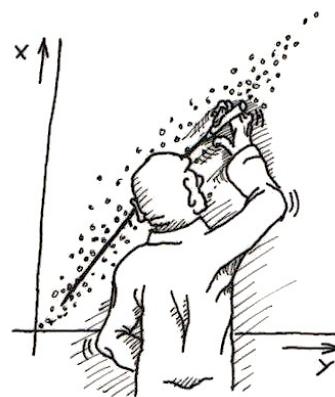


GP vs NN?

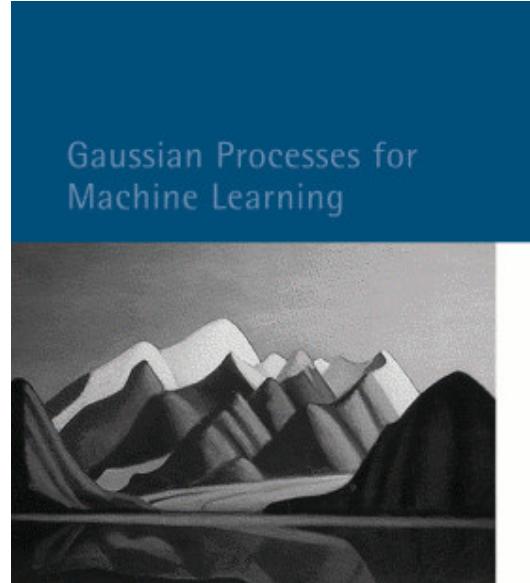
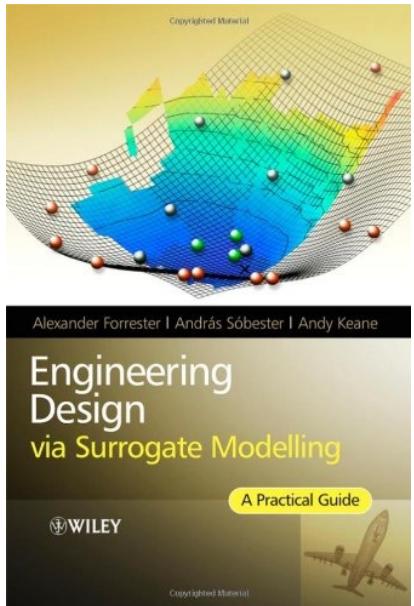
Prof. J. Morlier



Sustainable Aerostructures & Interactions

<https://github.com/jomorlier/mdocourse>

XO



X₀ in practice

Since 2017

<https://smt.readthedocs.io/en/latest>

<https://github.com/SMTorg/smt>

SMT 2.0b1 documentation » SMT: Surrogate Modeling Toolbox

next | index



SMT: Surrogate Modeling Toolbox

The surrogate modeling toolbox (SMT) is an open-source Python package consisting of libraries of surrogate modeling methods (e.g., radial basis functions, kriging), sampling methods, and benchmarking problems. SMT is designed to make it easy for developers to implement new surrogate models in a well-tested and well-documented platform, and for users to have a library of surrogate modeling methods with which to use and compare methods.

The code is available open-source on [GitHub](#).

Cite us

To cite SMT: M. A. Bouhlel and J. T. Hwang and N. Bartoli and R. Lafage and J. Morlier and J. R. R. Martins.

[A Python surrogate modeling framework with derivatives. Advances in Engineering Software, 2019.](#)

```
@article{SMT2019,
  Author = {Mohamed Amine Bouhlel and John T. Hwang and Nathalie Bartoli and Rémi Lafage and Joseph Morlier and Joaquim R. R. Martins},
  Journal = {Advances in Engineering Software},
  Title = {A Python surrogate modeling framework with derivatives},
  pages = {102662},
  year = {2019},
  issn = {0965-9978},
  doi = {https://doi.org/10.1016/j.advengsoft.2019.03.005},
  Year = {2019}}
```

Focus on derivatives

SMT is meant to be a general library for surrogate modeling (also known as metamodeling, interpolation, and regression), but its distinguishing characteristic is its focus on derivatives, e.g., to be used for gradient-based optimization. A surrogate model can be represented mathematically as

$$y = f(\mathbf{x}, \mathbf{xt}, \mathbf{yt}),$$

where $\mathbf{xt} \in \mathbb{R}^{nt \times nx}$ contains the training inputs, $\mathbf{yt} \in \mathbb{R}^{nt}$ contains the training outputs, $\mathbf{x} \in \mathbb{R}^{nx}$ contains the prediction inputs, and $y \in \mathbb{R}$ contains the prediction outputs. There are three types of derivatives of interest in SMT:

v: latest ▾

SM311 - GP vs NN

Au programme des 2 heures

Part 1. Régression par processus gaussiens

Introduction aux processus gaussiens, fondements mathématiques en 30' Exercice: Je programme mon GPR 30'

