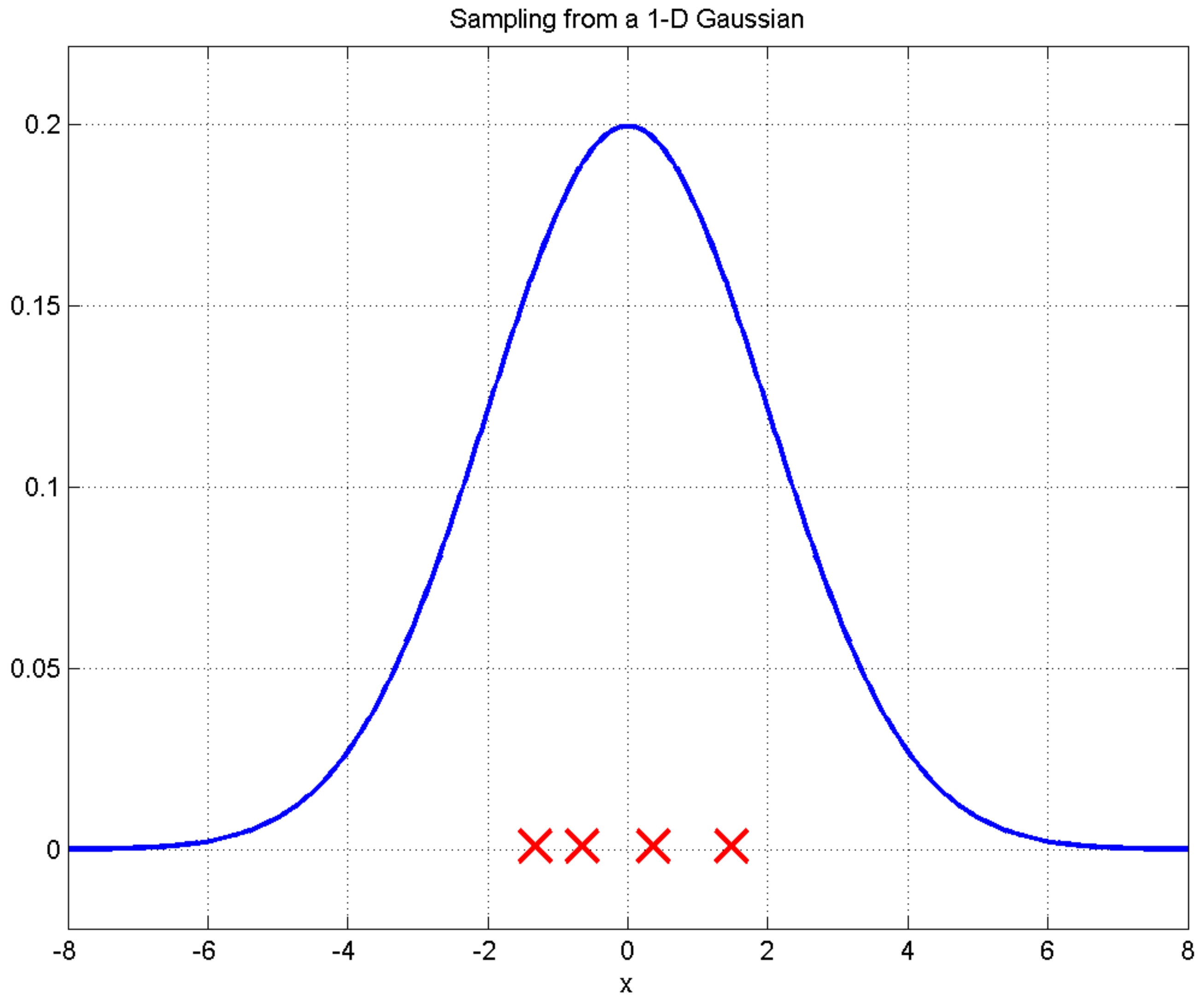
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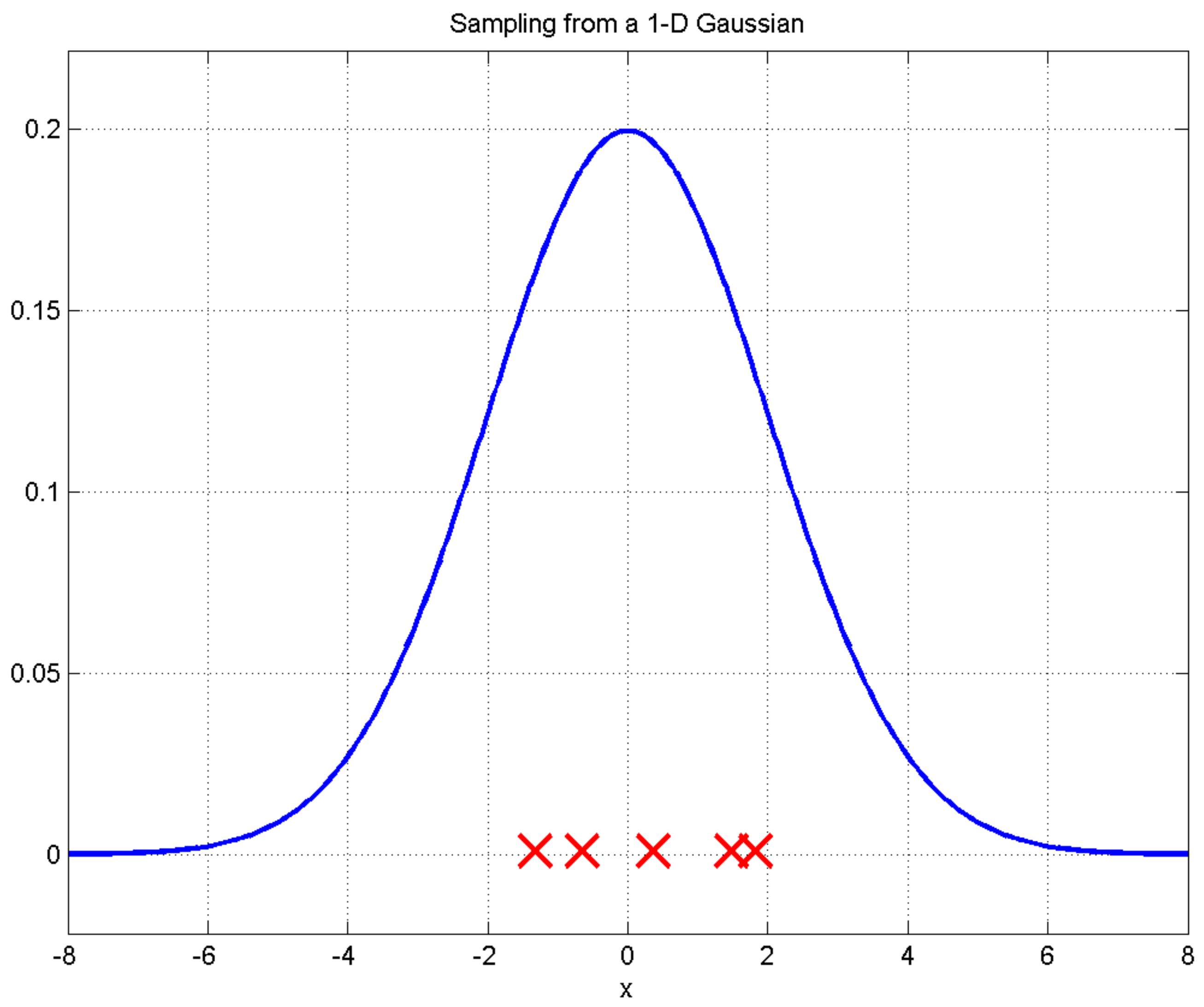

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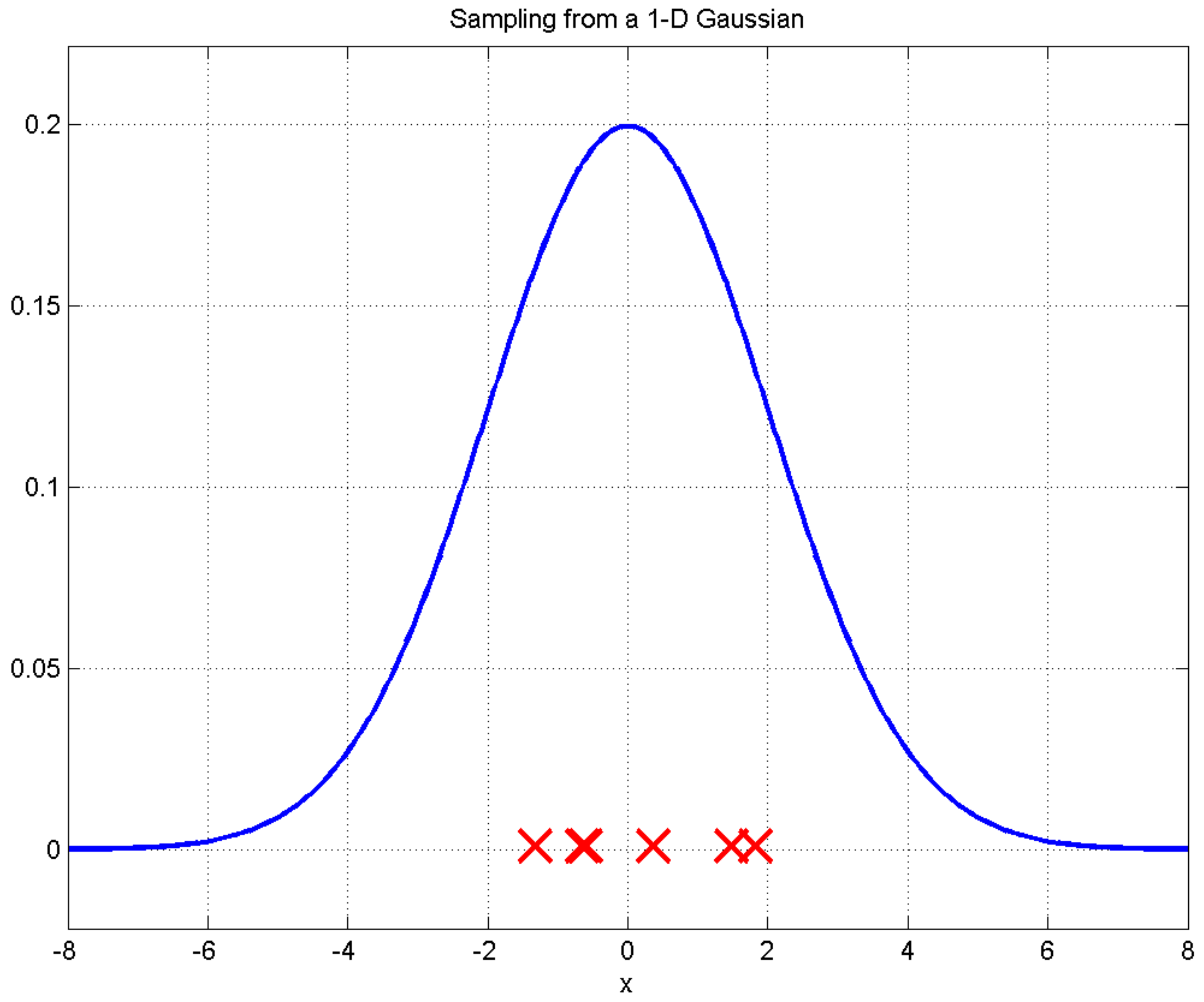
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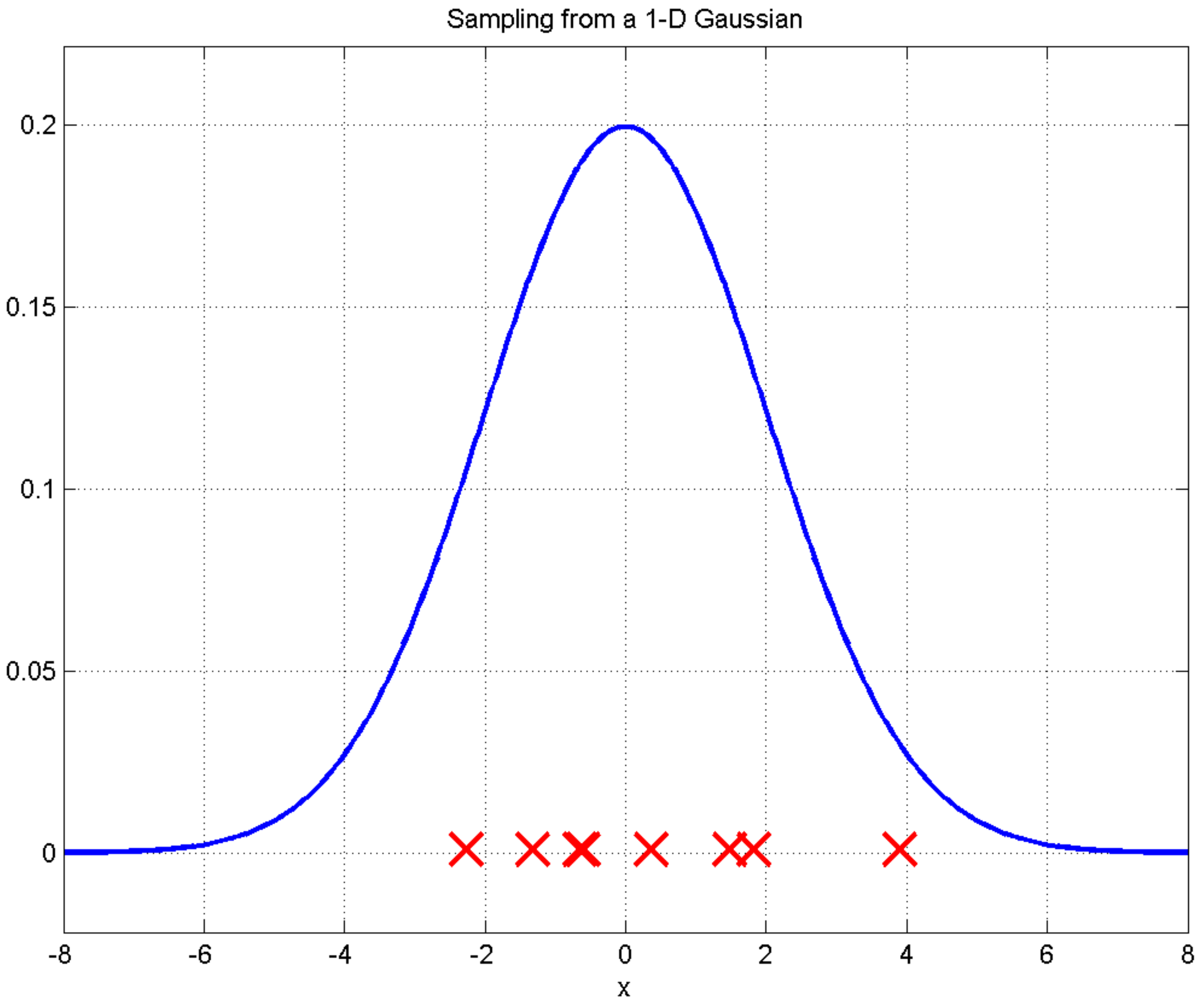

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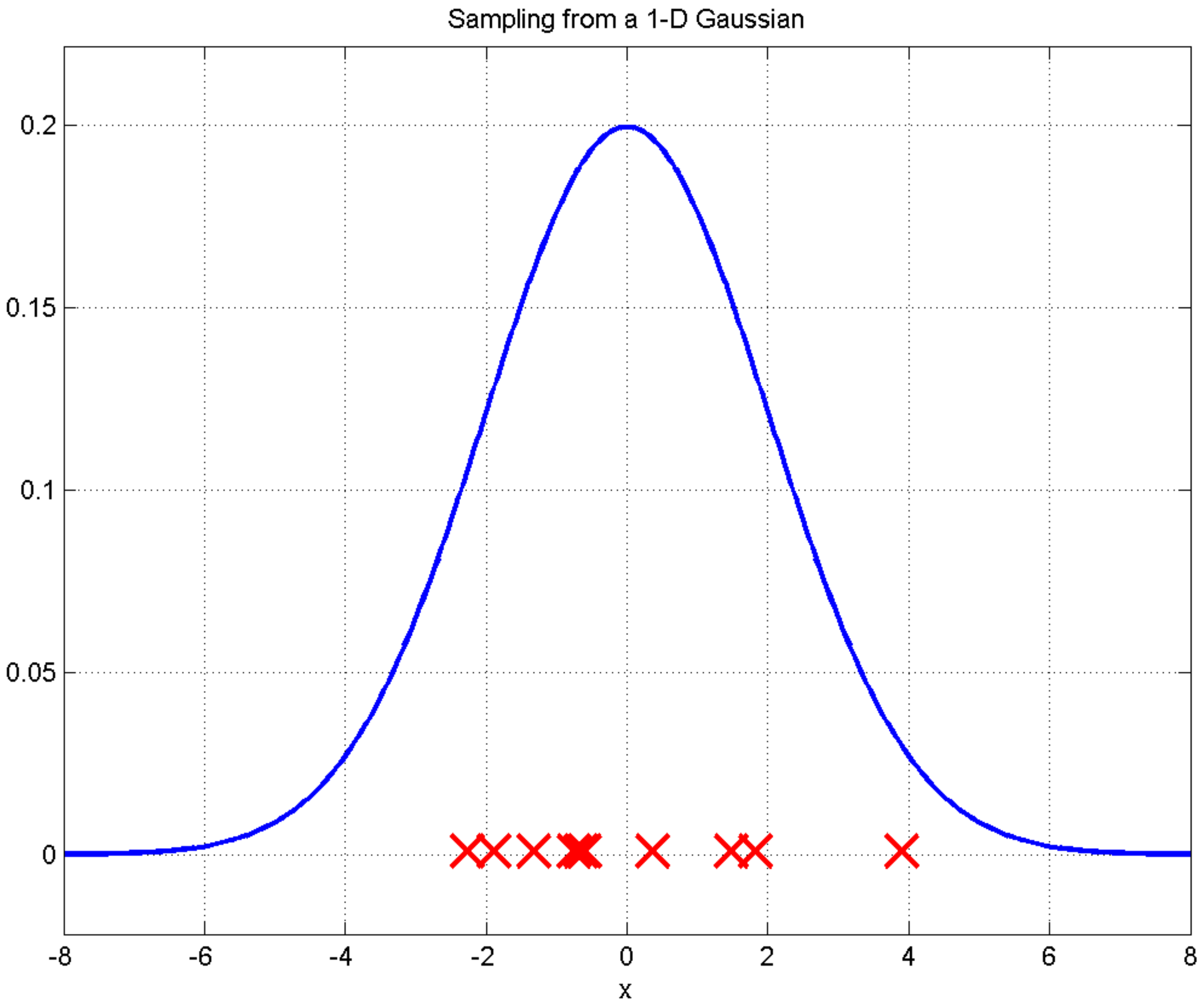
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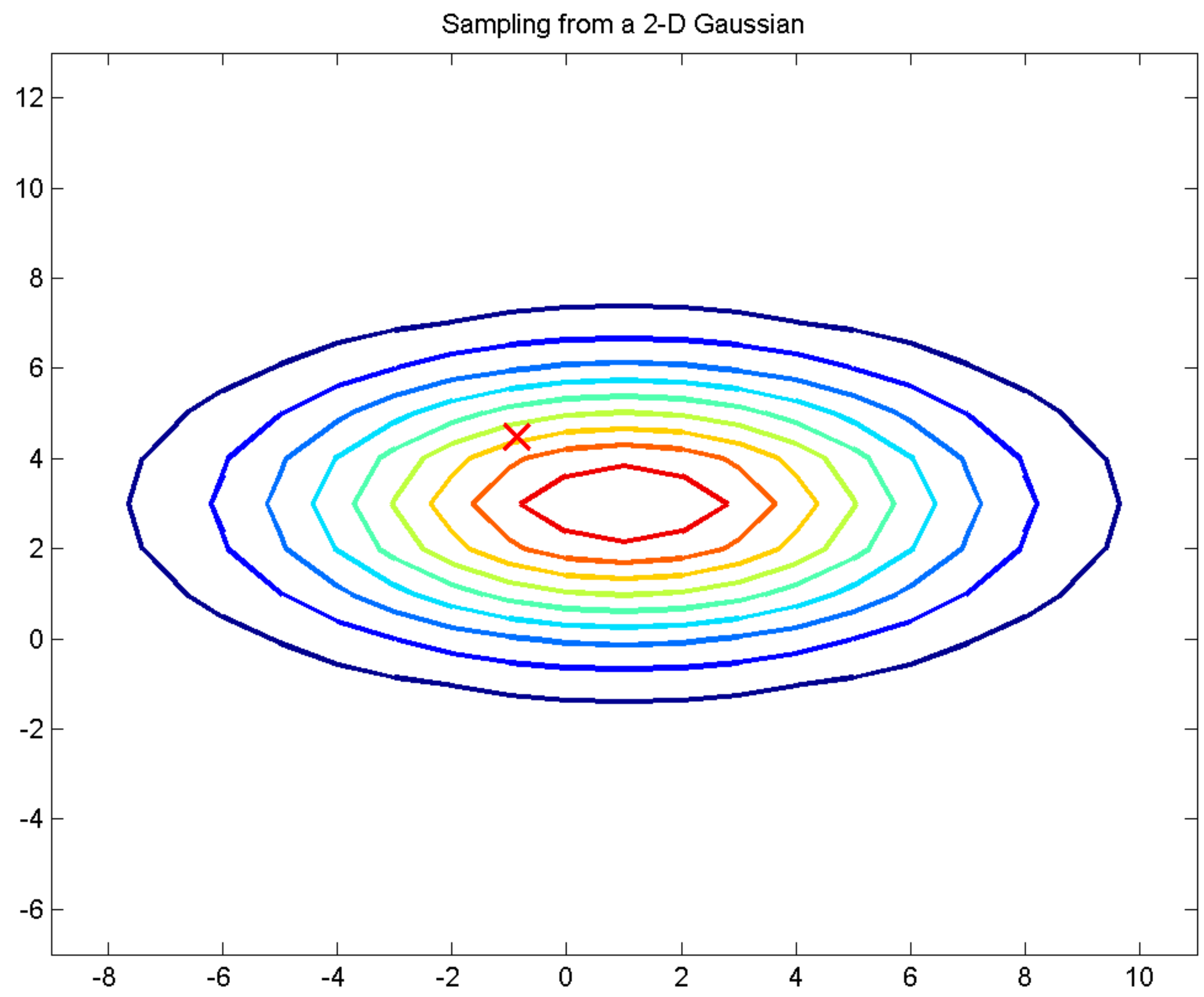
Sampling from a 2-D Gaussian
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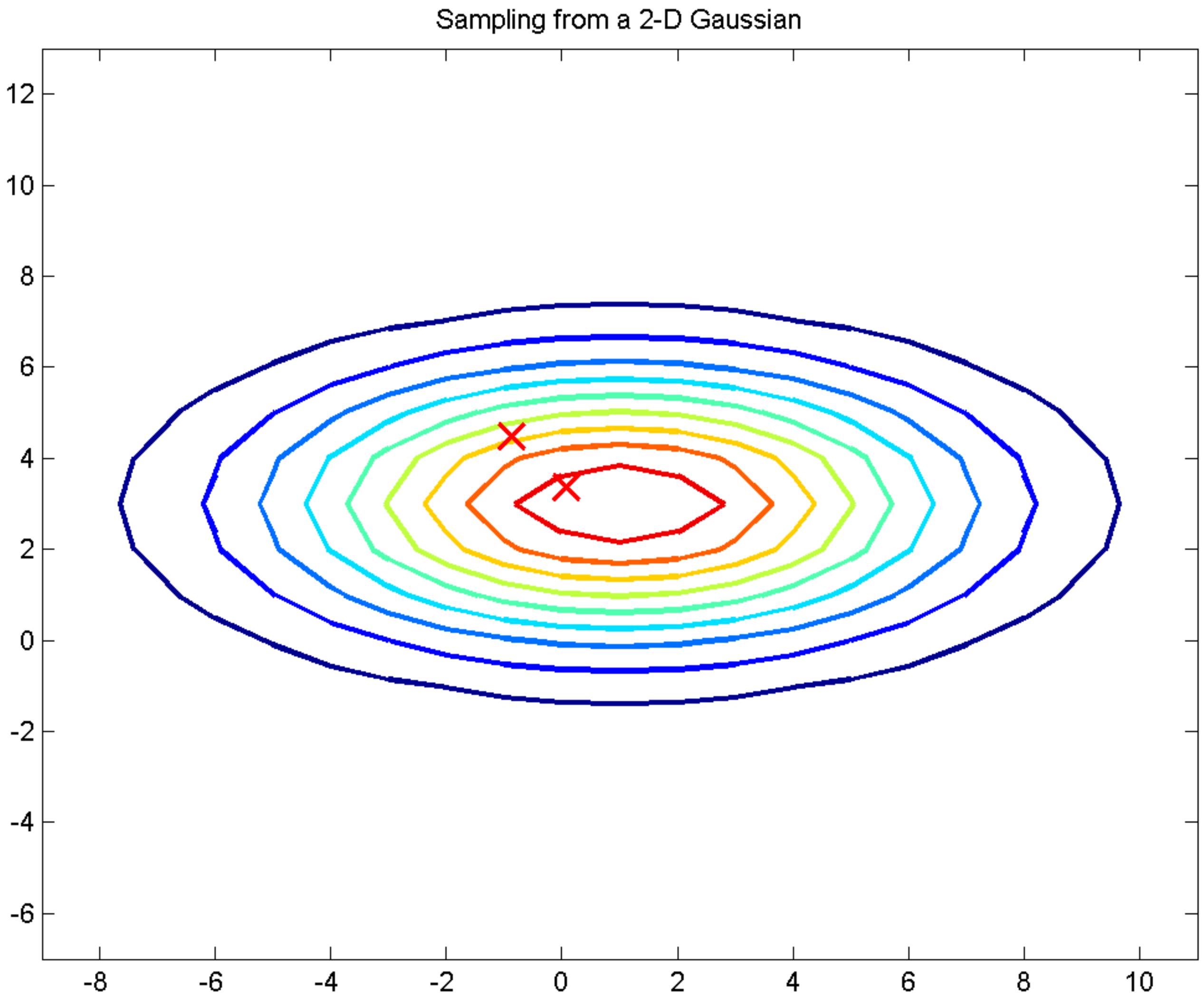
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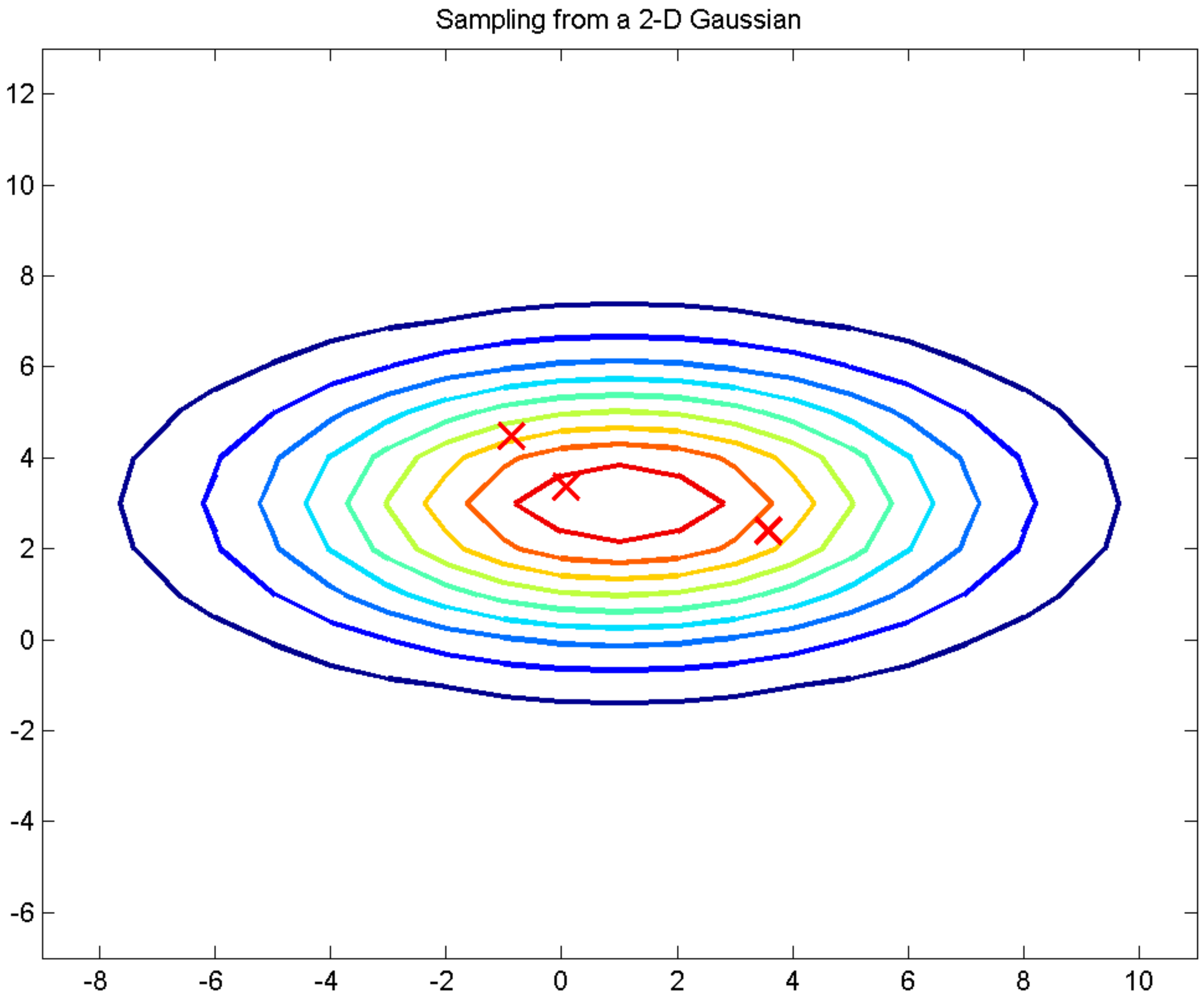
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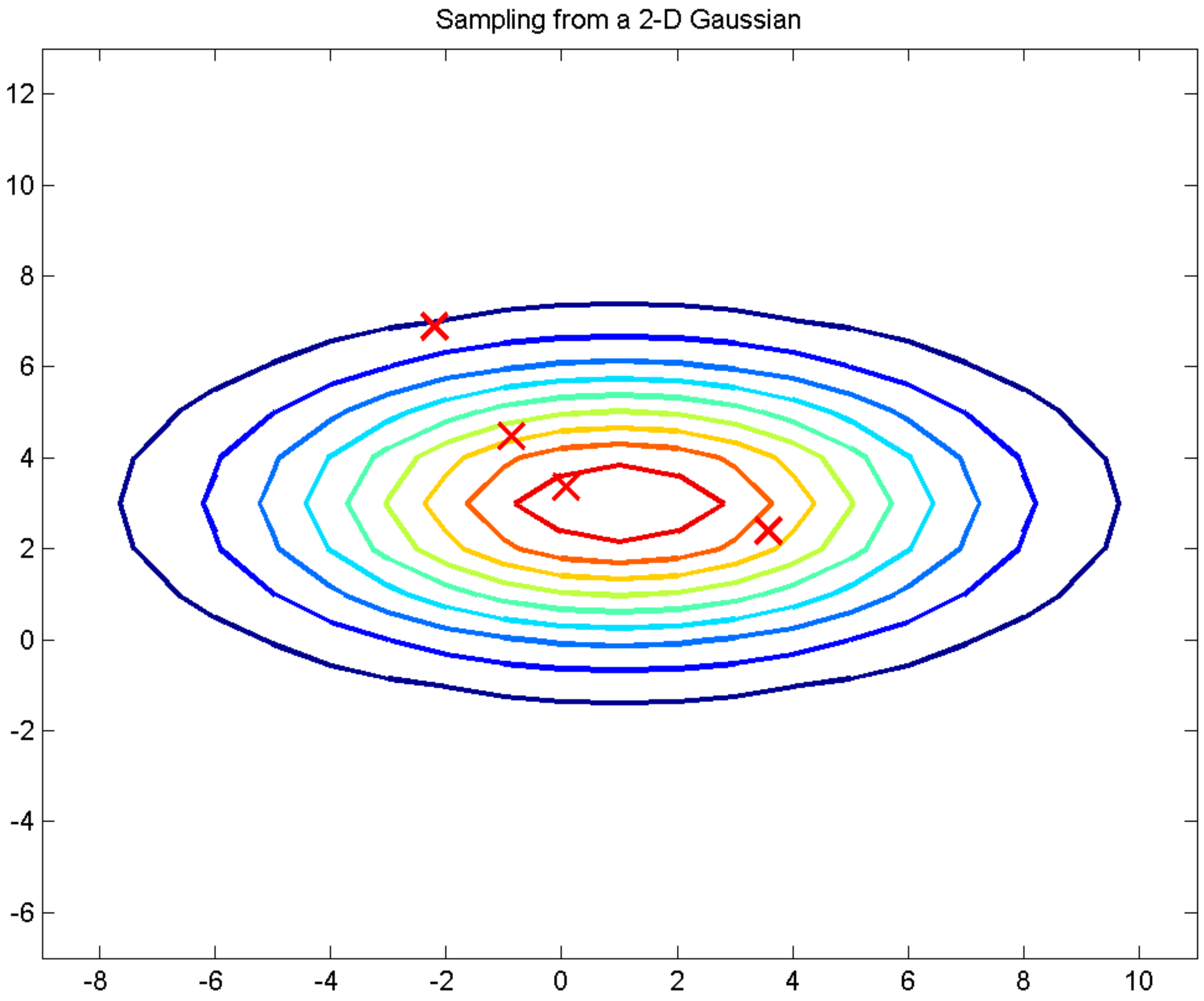
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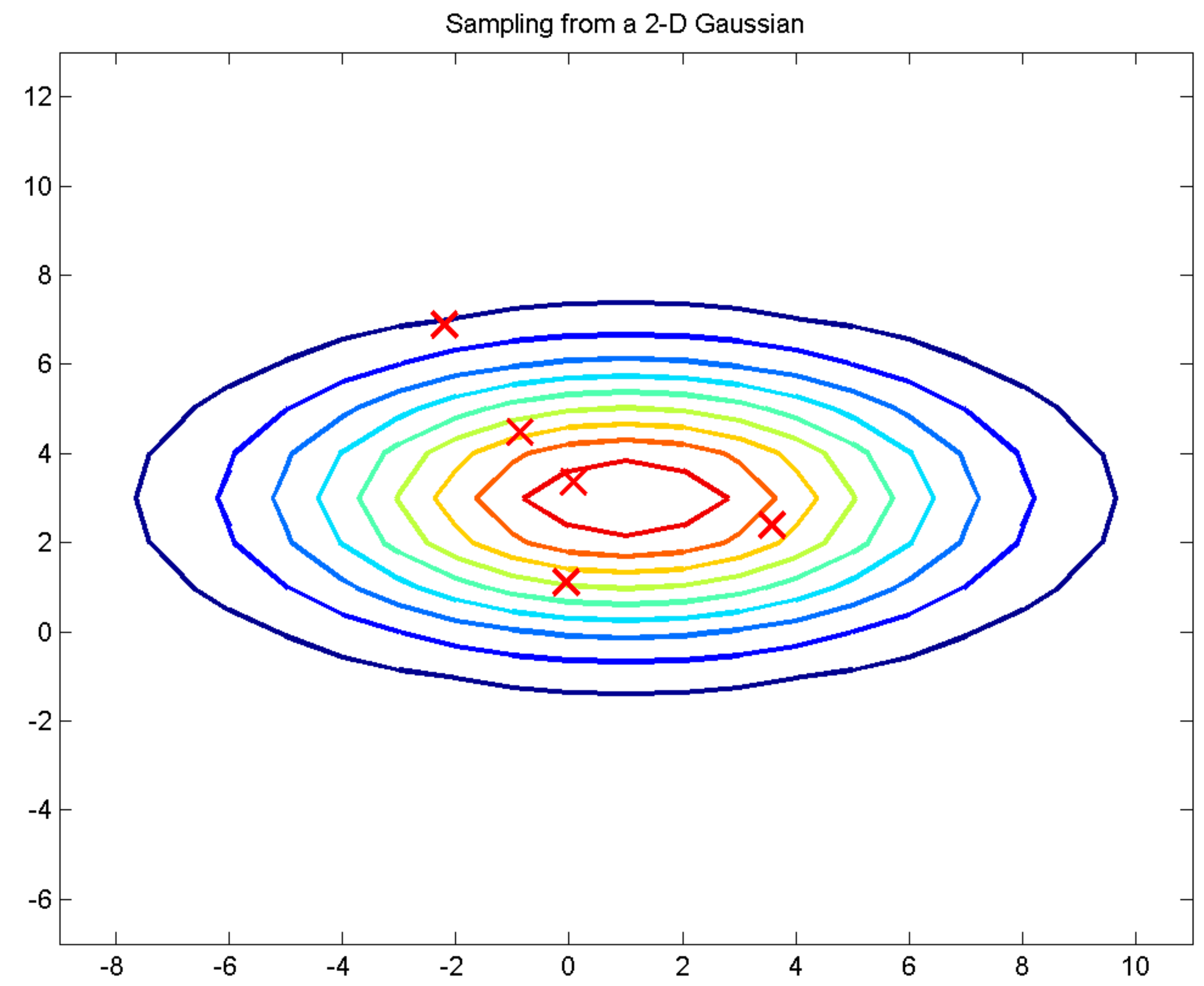
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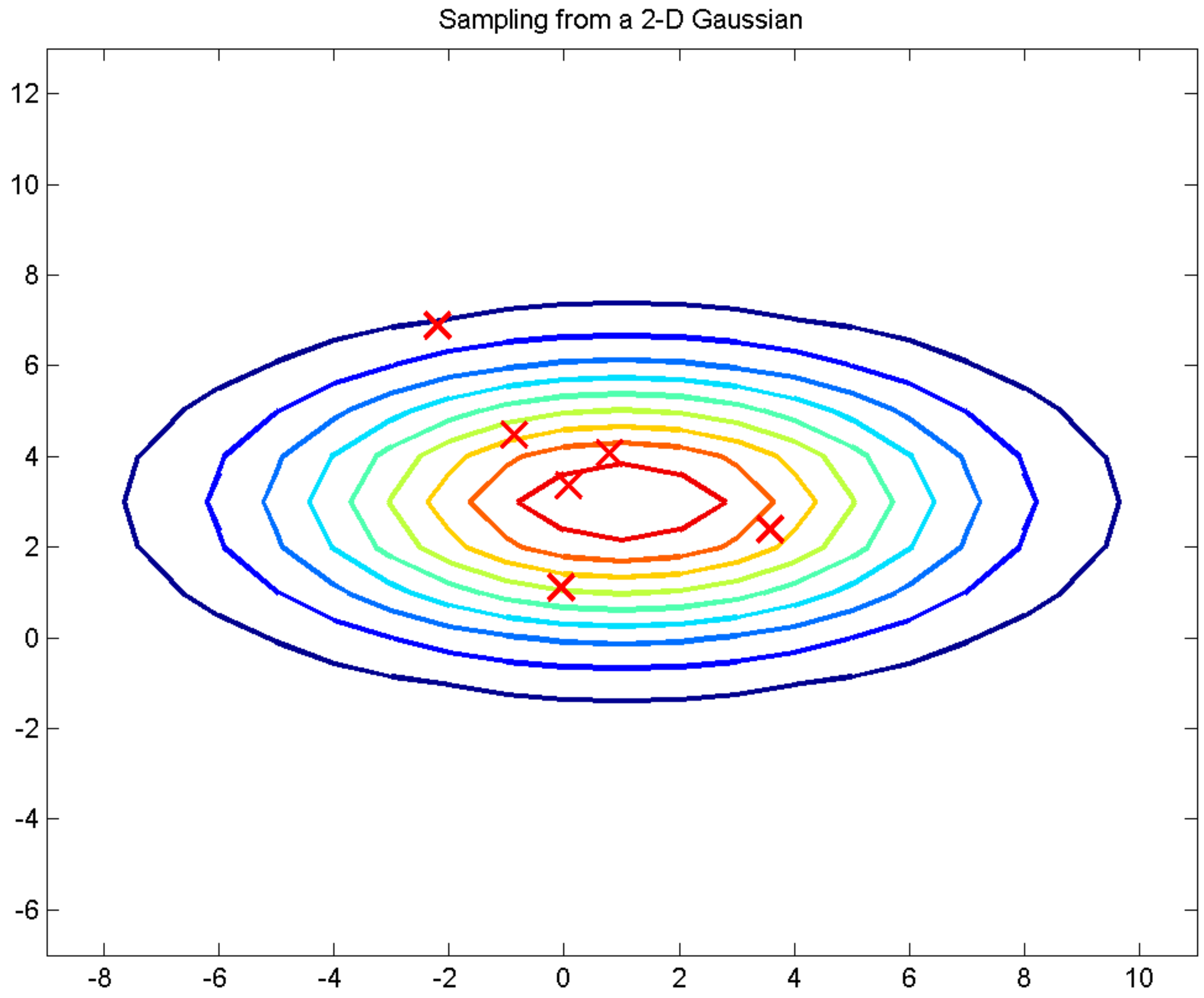