Part 2. processus gaussiens versus réseaux de neurones

Illustration en grande dimension, hyper parameter tuning, BO en 30' Exercice:

J'utilise des toolboxes sur des exemples plus complexes 45'

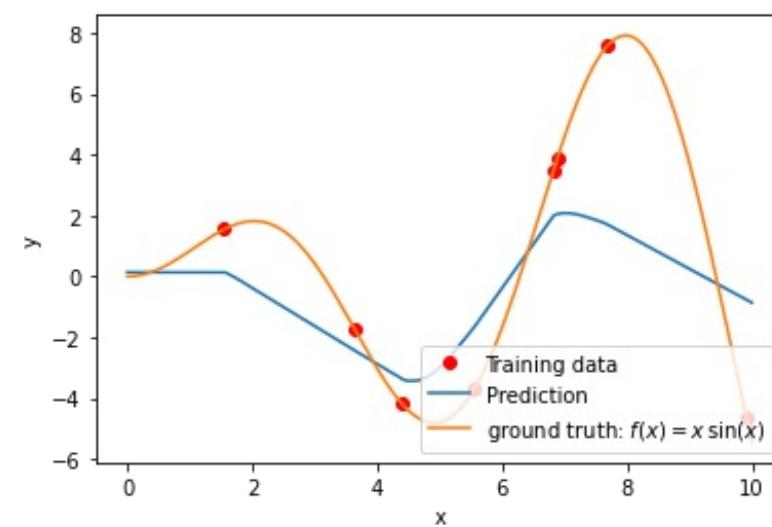
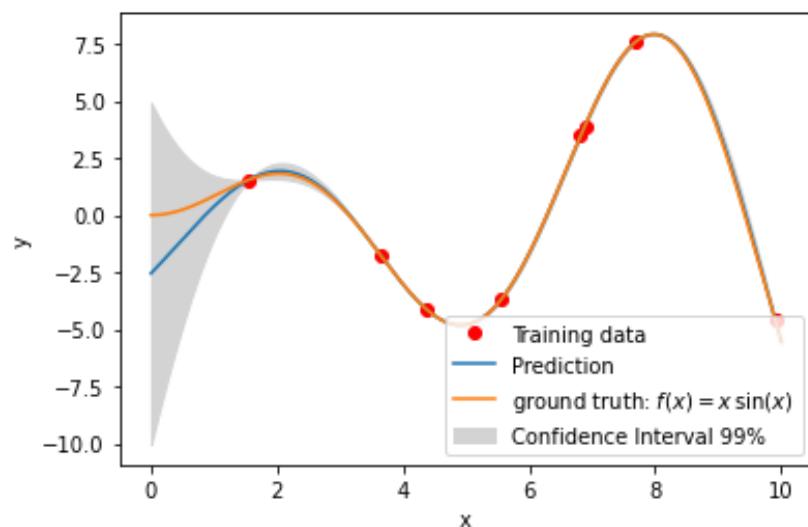
Travaux pratiques (Python)

sous colab Pour aller plus loin: Tutoriels SMT sur les processus gaussiens multi-fidélité, l'optimisation bayesienne
<https://github.com/SMTorg/smt/tree/master/tutorial>

1/Comparaison sur une simple fonction 1D : $x \sin(x)$. Sait-on à priori si l'on dispose d'assez de points ? Quel est l'effet des hyperparamètres (noyaux, degrés des polynômes, ...) ? Comparaison moindres carrés avec modèle linéaire/quadratique.

2/Entraîner un réseau de neurones (et/ou un processus gaussien) sur un dataset donné (sur une poutre encastrée).