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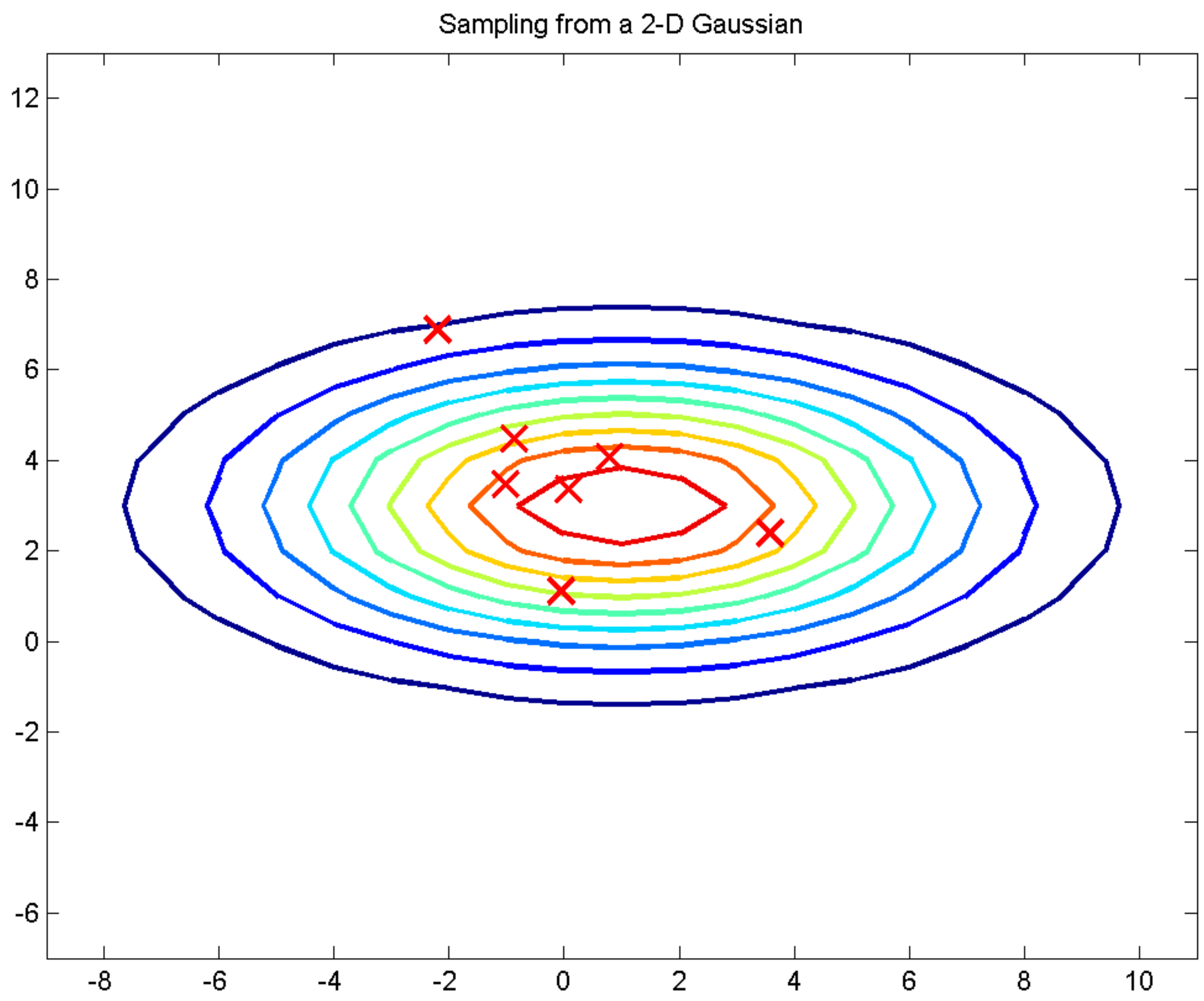
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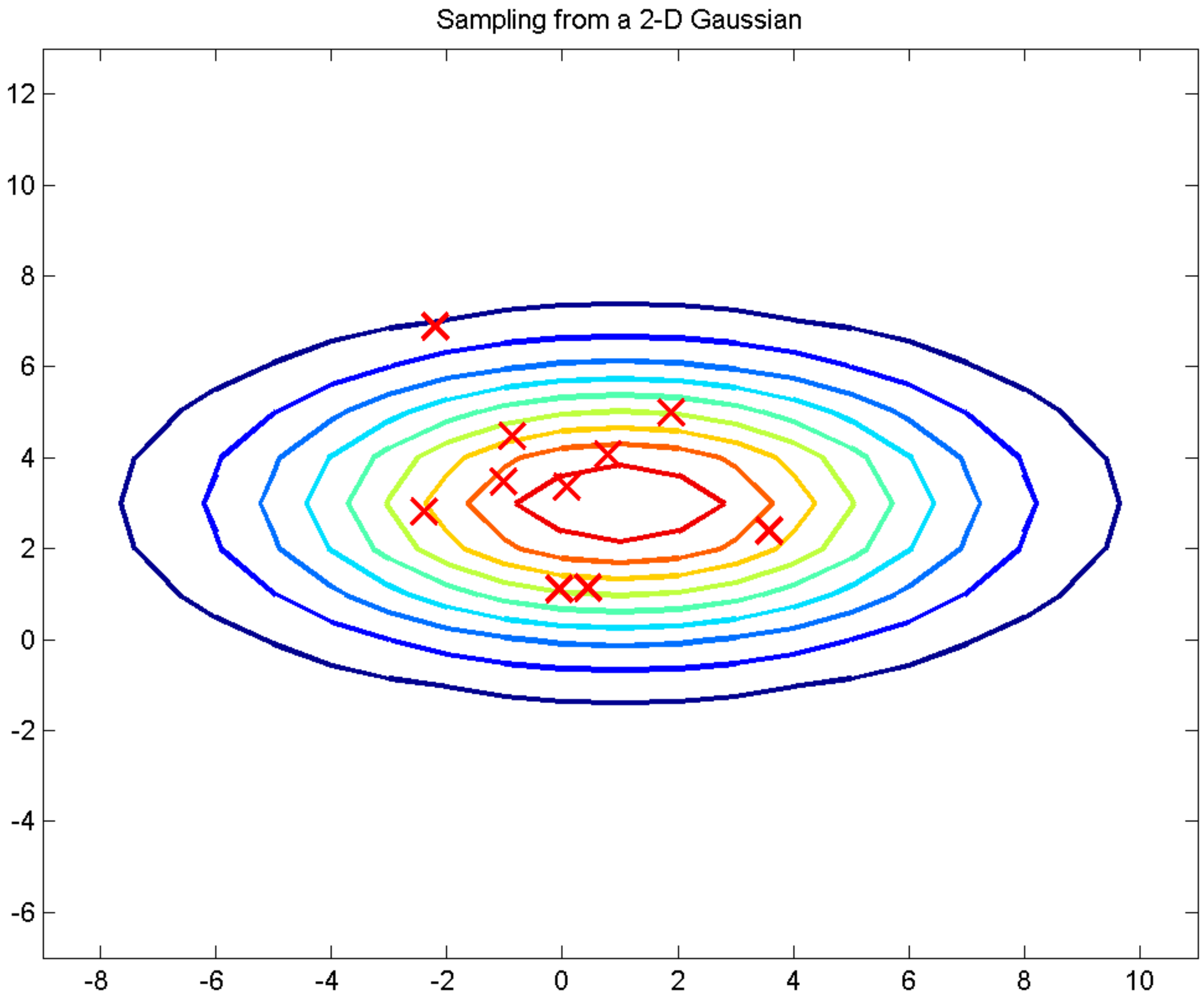
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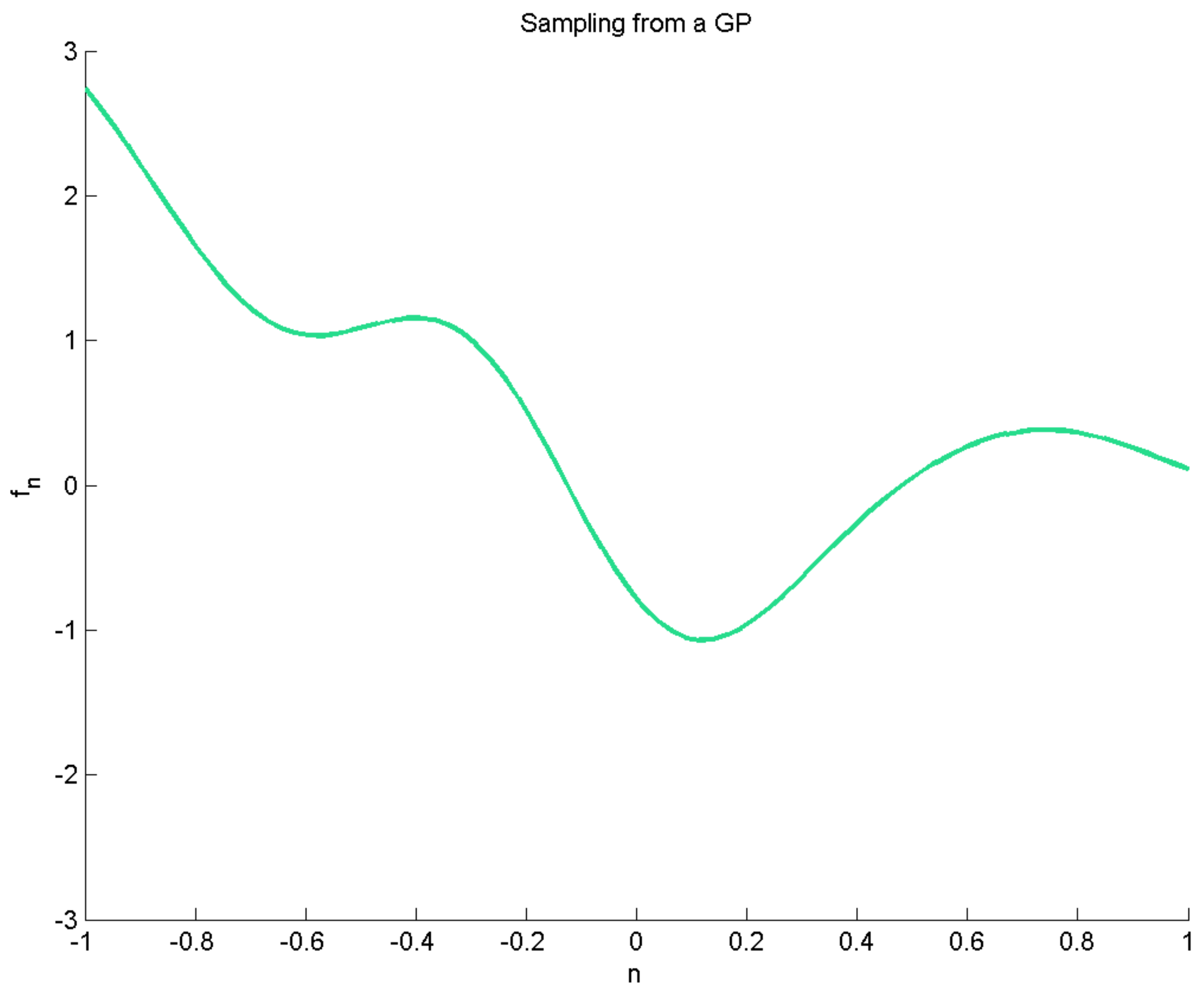

Sampling from a GP
3
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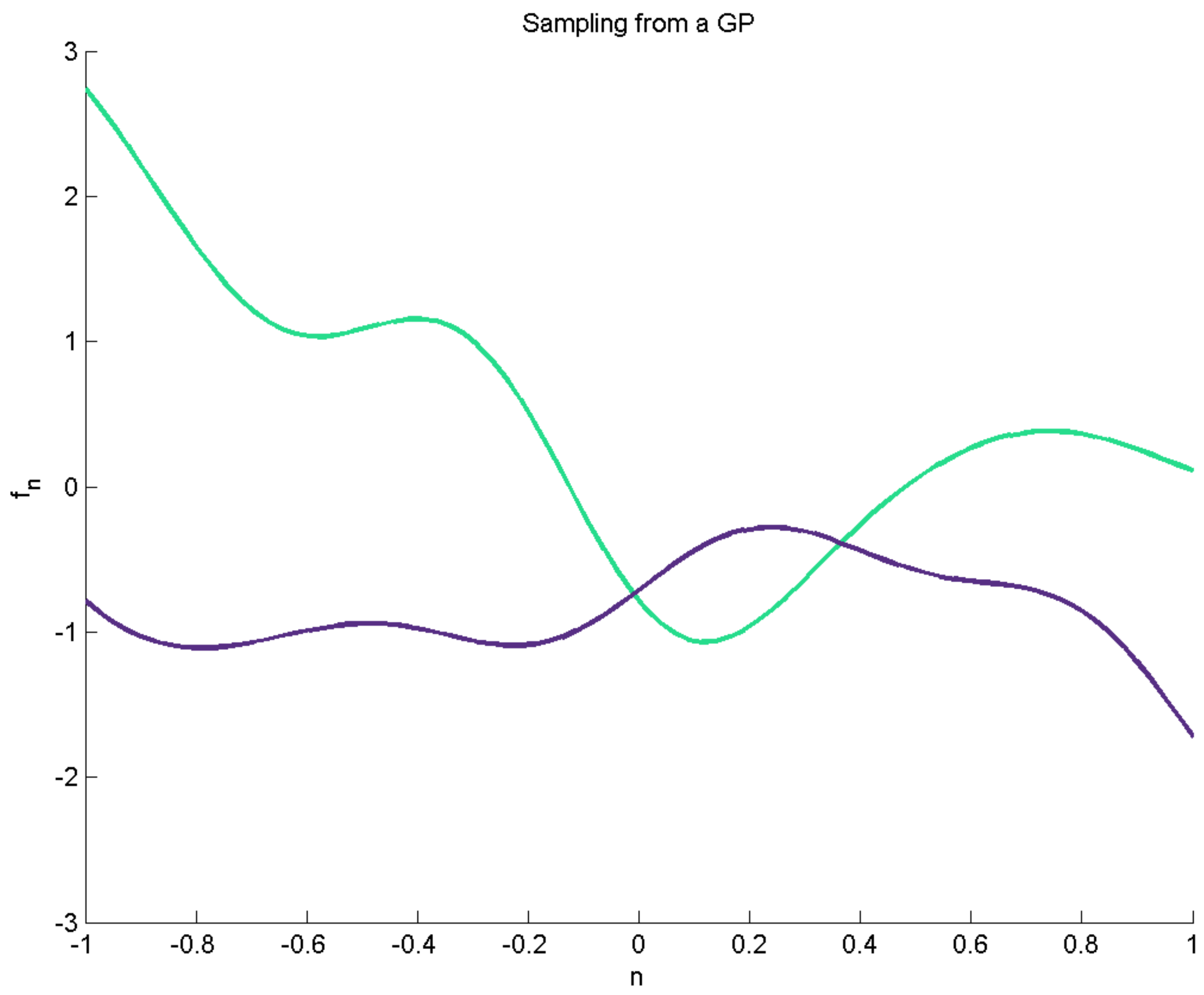
1
0
-1
-2
-3
f_n
-1
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
1
n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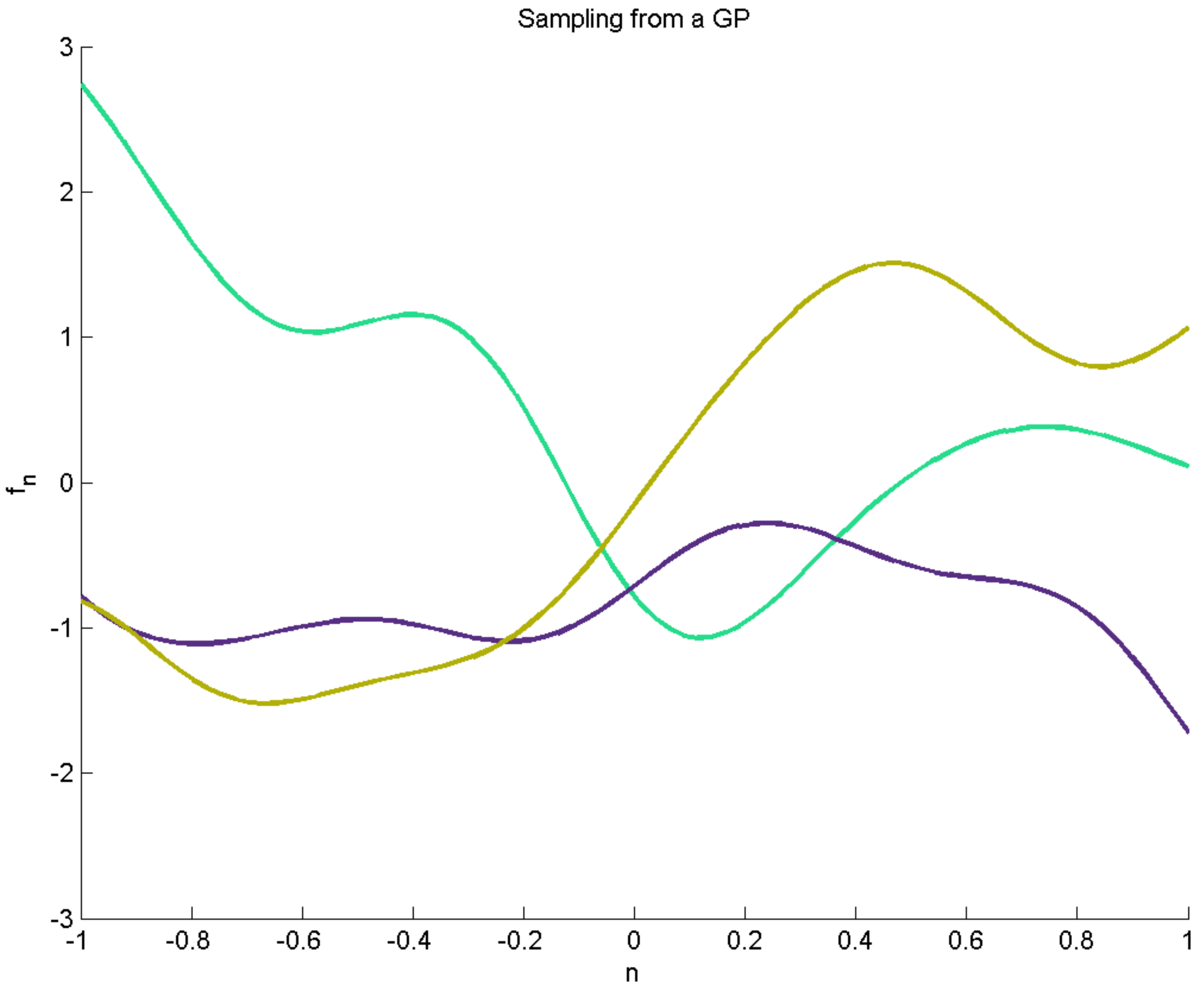
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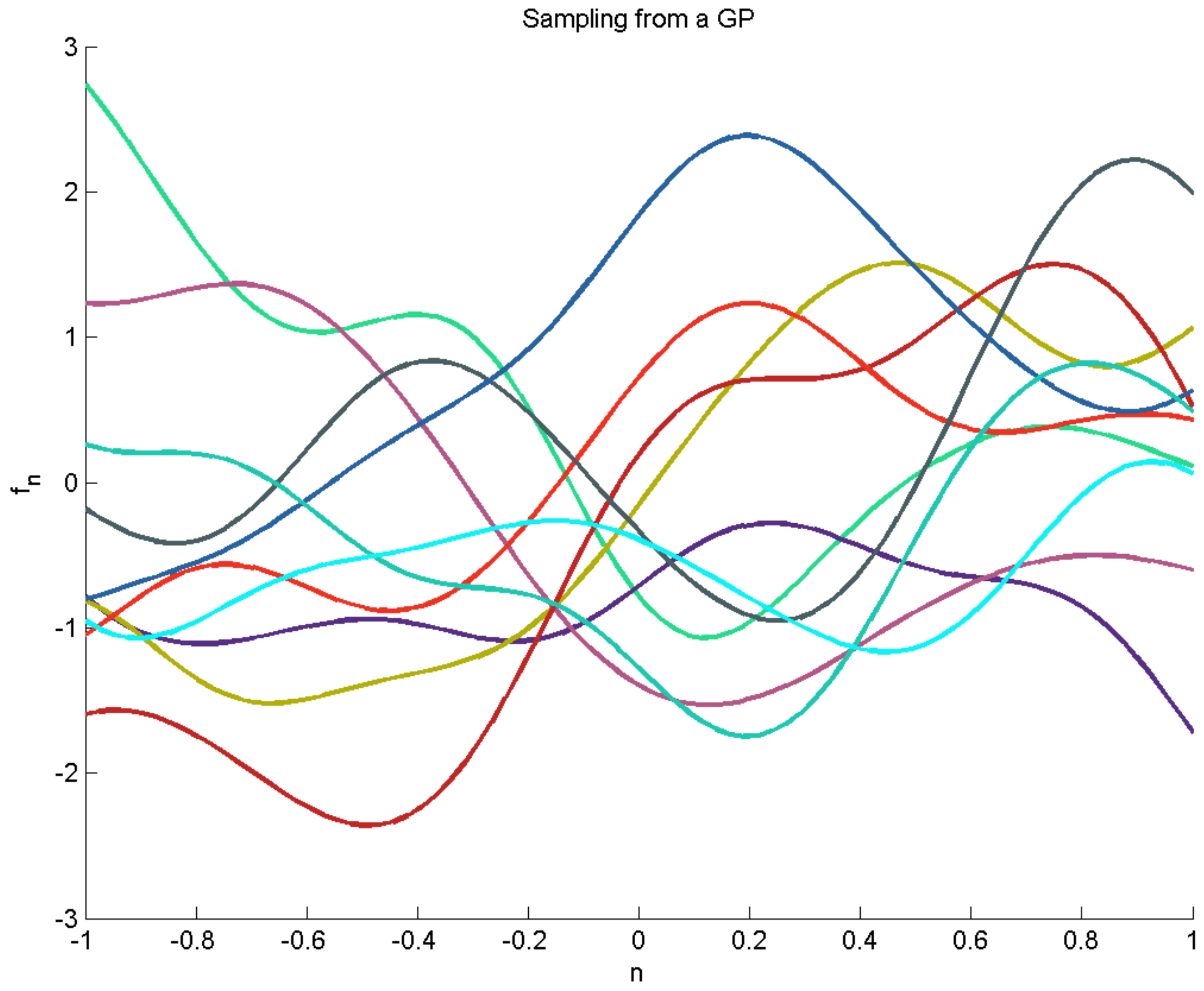
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0.8
1
n

Infinite model... but we *always* work with finite sets!

Let's start with a multivariate Gaussian:

$$p(\underbrace{f_1, f_2, \cdots, f_s}_{\mathbf{f}_A}, \underbrace{f_{s+1}, f_{s+2}, \cdots, f_N}_{\mathbf{f}_B}) \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{K}).$$

with:

$$\boldsymbol{\mu} = \begin{bmatrix} \boldsymbol{\mu}_A \\ \boldsymbol{\mu}_B \end{bmatrix} \text{ and } \mathbf{K} = \begin{bmatrix} \mathbf{K}_{AA} & \mathbf{K}_{AB} \\ \mathbf{K}_{BA} & \mathbf{K}_{BB} \end{bmatrix}$$

Marginalisation property:

$$p(\mathbf{f}_A, \mathbf{f}_B) \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{K}). \quad \text{Then:}$$

$$p(\mathbf{f}_A) = \int_{\mathbf{f}_B} p(\mathbf{f}_A, \mathbf{f}_B) d\mathbf{f}_B = \mathcal{N}(\boldsymbol{\mu}_A, \mathbf{K}_{AA})$$

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Infinite model... but we *always* work with finite sets!

In the GP context $\mathbf{f} = f(x)$:

$$\boldsymbol{\mu}_{\infty} = \begin{bmatrix} \boldsymbol{\mu}_{\mathbf{f}} \\ \cdots \\ \cdots \end{bmatrix} \quad \text{and} \quad \mathbf{K}_{\infty} = \begin{bmatrix} \mathbf{K}_{\mathbf{ff}} & \cdots \\ \cdots & \cdots \end{bmatrix}$$

Infinite model... but we *always* work with finite sets!

In the GP context $\mathbf{f} = f(x)$:

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Covariance function: Maps locations x_i, x_j of the input domain $\mathcal{X}$ to an entry in the covariance matrix:

$$\mathbf{K}_{i,j} = k(\mathbf{x}_i, \mathbf{x}_j)$$

For all available inputs:

$$\mathbf{K} = \mathbf{K}_\mathbf{ff} = k(\mathbf{X}, \mathbf{X})$$

GP: joint Gaussian distribution of the training and the (potentially infinite!) test data:

$\mathbf{f}^* = f(\mathbf{x}^*)$

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

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$\mathbf{K}_*$ is the (cross)-covariance matrix obtained by evaluating the covariance function in pairs of training inputs $\mathbf{X}$ and test inputs $\mathbf{X}_*$, ie.

$$\mathbf{f}_* = k(\mathbf{X}, \mathbf{X}_*).$$

Similarly:

$$\mathbf{K}_{**} = k(\mathbf{X}_*, \mathbf{X}_*).$$

Posterior is also Gaussian!

$p(\mathbf{f}_A, \mathbf{f}_B) \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{K}).$ Then:

$$p(\mathbf{f}_A|\mathbf{f}_B) = \mathcal{N}(\boldsymbol{\mu}_A + \mathbf{K}_{AB}\mathbf{K}_{BB}^{-1}(\mathbf{f}_B - \boldsymbol{\mu}_B), \mathbf{K}_{AA} - \mathbf{K}_{AB}\mathbf{K}_{BB}^{-1}\mathbf{K}_{BA})$$

In the GP context this can be used for inter/extrapolation:

$$p(f_*|f_1, \cdots, f_N) = p(f(x_*)|f(x_1), \cdots, f(x_N)) \sim \mathcal{N}$$

$$p(\mathbf{f}_*|\mathbf{f_1}, \cdots, \mathbf{f_N}) = p(f(x_*)|f(x_1), \cdots, f(x_N))$$

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

$p(f(x_*)|f(x_1), \cdots, f(x_N))$ is a posterior **process**!

Posterior is also Gaussian!

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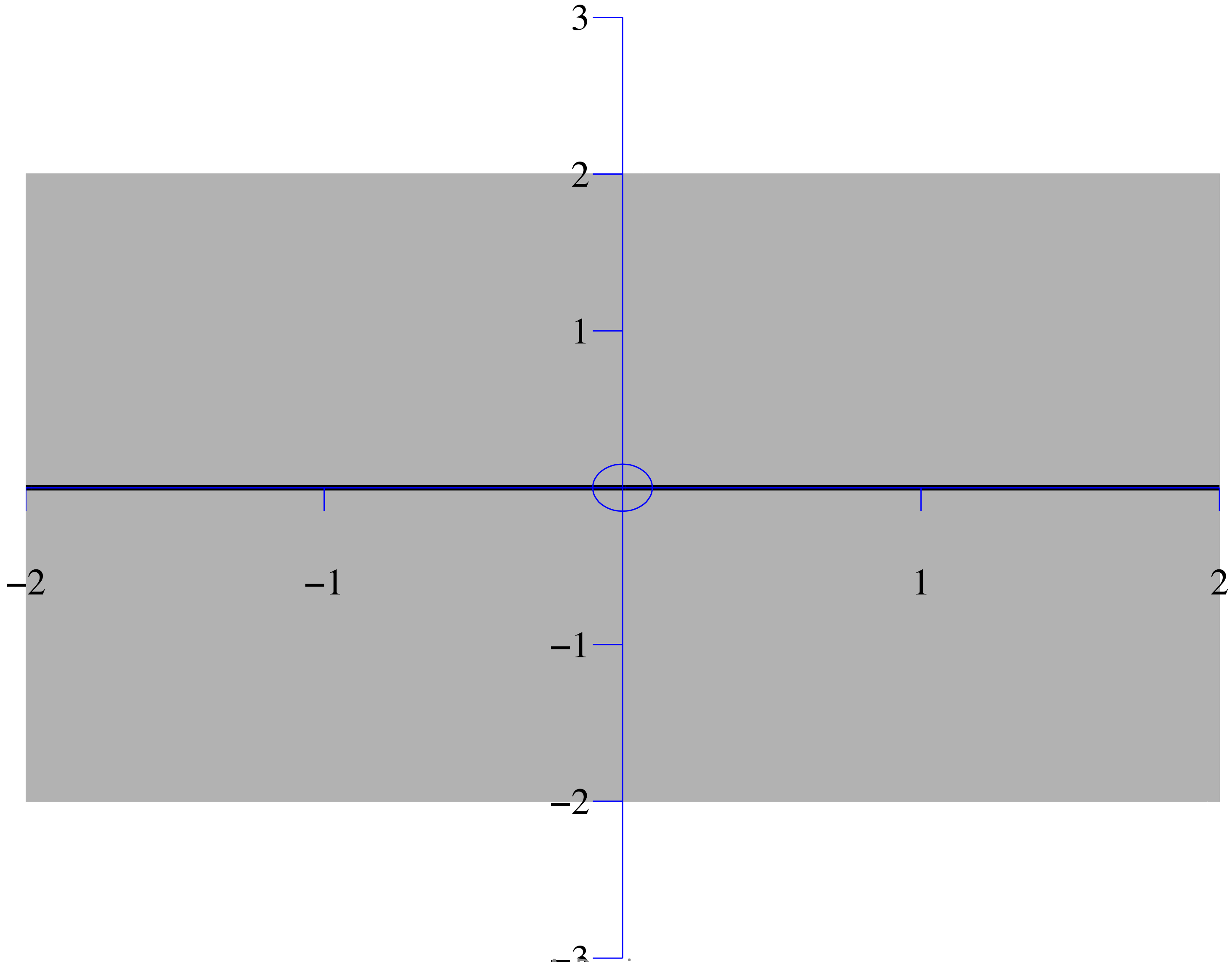
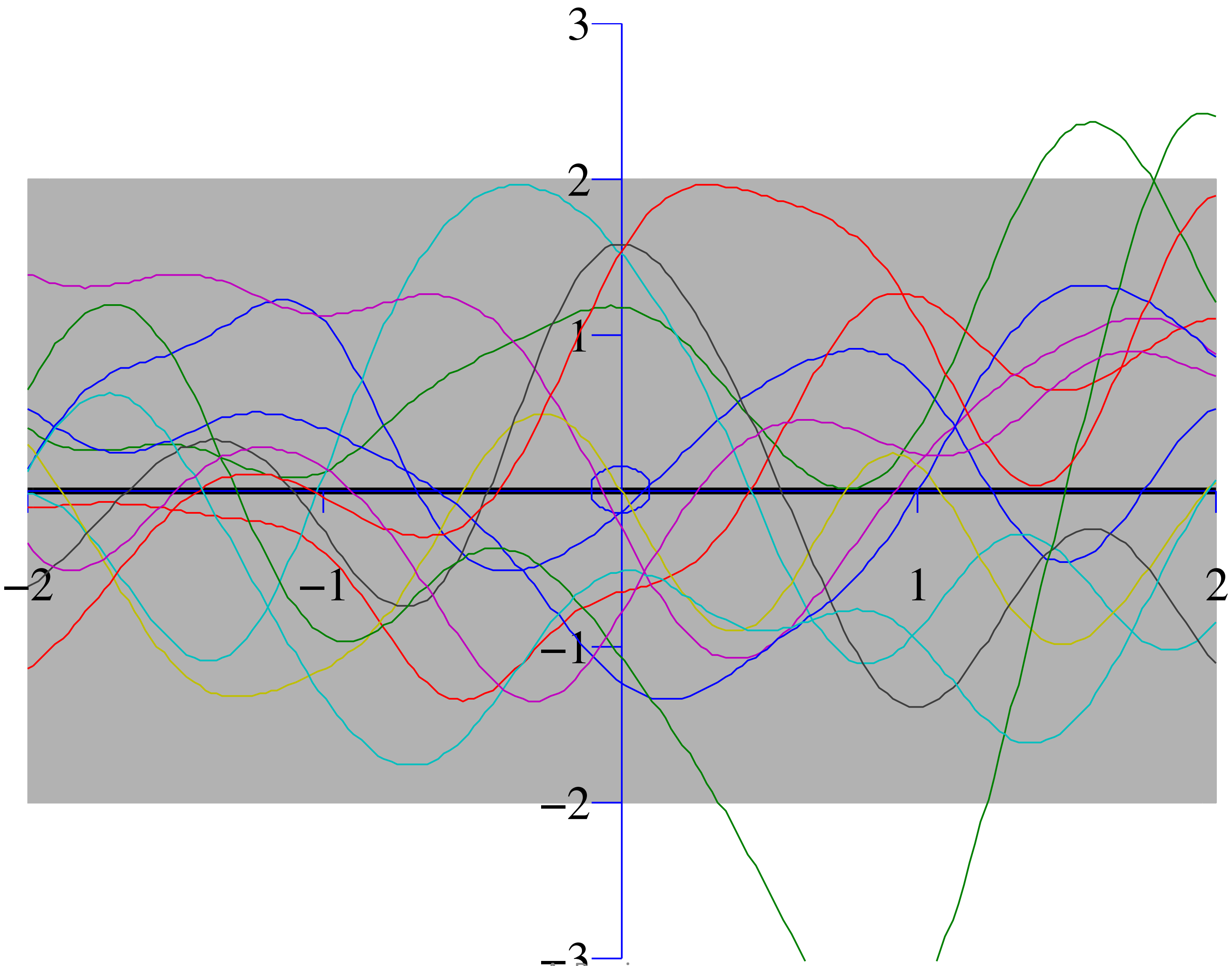
$$\begin{aligned} p(\mathbf{f}_*|\mathbf{f_1}, \cdots, \mathbf{f_N}) &= p(f(x_*)|f(x_1), \cdots, f(x_N)) \\ &\sim \mathcal{N}(\mathbf{K}_*^\top \mathbf{K}^{-1}\mathbf{f}\ ,\ \mathbf{K}_{*,*} - \mathbf{K}_*^\top \mathbf{K}^{-1}\mathbf{K}_*) \end{aligned}$$

$p(f(x_*)|f(x_1), \cdots, f(x_N))$ is a posterior **process**!

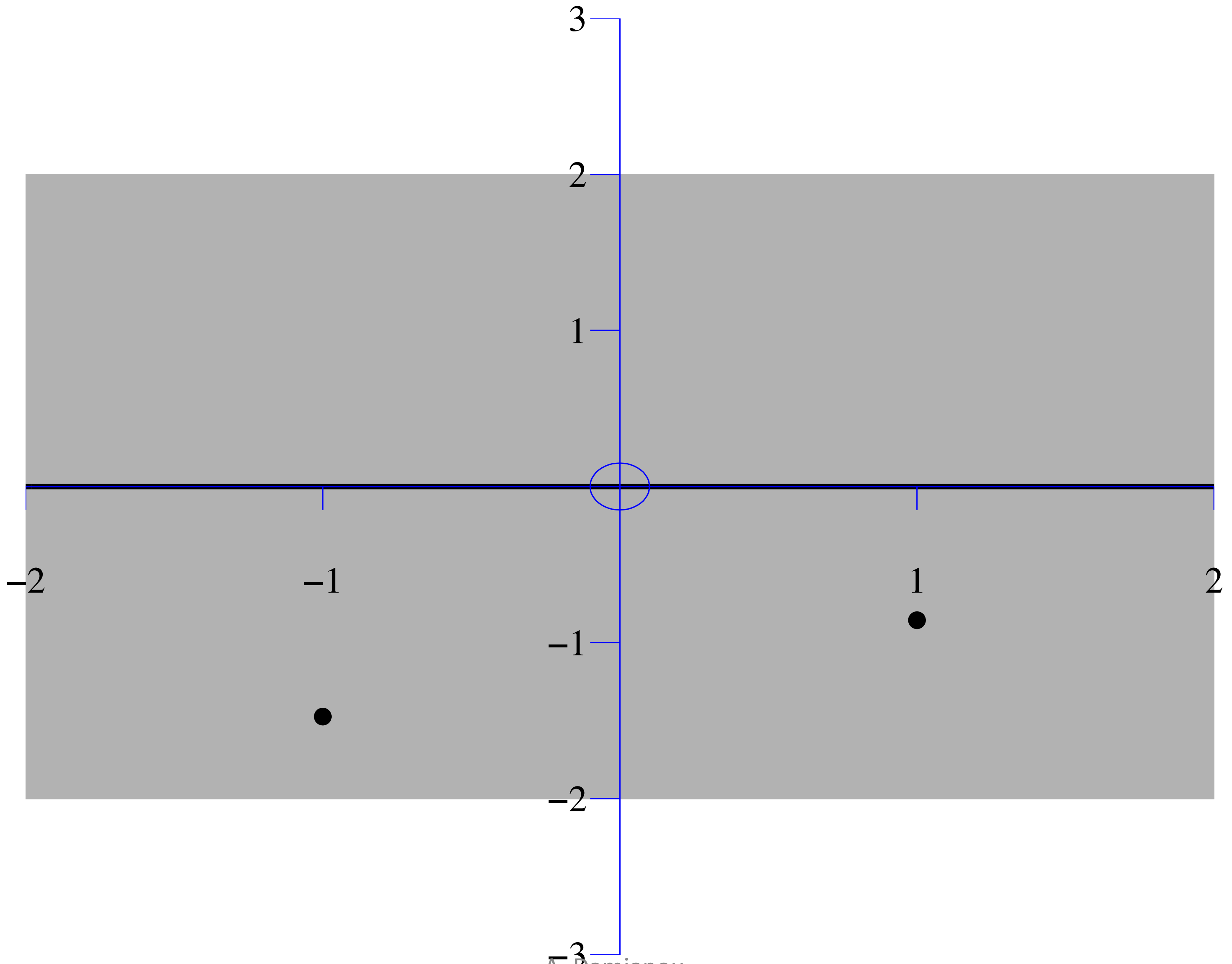
Fitting the data *(shaded area is* **uncertainty***)*



Fitting the data - Prior Samples



Fitting the data



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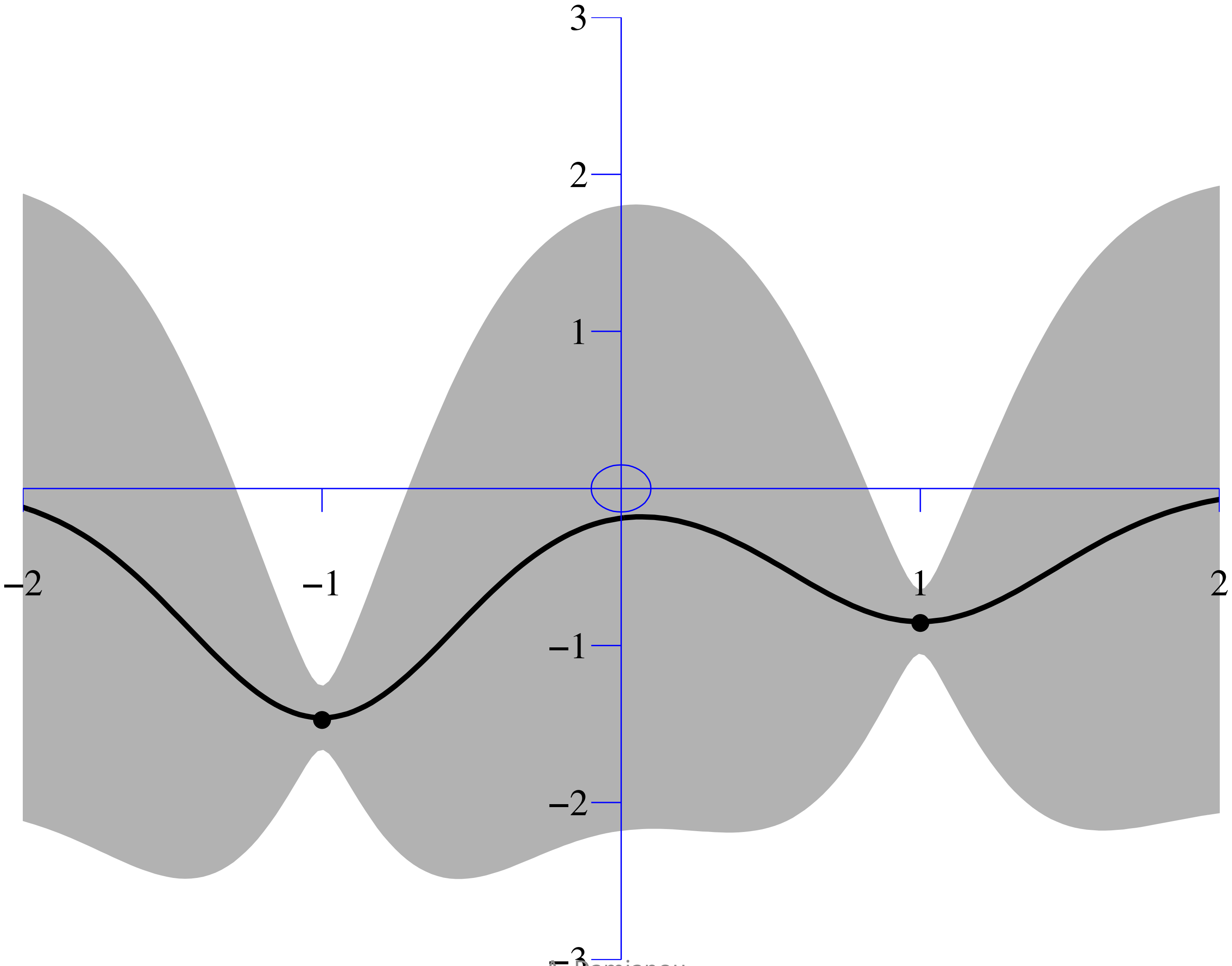
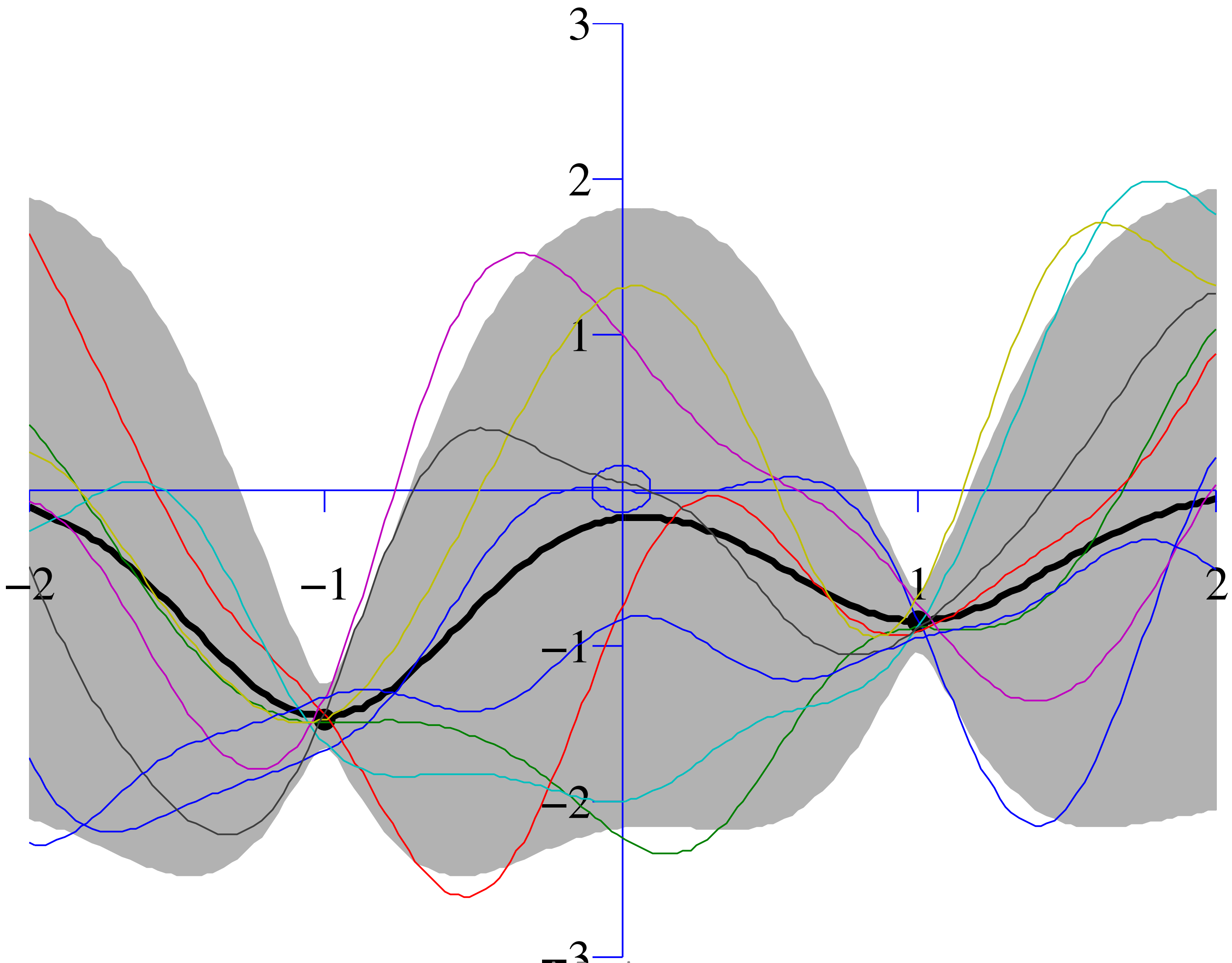