GPR vs NN



SM311 - GP vs NN

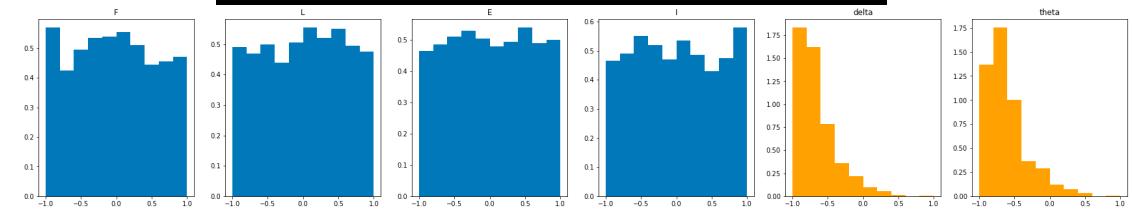
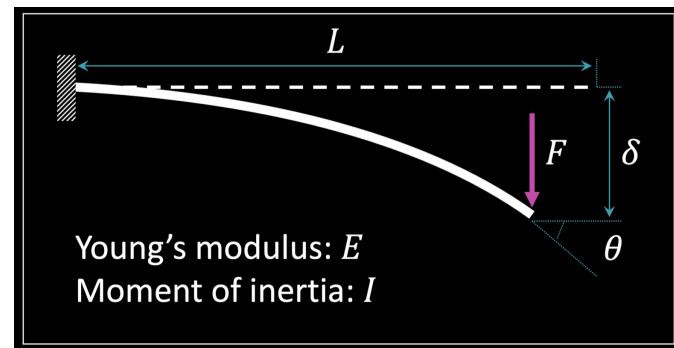
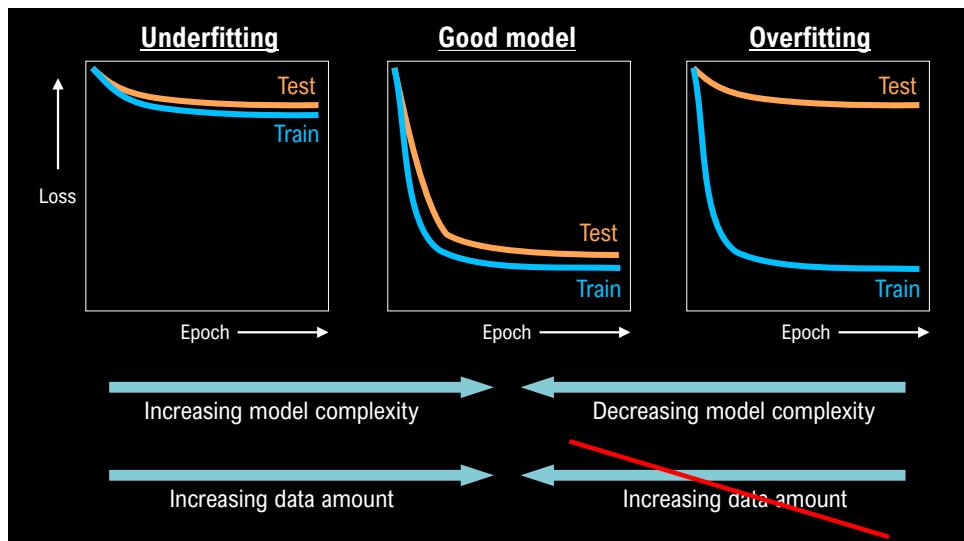
Travaux pratiques (Python)

sous colab

1/Best activation function (link to derivative)

<https://github.com/christianversloot/machine-learning-articles/blob/main/using-relu-sigmoid-and-tanh-with-pytorch-ignite-and-lightning.md>

2/Question on data generation (experiments / cheap code / costly code)



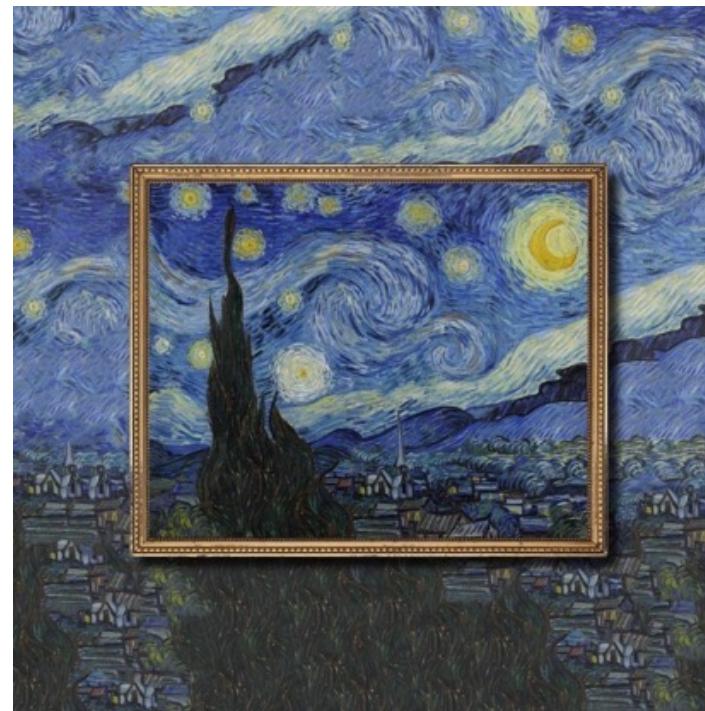
Part 1. Régression par processus gaussiens

Part 2. processus gaussiens versus réseaux de neurones

Part 3. Physics Informed Neural Networks {PINN}

ML vs Engineering

Kriging (Pioneer)	Gaussian Processes (link with AI)
Developed by Daniel Krige – 1951; formalized by Georges Mathéron in the 60's (Mines Paris) Krig, D. G., 1951, A statistical approach to some basic mine valuation problems on the Witwatersrand: J. Chem. Metal. Min. Soc. South Africa, v. 52, p. 119-139. Matheron, G., 1963b, Principles of geostatistics: Economic Geol., v. 58, p. 1246-1266.	Neural network with infinite neurons tend to Gaussian Process 1994 Neal, R. Priors for infinite networks. Tech. rep., University of Toronto, 1994. Williams, C. K. I., and Rasmussen, C. E. Gaussian processes for regression. <i>Advances in Neural Information Processing Systems 8</i> (1996), 514–520.