Fitting the data - Posterior samples

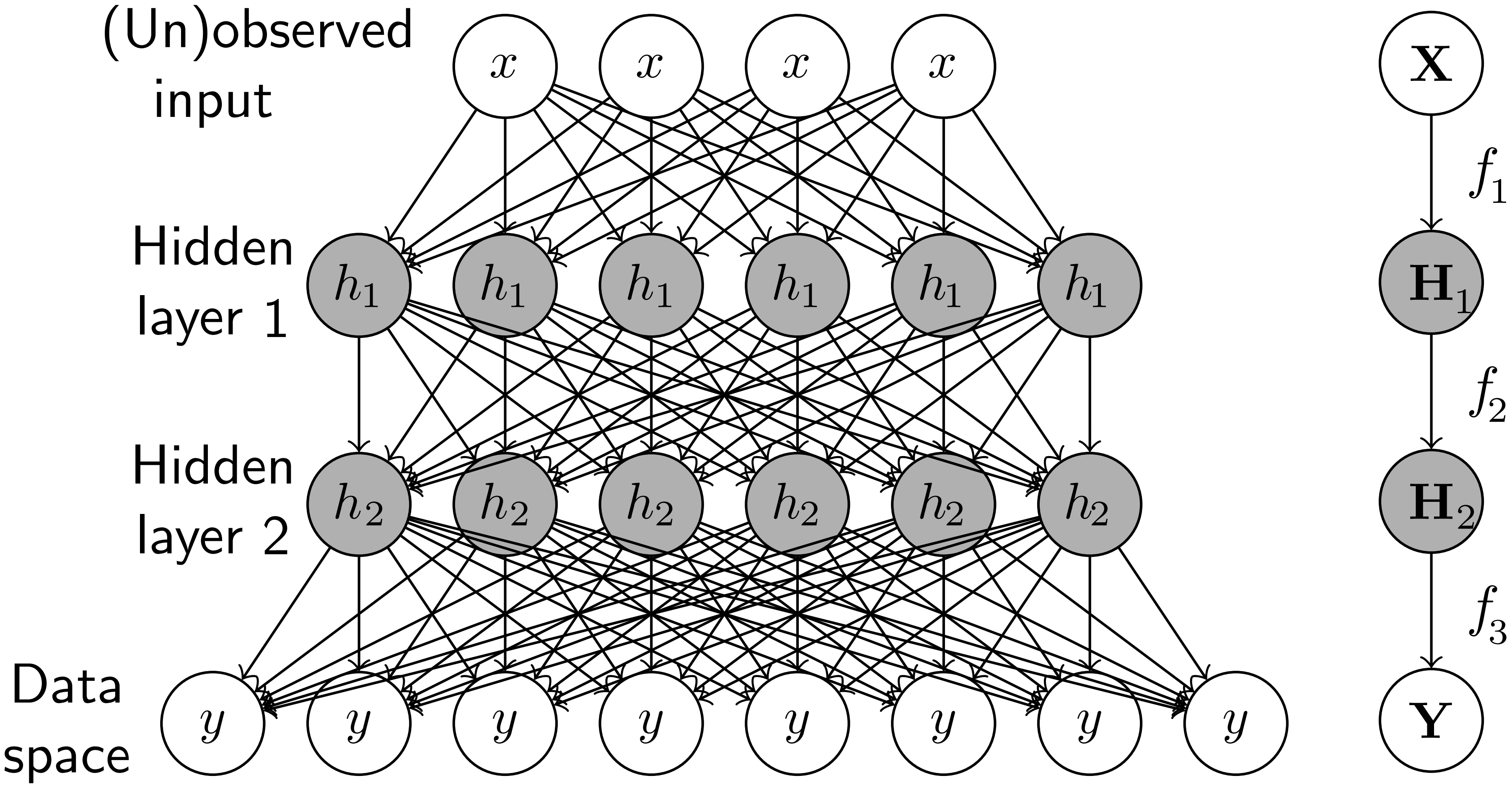


Summary – Gaussian processes

- GPs generalize Gaussian distributions to infinite dimensions (i.e. functions)
- A GP does not have parameters. We only make implicit assumptions about the properties of the functions (e.g. smoothness).
- Predictions are analytic and come with uncertainty.

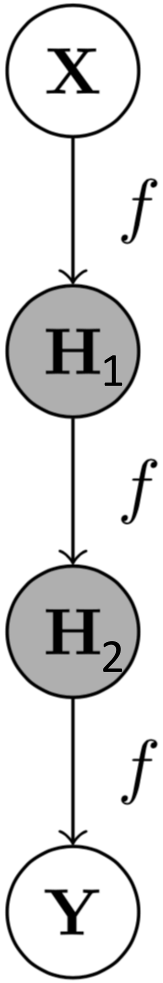
Part 2: Deep Gaussian processes

A general *family* of probabilistic models



$$\mathbf{Y} = f_3(f_2(\cdots f_1(\mathbf{X}))), \qquad \mathbf{H}_i = f_i(\mathbf{H}_{i-1})$$

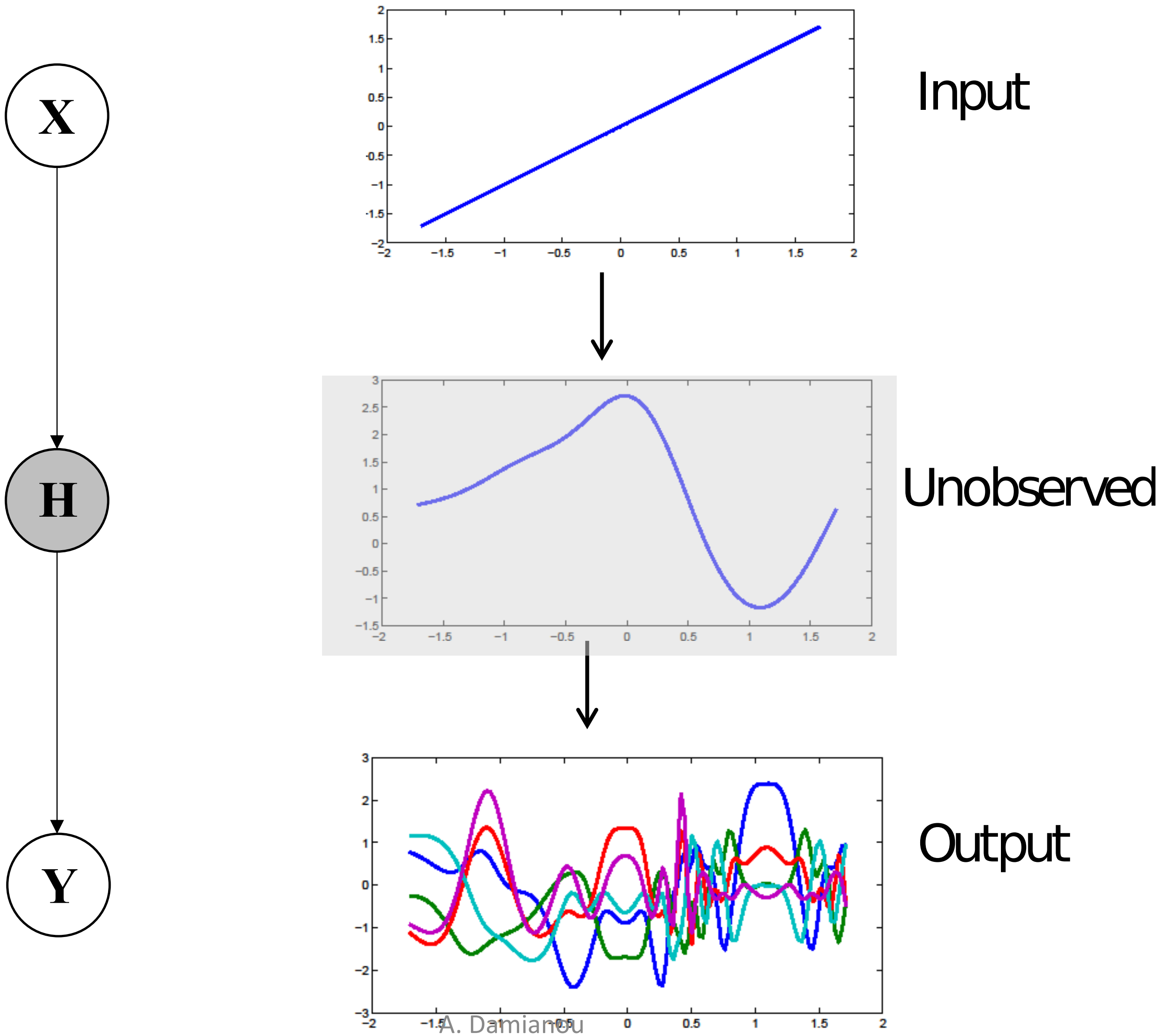
Deep Gaussian process



- Nested function composition
- Non-parametric, non-linear mappings *f*
- Mappings *f* marginalized out analytically
- NOT a GP!

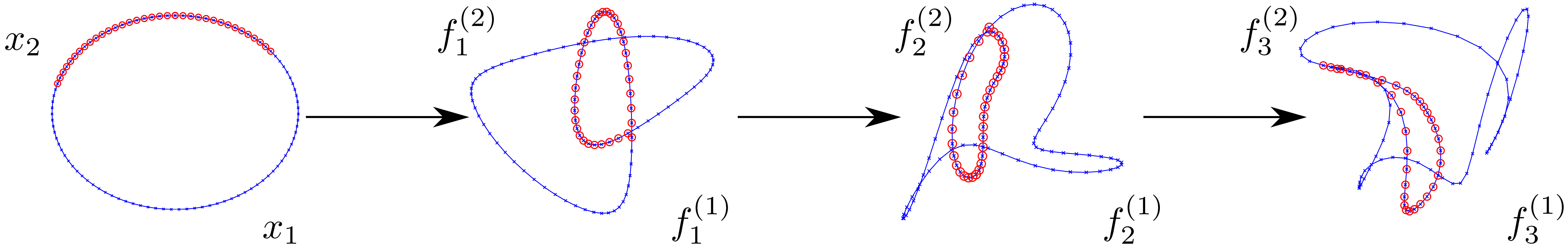
Damianou & Lawrence, 2013, Damianou, PhD Thesis 2015

Sampling from a Deep GP

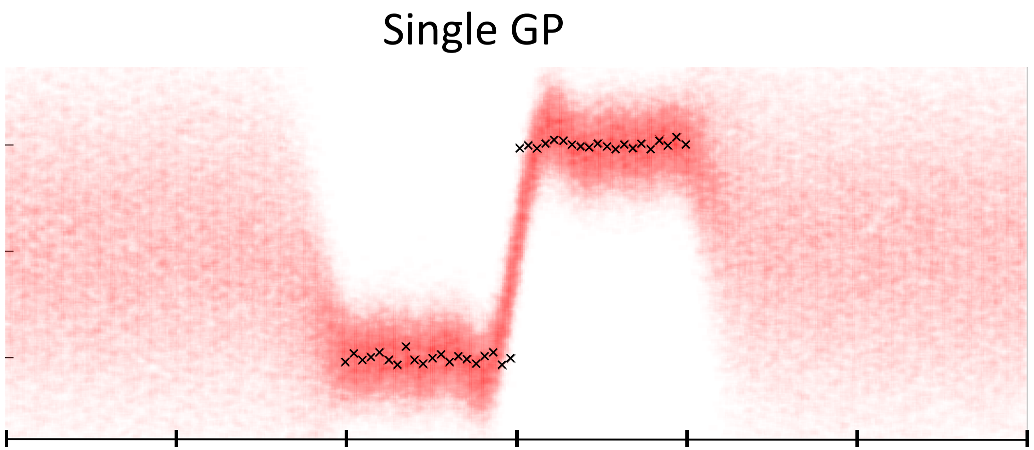


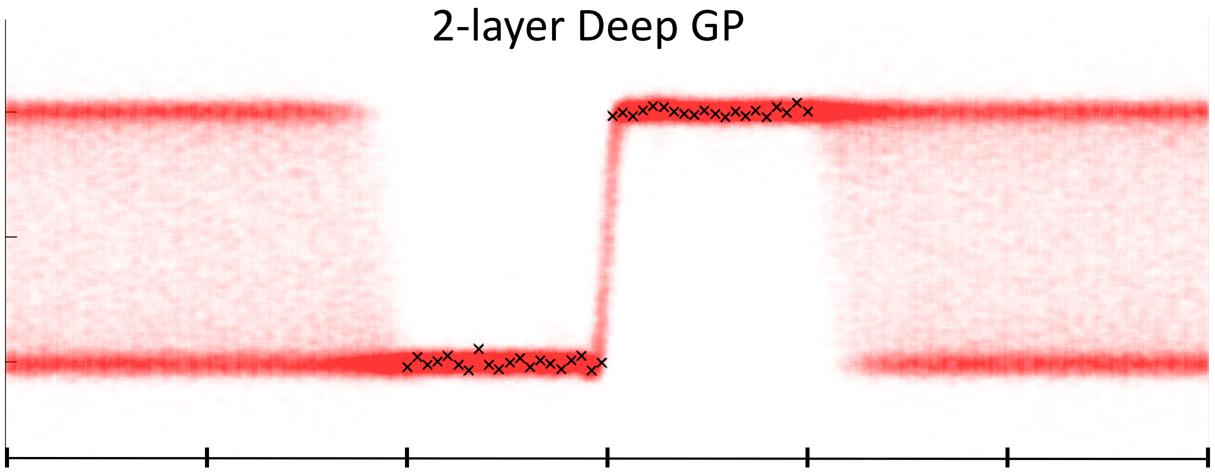
Feature learning

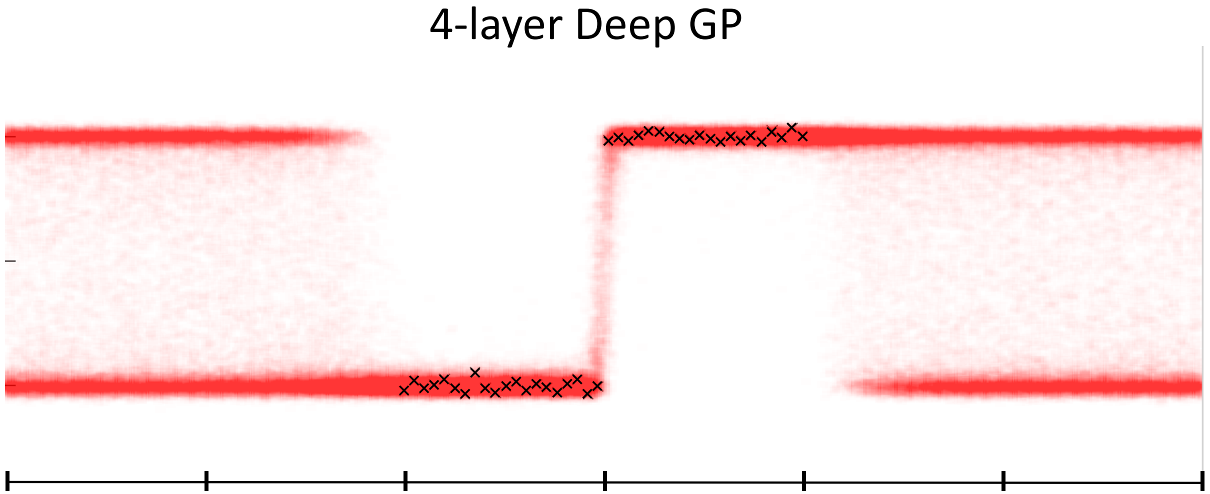
Regularities are learned as “knots” in the latent space, carried over from layer to layer.



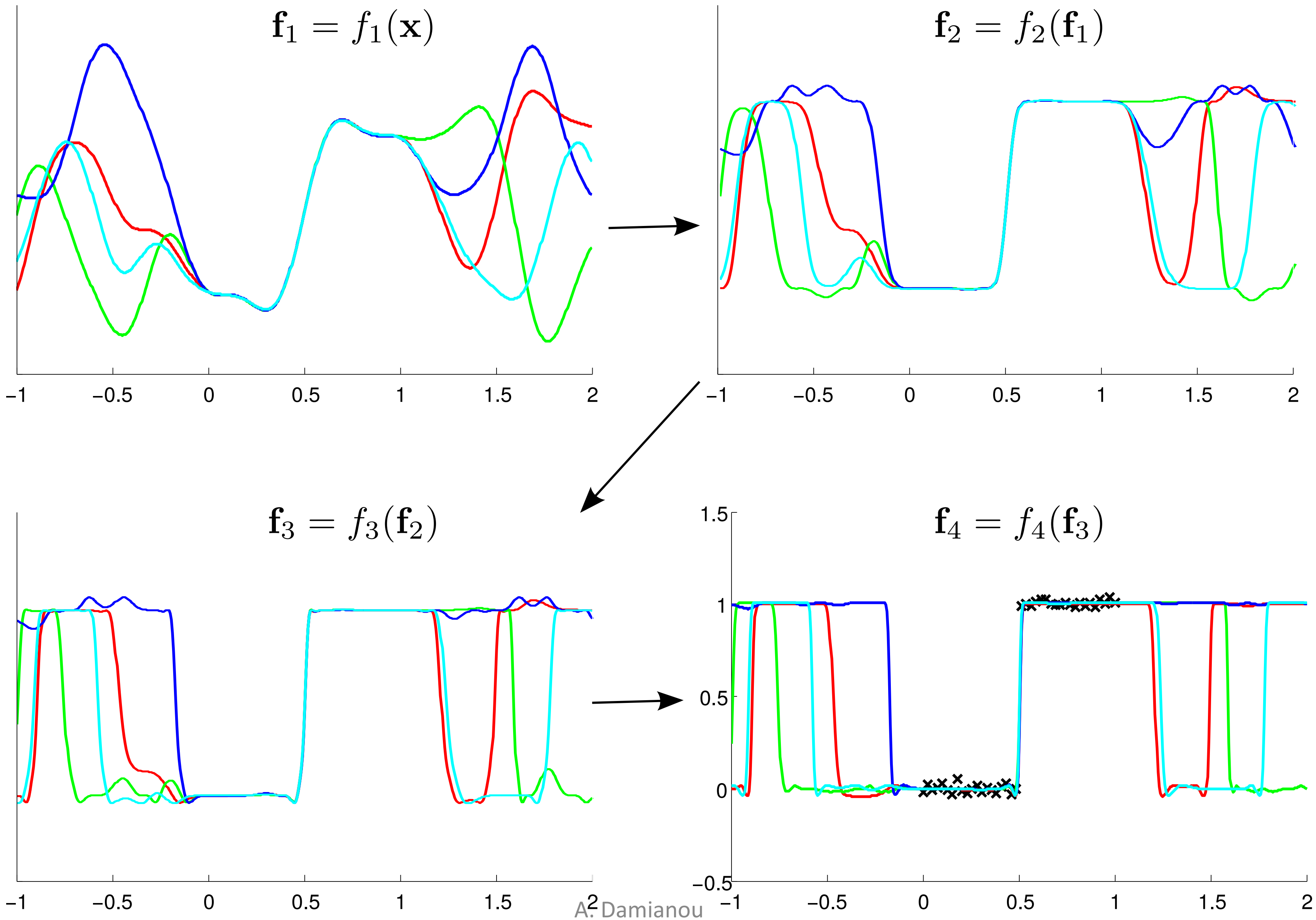
Step function example







Successive warping to learn the step function



Properties

- Unsupervised learning possible due to Bayesian regularization
- Very data efficient
- Scalability also possible with newer techniques

- Intractable objective
- Classification is more challenging

Summary – Deep Gaussian processes

- A DGP is a GP whose input is a GP, whose input is a GP…

- Propagate uncertainty across layers (not only point estimates)

Summary – Deep Gaussian processes

- A DGP is a GP whose input is a GP, whose input is a GP…

- Propagate uncertainty across layers (not only point estimates)

- What if layers represent different *kinds* of observation spaces? E.g. different *fidelities*?

Part 3: Multi-fidelity modeling

Multi-fidelity data

High fidelity observations

Low fidelity observations

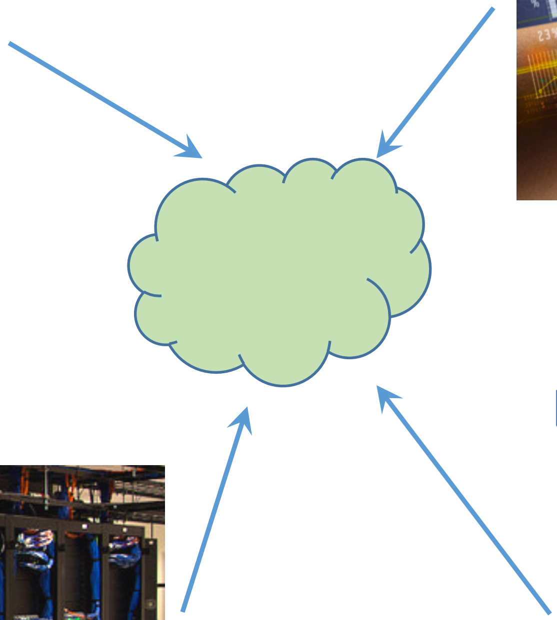
High fidelity simulations

Low fidelity simulations

Multi-fidelity data

High fidelity observations

Low fidelity observations



High fidelity simulations

Low fidelity simulations

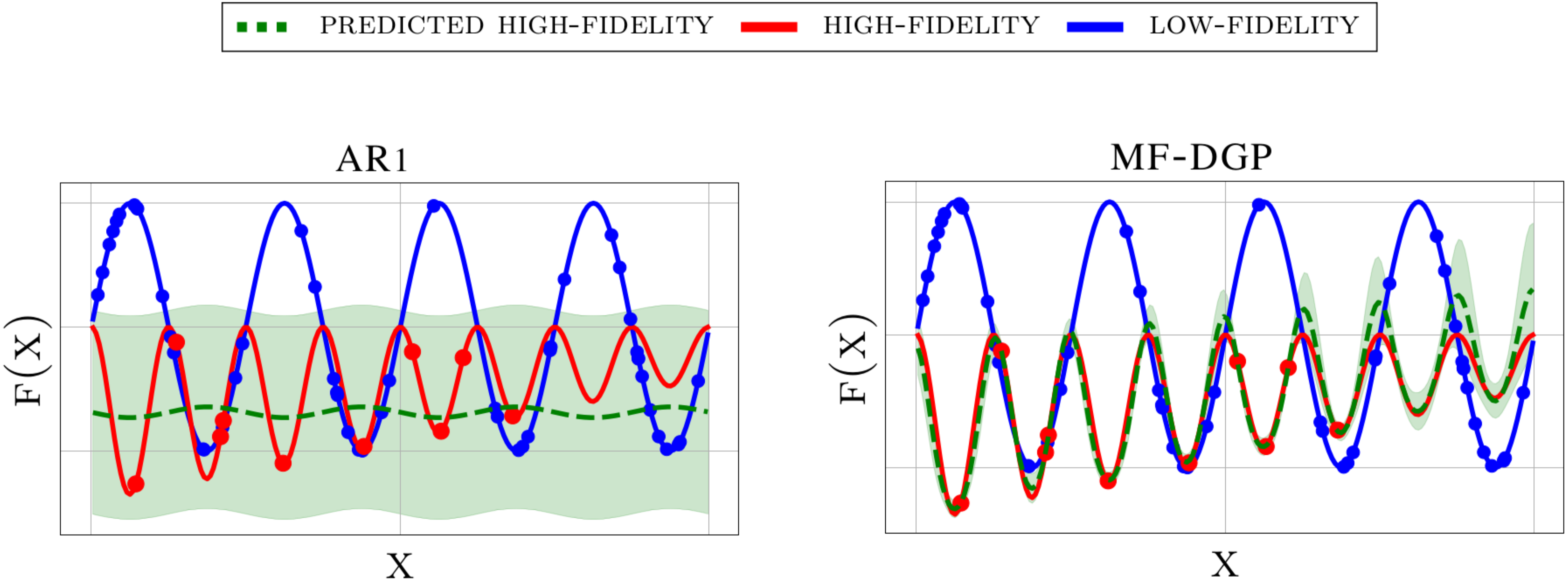
X_H

$Y_H =$ OK
OK
OK
OK
ERROR!
OK
OK

X_L

$Y_L =$ OK
OK
ERROR!
OK
ERROR!
OK
ERROR!

Fusing information from multiple fidelities



We want to trust the high-fidelity data, where we have them, and where we don't have them to learn how to reason based on low-fidelity data.

Linear GP multi-fidelity

$$f_H(x) = \rho_H f_L(x) + \delta_H(x)$$

f_H High fidelity function (GP)

ρ_H Contribution of low fidelity (const)

f_L Low fidelity function (GP)

δ_H Bias between fidelities (GP)

Kennedy & O'Hagan 2000, Le Gratiet & Garnier 2014

Non-linear multi-fidelity GP => Deep GP

$$f_H(x) = \rho_H f_L(x) + \delta_H(x)$$

Linear relationship between fidelities

$$f_H(x) = \rho_H(f_L(x), x) + \delta_H(x)$$

Non-linear relationship between fidelities
(if ρ is a GP -> overall a deep GP!)

Non-linear multi-fidelity GP => Deep GP

$$f_H(x) = \rho_H f_L(x) + \delta_H(x)$$

Linear relationship between fidelities

$$f_H(x) = \rho_H(f_L(x), x) + \delta_H(x)$$

Non-linear relationship between fidelities
(if ρ is a GP -> overall a deep GP!)

$$\Downarrow$$

$$f_H(x) = g_H(f_L^*(x), x)$$

δ absorbed into g

$f_L^*(x)$ denotes the posterior of the GP modeling the low-fidelity data.

Perdikaris et al., Proc. Royal Society, 2017

Algorithm

1. Train f_L on (X_L, Y_L)

2. Compute $f_L^*(X_H)$

3. Train f_H on $((X_L, Y_L), f_L^*(X_H))$

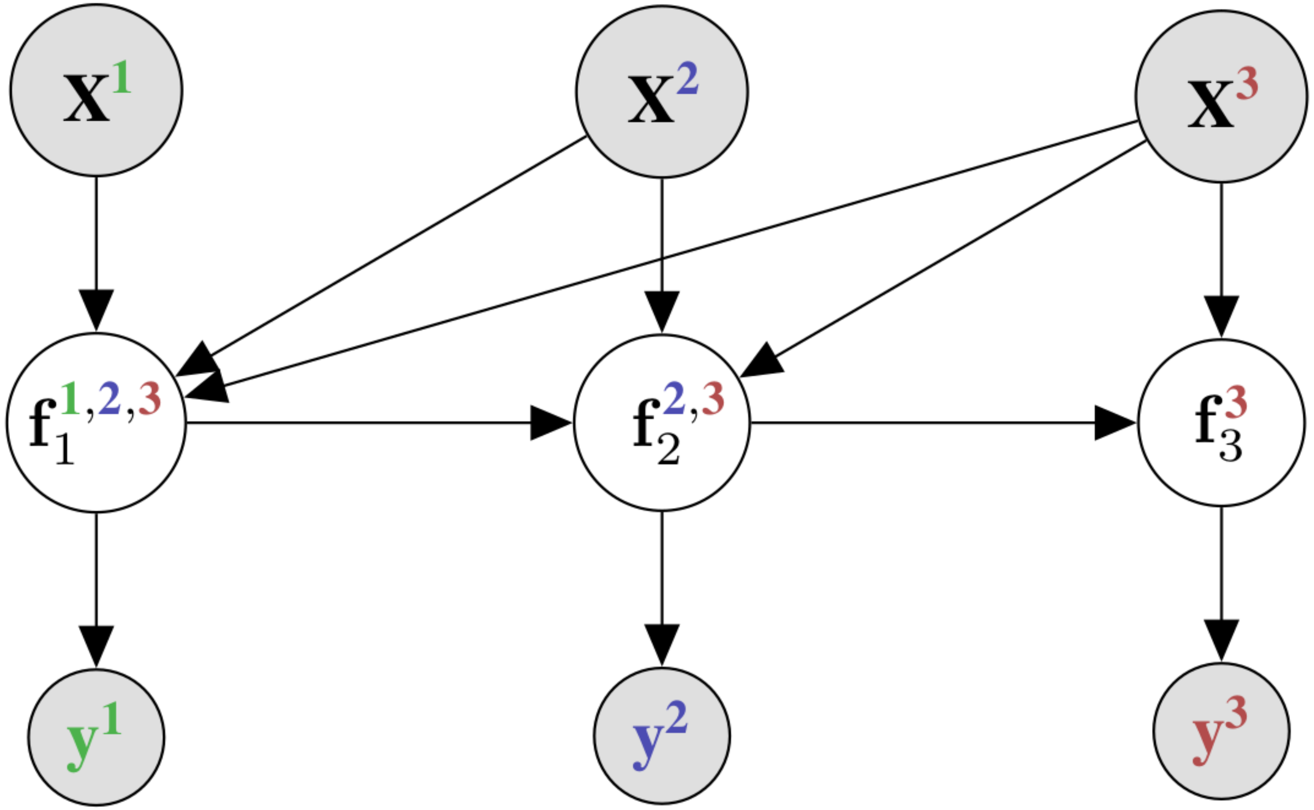
Predictions

$$p(f_H^*(x^*)) =$$

$$\int \underbrace{p(f_H(x^*, f_L^*(x^*))|y_H, x_H, x^*)}_{\text{Local posterior from fidelity } H} \; \underbrace{p(f_L^*(x^*))}_{\text{Predictive from fidelity } L} \, df_L^*$$

Communication between fidelities during training

$f_{\text{layer}}^{\text{fidelity}}$



Cutajar et al. arXiv: 1903.07320

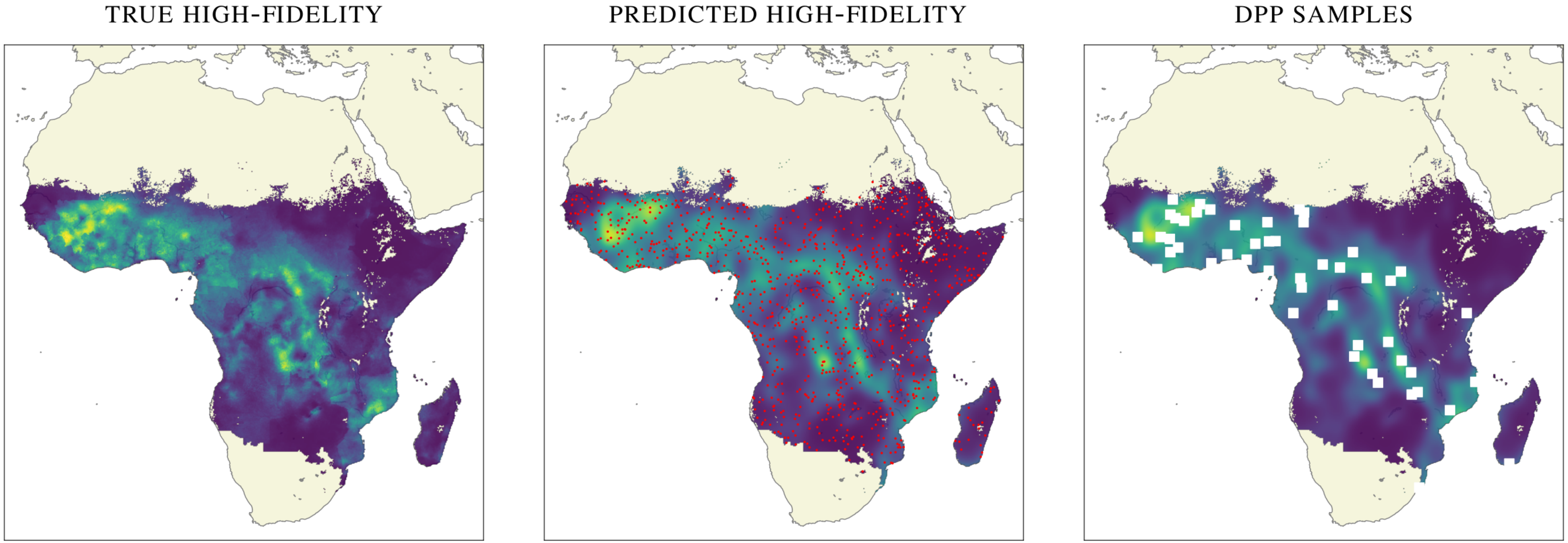


Figure 5: Real-world experiment indicating the infection rate of *Plasmodium falciparum* among African children. Lighter-shaded regions denote higher infection rates in that area of the continent. *Left:* True infection rates recorded for the year 2015. *Center:* MF-DGP predictions given low-fidelity data from 2005 and limited high-fidelity training points (marked in red) from 2015. *Right:* White squares show the samples drawn from a DPP using the posterior covariance of the MF-DGP model as its kernel.

Sequential design for multi-fidelity GP

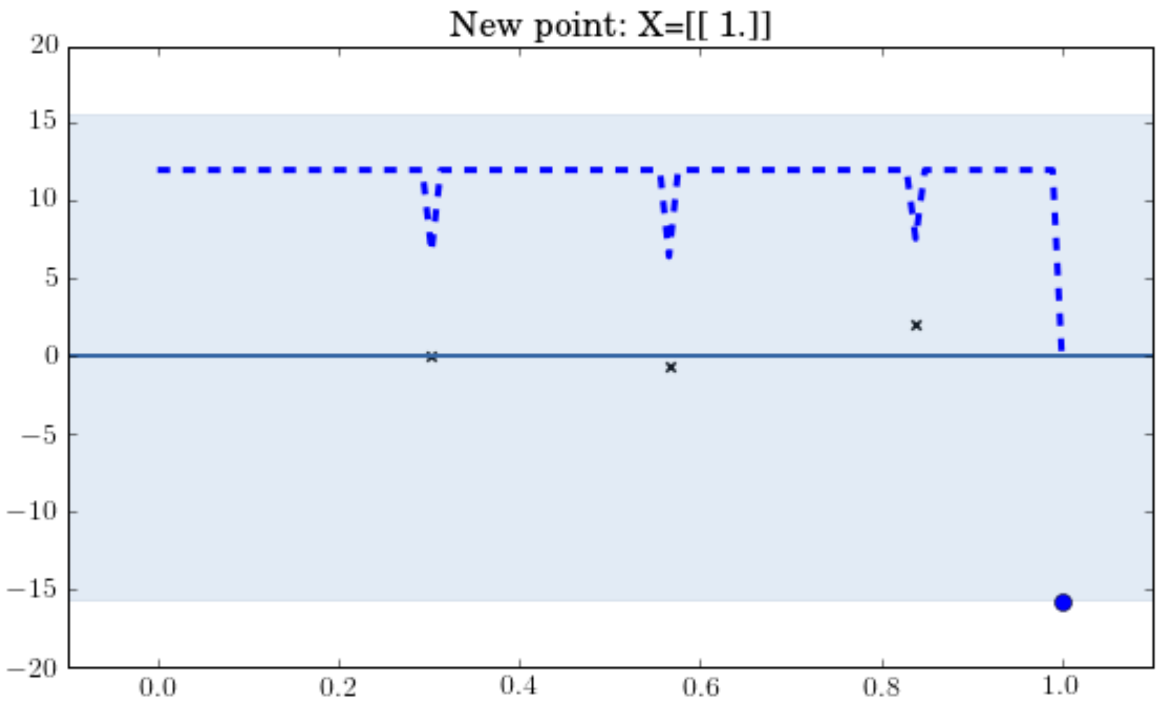
- **Strategy for collecting data points** across fidelities

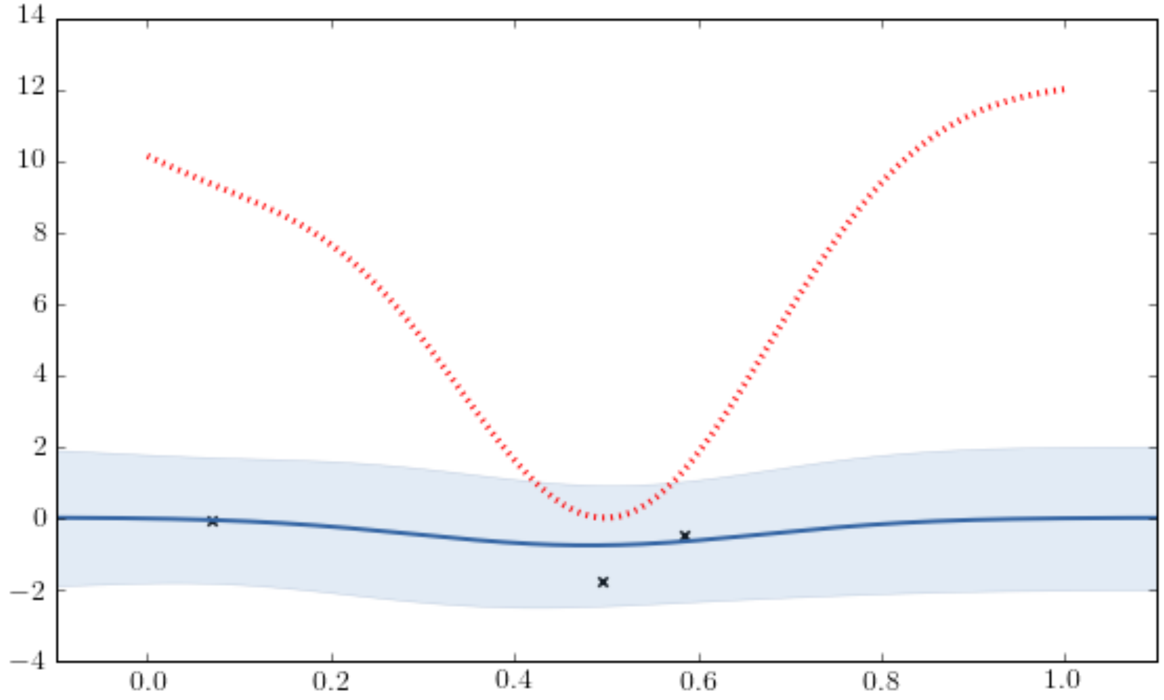
- Each fidelity evaluation comes with a different **cost**, proportional to the level of fidelity

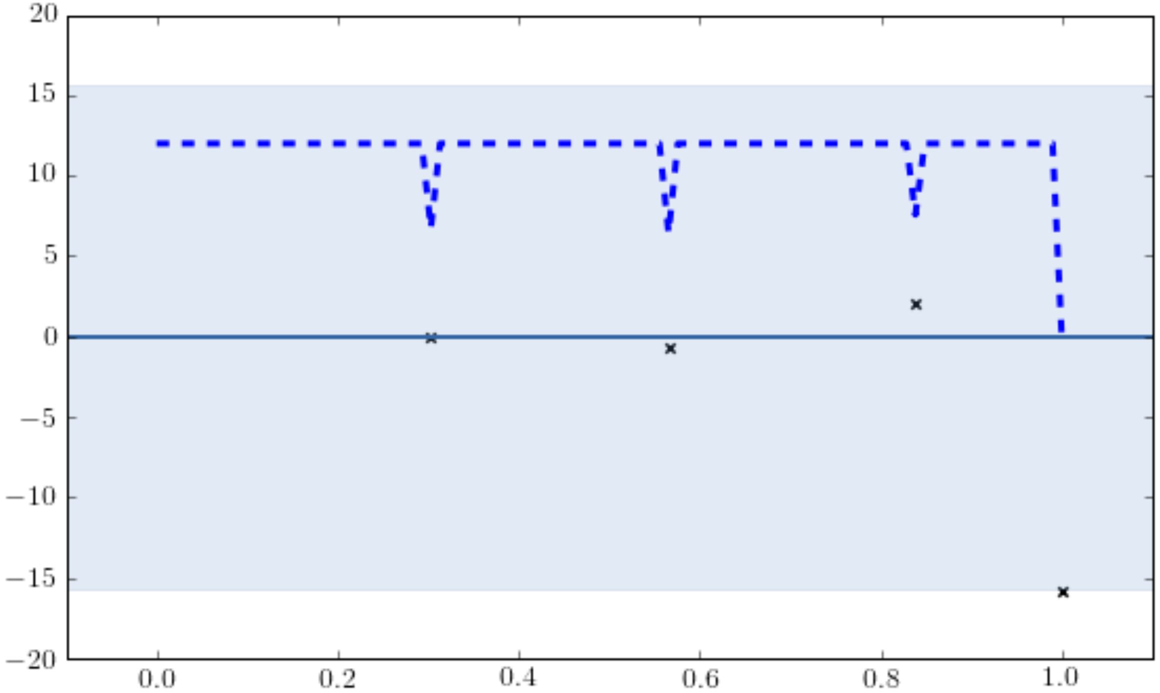
- Approach: Formulation as a multi-fidelity **bandit** GP problem in the UCB setting *(Kandasamy et al. 2016)*

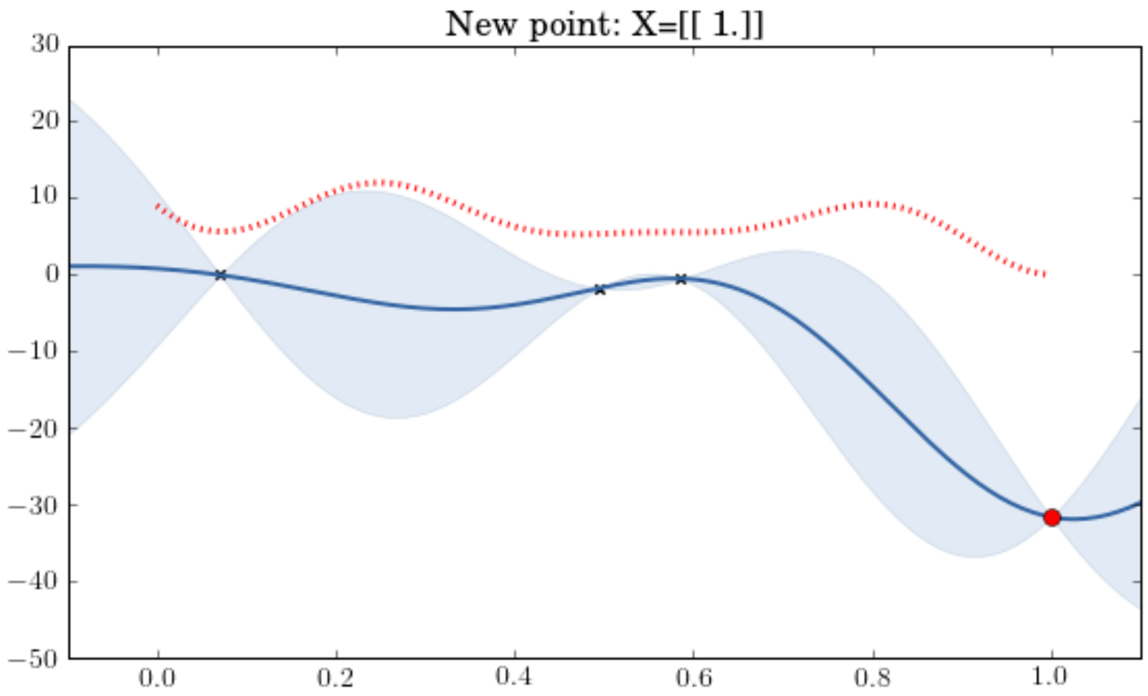
Demonstration

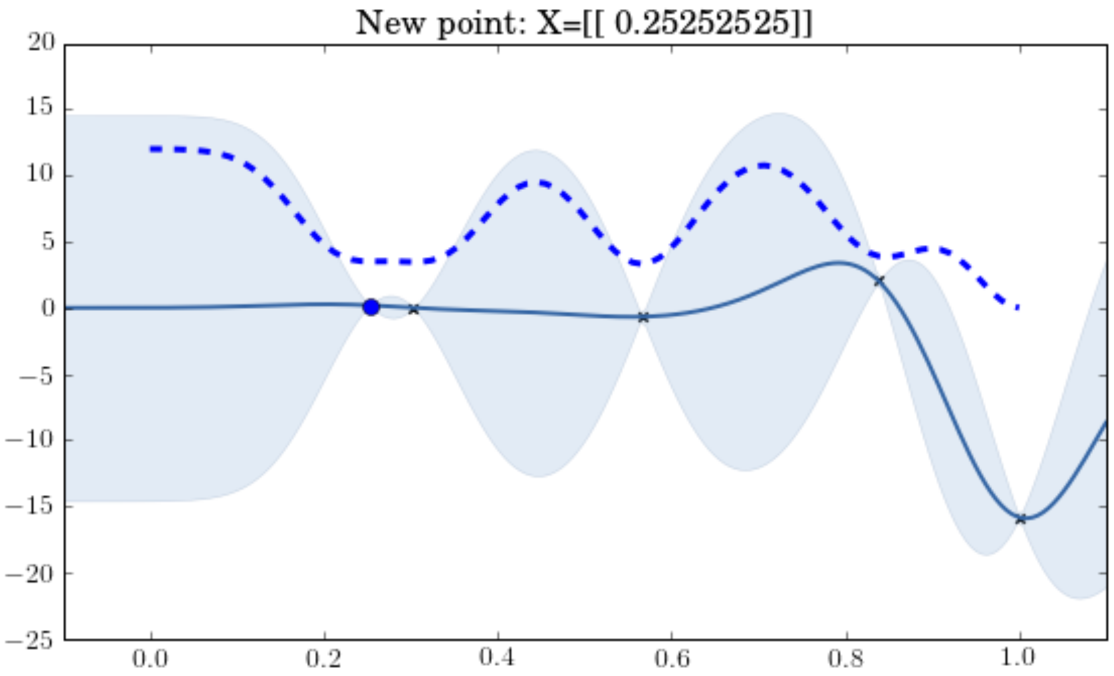
- Find the maximum of the high-fidelity function
- Consider cost while collecting points from each fidelity


New point: X=[[1.]]
20
15
10
5
0
−5
−10
−15
−20
0.0
0.2
0.4
0.6
0.8
1.0


14
12
10
8
6
4
2
0
−2
−4
0.0
0.2
0.4
0.6
0.8
1.0


20
15
10
5
0
−5
−10
−15
−20
0.0
0.2
0.4
0.6
0.8
1.0


New point: X=[[1.]]
30
20
10
0
−10
−20
−30
−40
−50
0.0
0.2
0.4
0.6
0.8
1.0


New point: X=[[0.25252525]]
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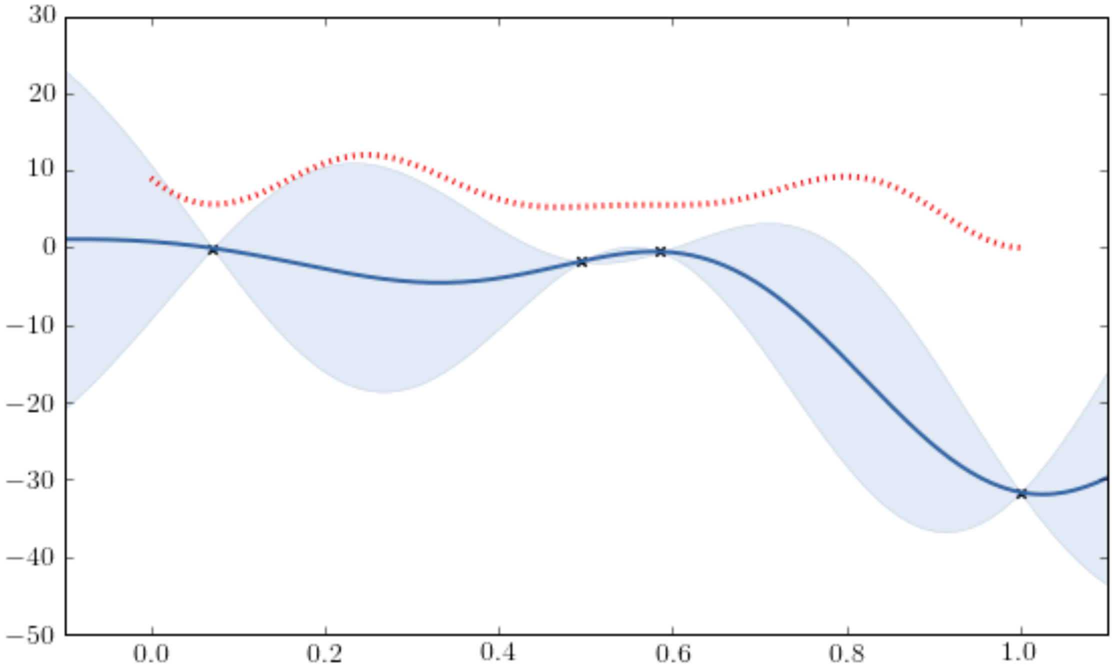
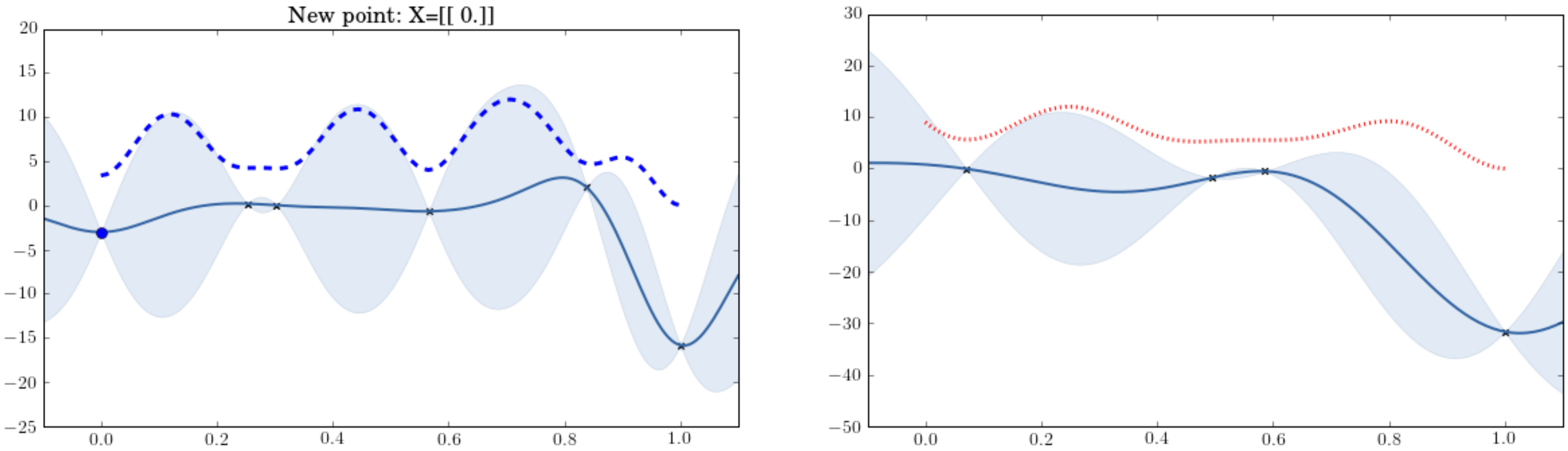
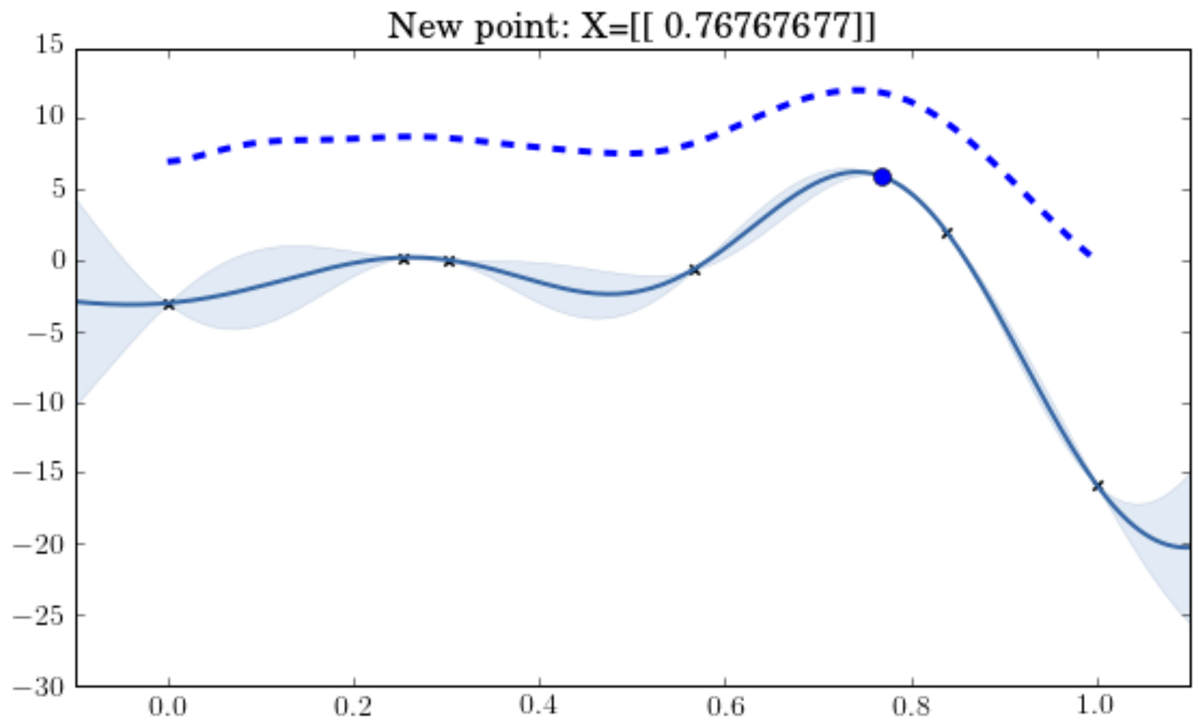
15
10
5
0
−5
−10
−15
−20
−25
0.0
0.2
0.4
0.6
0.8
1.0


30
20
10
0
−10
−20
−30
−40
−50
0.0
0.2
0.4
0.6
0.8
1.0



New point: X=[[0.]]


New point: X=[[0.76767677]]
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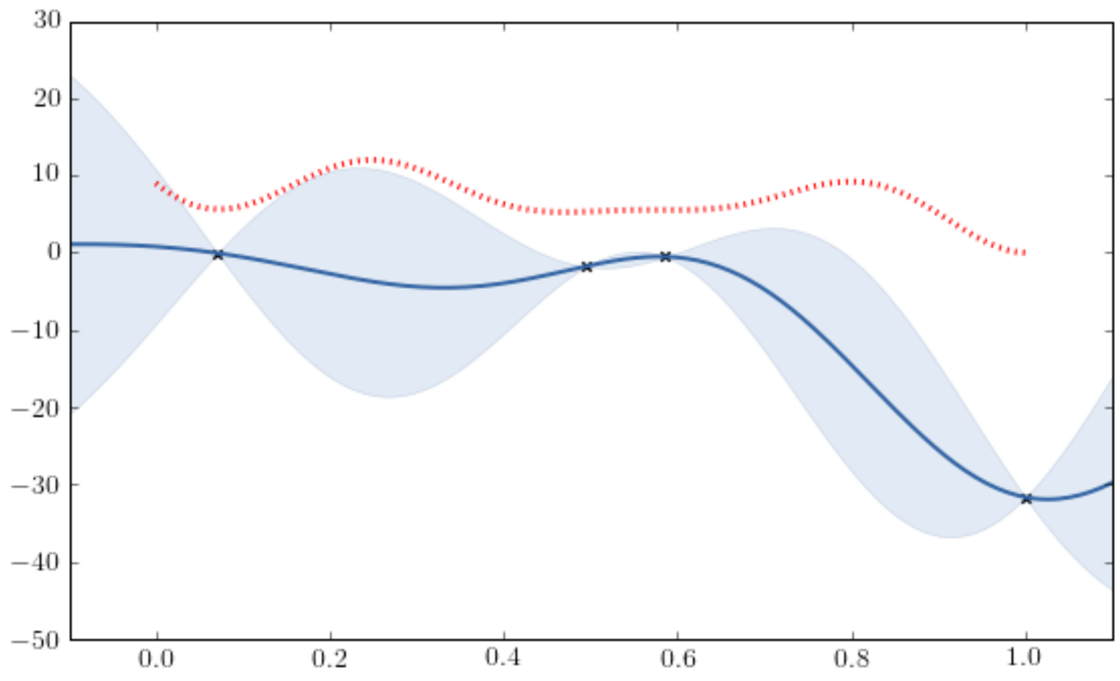
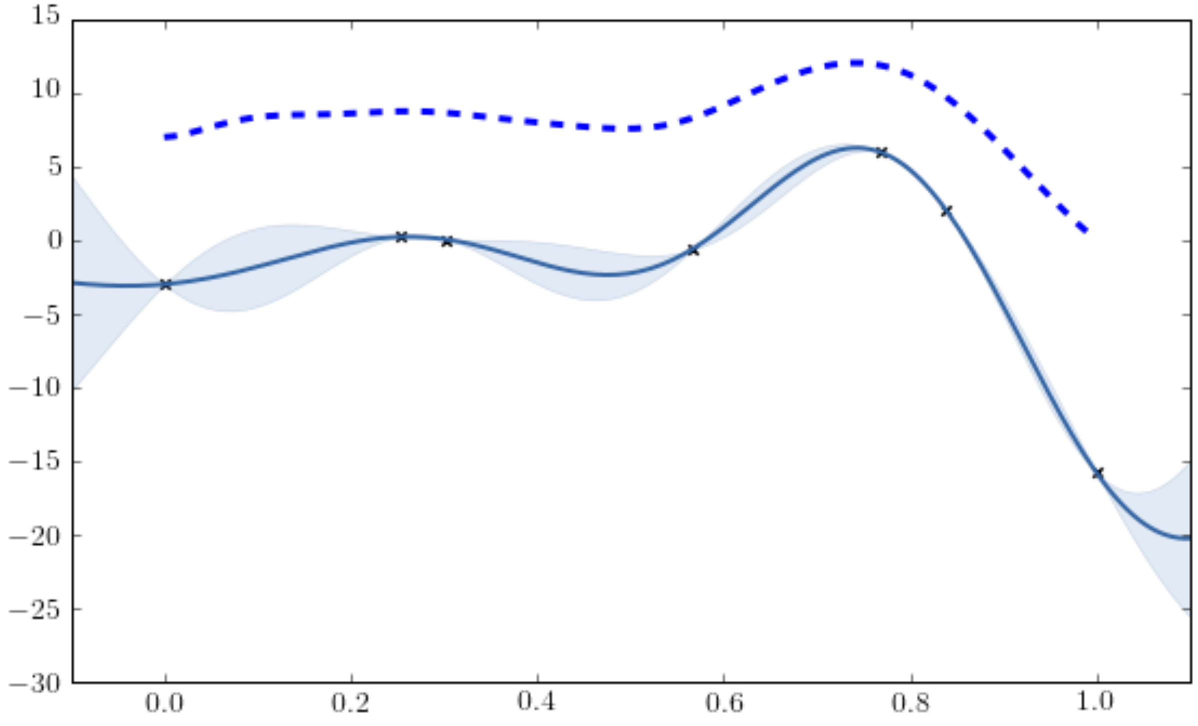
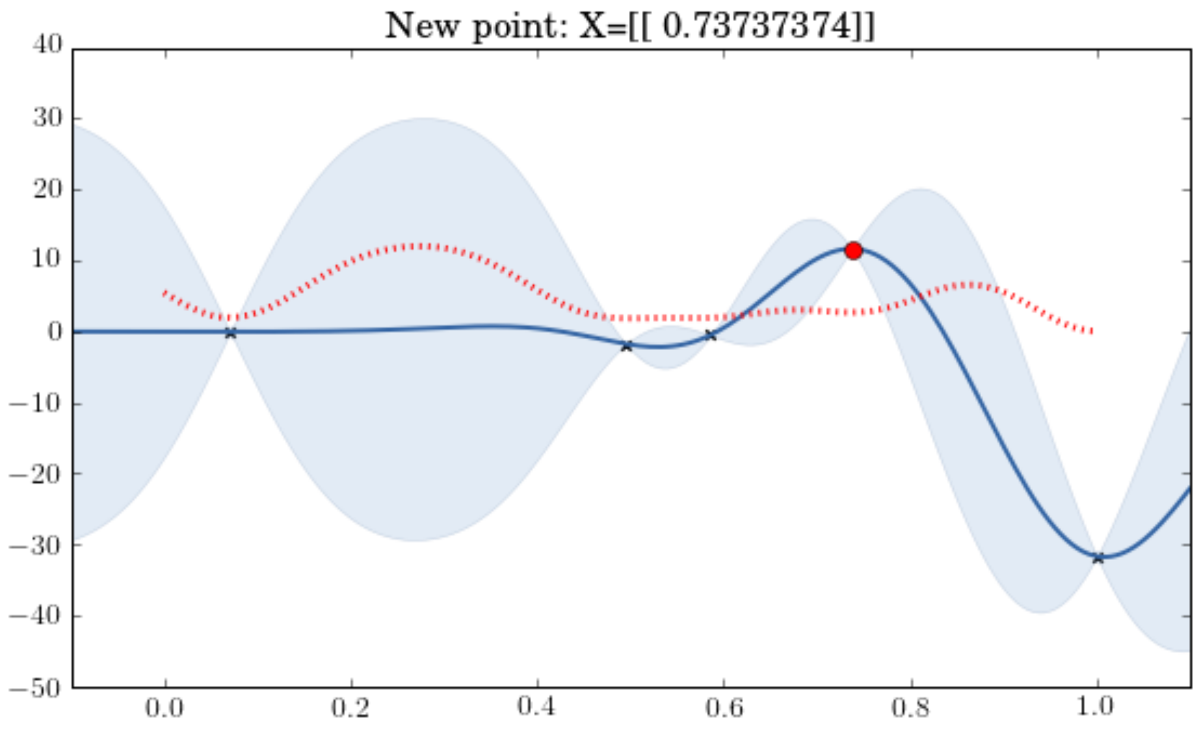
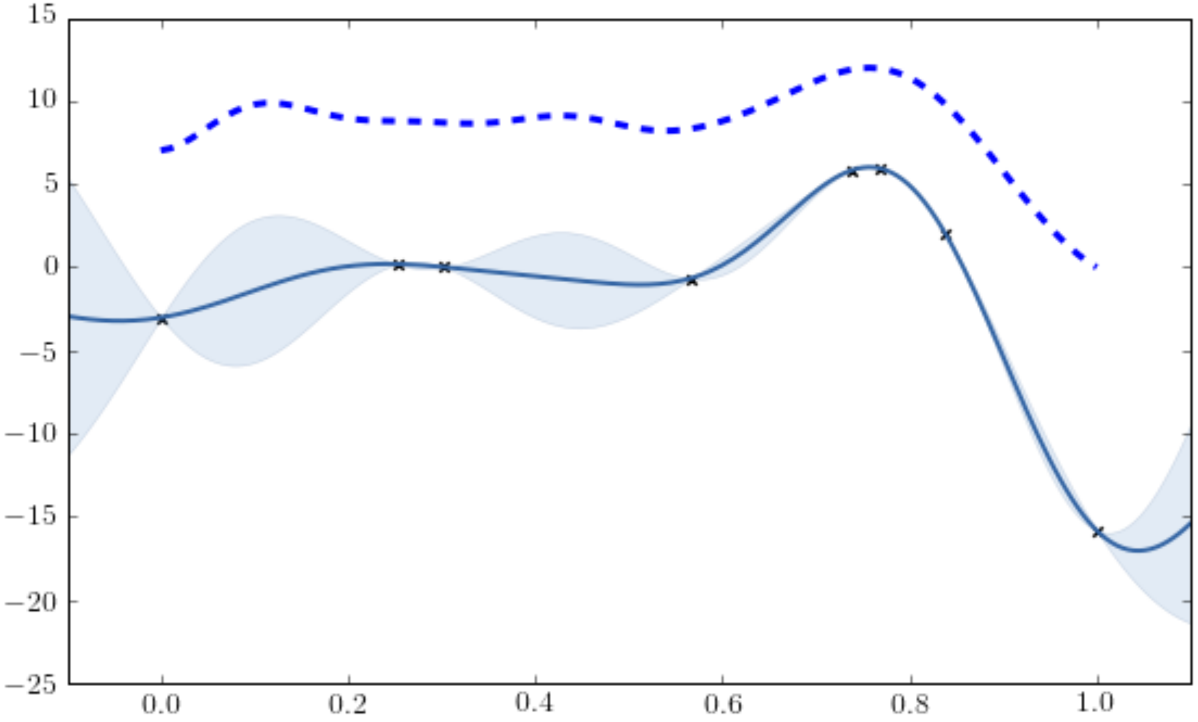
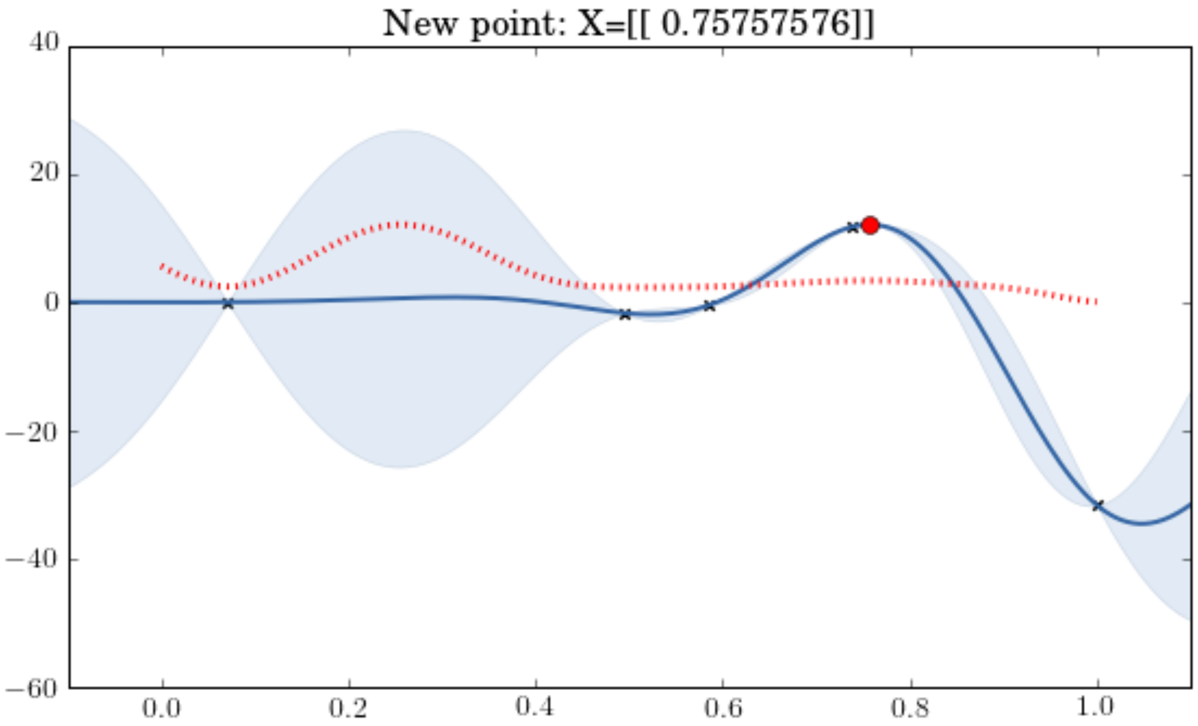
10
5
0
−5
−10
−15
−20
−25
−30
0.0
0.2
0.4
0.6
0.8
1.0


30
20
10
0
−10
−20
−30
−40
−50
0.0
0.2
0.4
0.6
0.8
1.0


15
10
5
0
−5
−10
−15
−20
−25
−30
0.0
0.2
0.4
0.6
0.8
1.0


New point: X=[[0.73737374]]
40
30
20
10
0
−10
−20
−30
−40
−50
0.0
0.2
0.4
0.6
0.8
1.0


15
10
5
0
−5
−10
−15
−20
−25
0.0
0.2
0.4
0.6
0.8
1.0


New point: X=[[0.75757576]]
40
20
0
−20
−40
−60
0.0
0.2
0.4
0.6
0.8
1.0

Conclusion

- GPs: Non-parametric inference over the space of functions
- Deep GPs learn rich mappings in a regularized and data efficient manner
- Multi-fidelity (D)GPs allow us to fuse multiple fidelity data
- We can actively acquire data of different fidelities using the GP emulators in each fidelity.

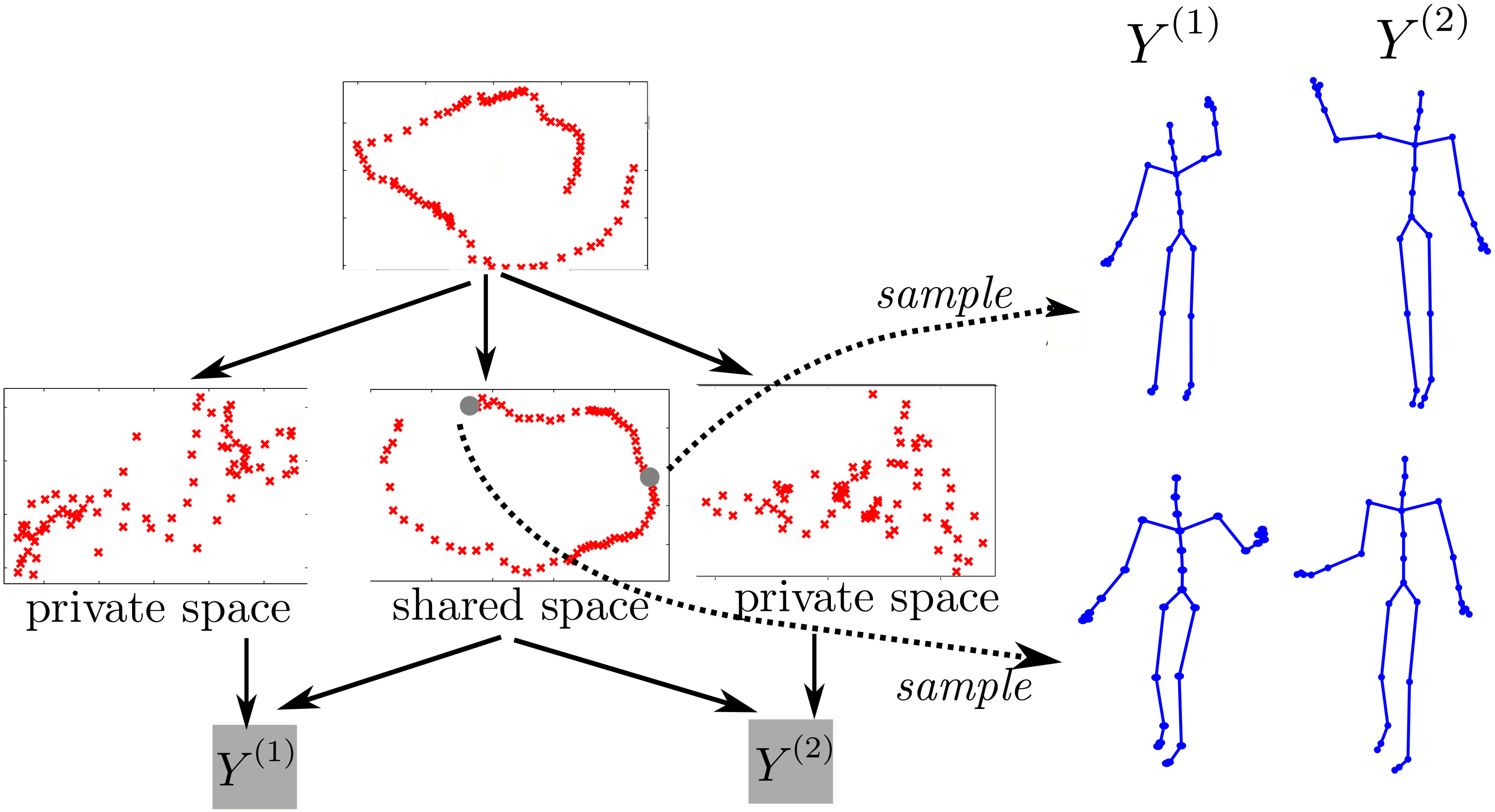
Thanks!

Questions?

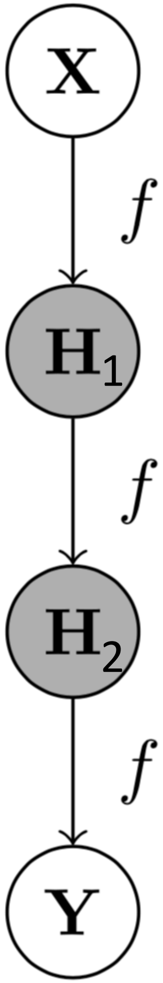
See also: http://adamian.github.io/talks/Damianou_GP_tutorial.html

Appendix

Unsupervised learning for multiple views



Deep Gaussian process

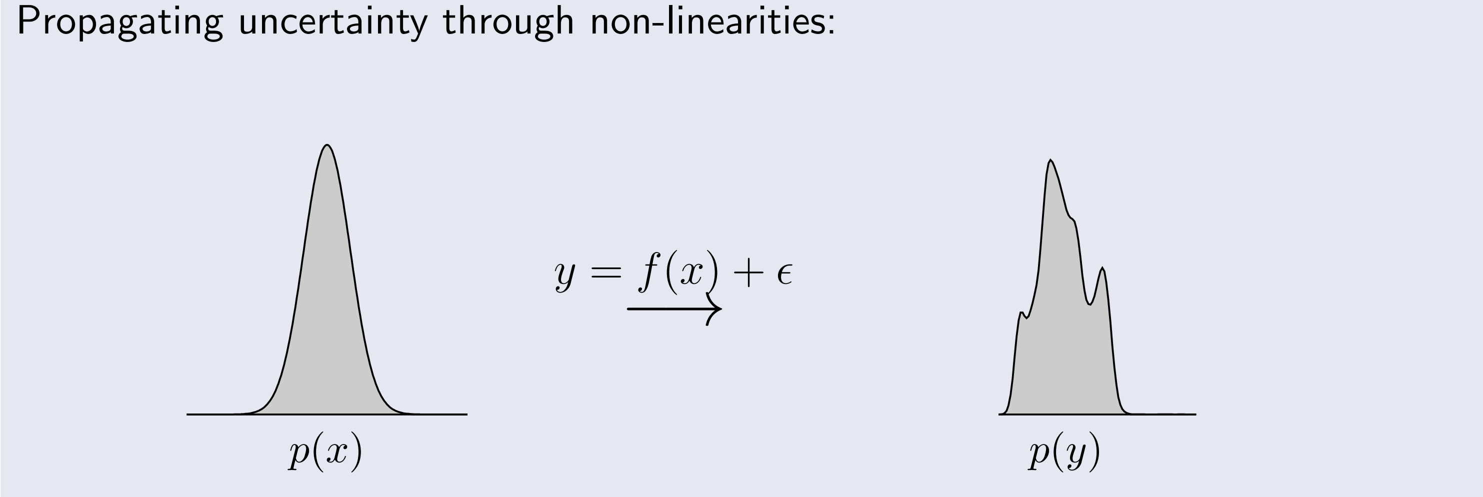


- Objective: $p(y|x) = \int_{h_2} \left(p(y|h_2) \int_{h_1} p(h_2|h_1) p(h_1|x) \right)$
- $p(h_2|x) \quad = \int_{h_1, f_2} \quad p(h_2|f_2) p(f_2|h_1) \quad p(h_1|x)$

Inference in Deep GPs: uncertainty propagation

- Objective: $p(y|x) = \int_{h_2} \left(p(y|h_2) \int_{h_1} p(h_2|h_1) p(h_1|x) \right)$

- $p(h_2|x) \quad = \int_{h_1, f_2} p(h_2|f_2) \underbrace{p(f_2|h_1)}_{\text{contains } (k(h_1,h_1))^{-1}} p(h_1|x)$



Variational bound and its properties

Bound on the log marginal likelihood *log p(y)*

$$\mathcal{F} = \overbrace{\sum_{l=2}^{L+1} \left\langle \sum_{n=1}^{N} \mathcal{L}(\mathbf{h}_l^{(n)}, \mathbf{u}_l) \right\rangle_{\mathcal{Q}}}^{\text{Data fit}} - \sum_{l=2}^{L+1} \mathsf{KL}\left(q(\mathbf{u}_l) \parallel p(\mathbf{u}_l)\right) \underbrace{- \mathsf{KL}\left(q(\mathbf{h}_1) \parallel p(\mathbf{h}_1)\right)}_{\text{Regularization}} + \sum_{l=2}^{L} \underbrace{\mathcal{H}\left(q(\mathbf{h}_l)\right)}_{\text{Regularization}}$$

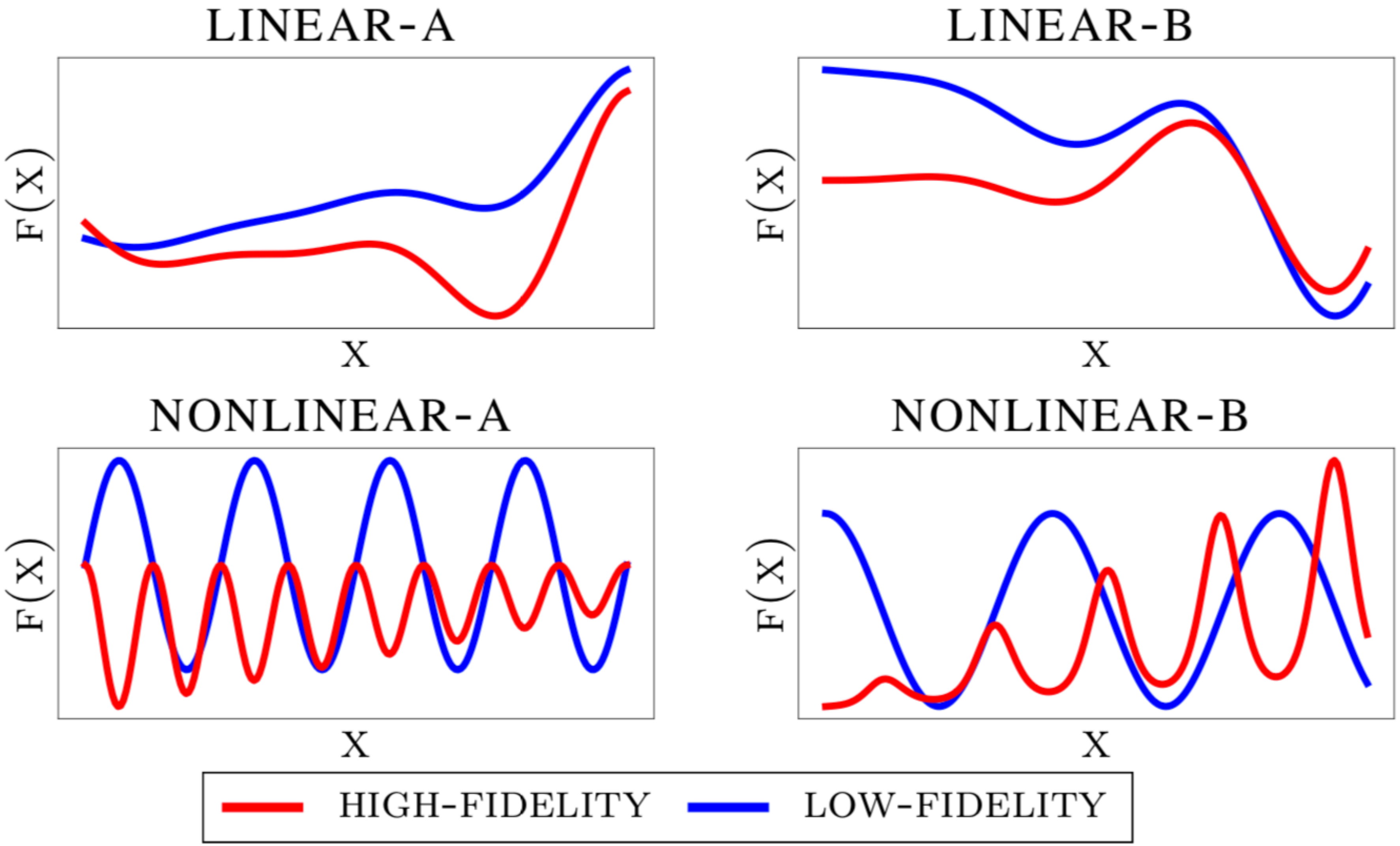


Figure 3: Synthetic examples. *Top:* Linear mapping between fidelities. *Bottom:* Nonlinear mapping.

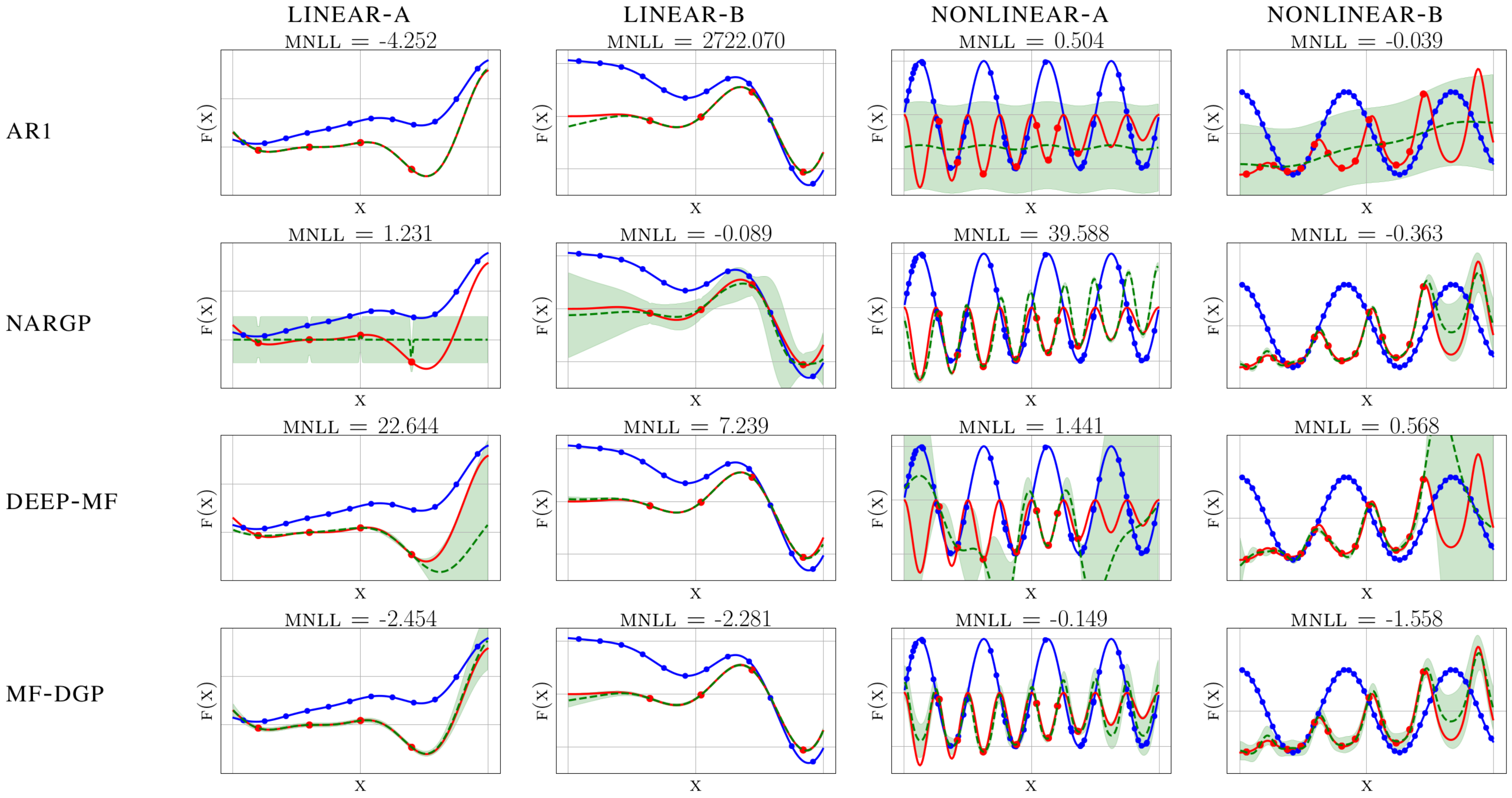


Figure 4: Cross-comparison across methods and synthetic examples for challenging multi-fidelity scenarios. MF-DGP yields conservative uncertainty estimates where few high-fidelity observations are available.

Benchmark examples

Table 1: Model Comparison on Multi-fidelity Benchmark Examples.

BENCHMARK	D_{in}	FIDELITY ALLOCATION	AR1 R^2	AR1 RMSE	AR1 MNLL	NARGP R^2	NARGP RMSE	NARGP MNLL	MF-DGP R^2	MF-DGP RMSE	MF-DGP MNLL
CURRIN	2	12-5	0.913	0.677	20.105	0.903	0.740	20.817	**0.935**	**0.601**	**0.763**
PARK	4	30-5	**0.985**	0.575	465.377	0.954	0.928	743.119	**0.985**	**0.565**	**1.383**
BOREHOLE	8	60-5	**1.000**	**0.005**	**-3.946**	0.973	0.063	-1.054	0.999	0.015	-2.031
BRANIN	2	80-30-10	0.891	0.044	-1.740	0.929	0.053	-1.223	**0.965**	**0.030**	**-2.572**
HARTMANN-3D	3	80-40-20	**0.998**	**0.043**	0.440	0.305	0.755	0.637	0.994	0.075	**-0.731**