SM311 - GP vs NN

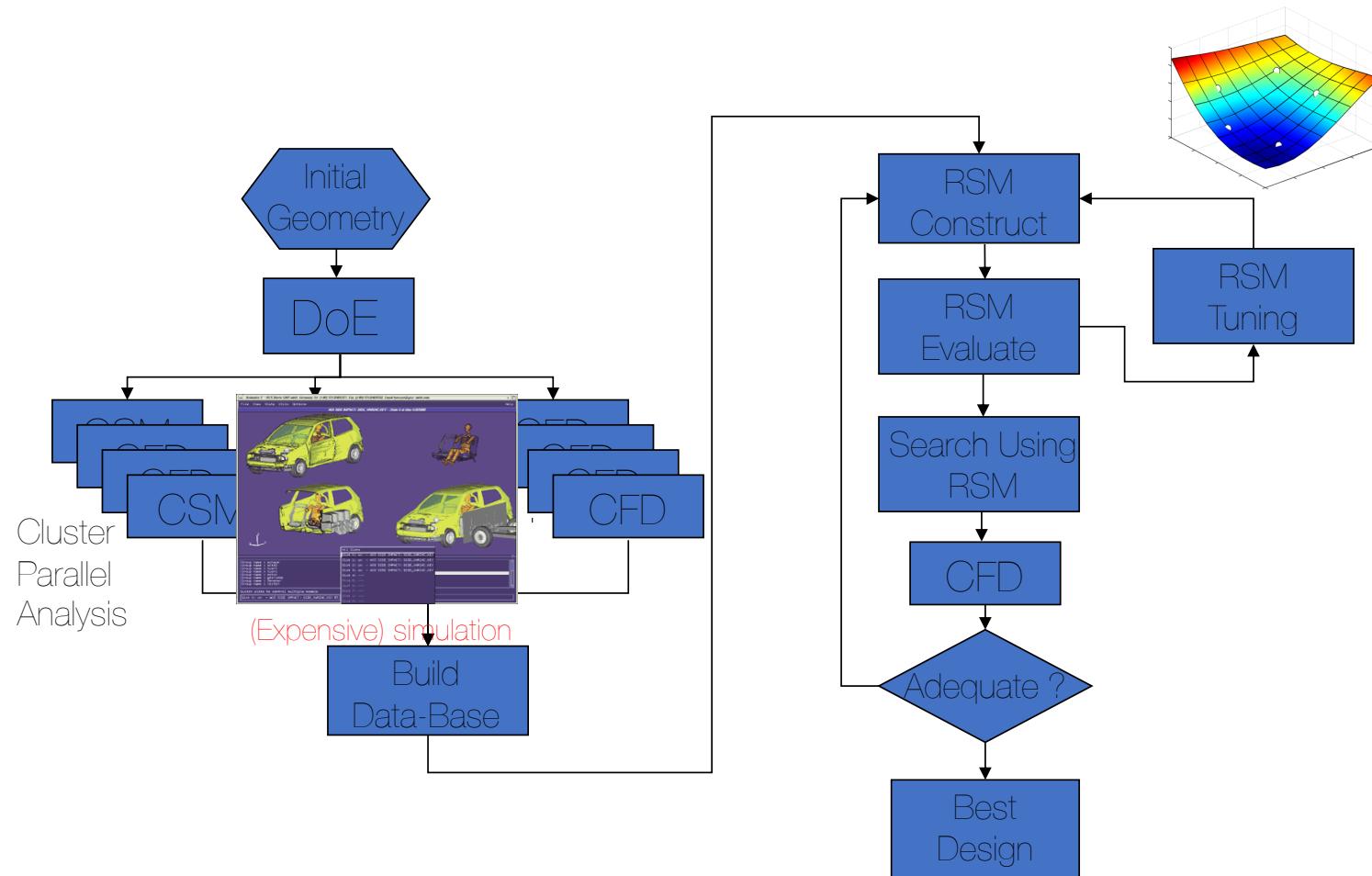
Qualitative claims such as "ML works OK for interpolation but doesn't work for extrapolation" are wrong.

<https://arxiv.org/abs/2110.0948>

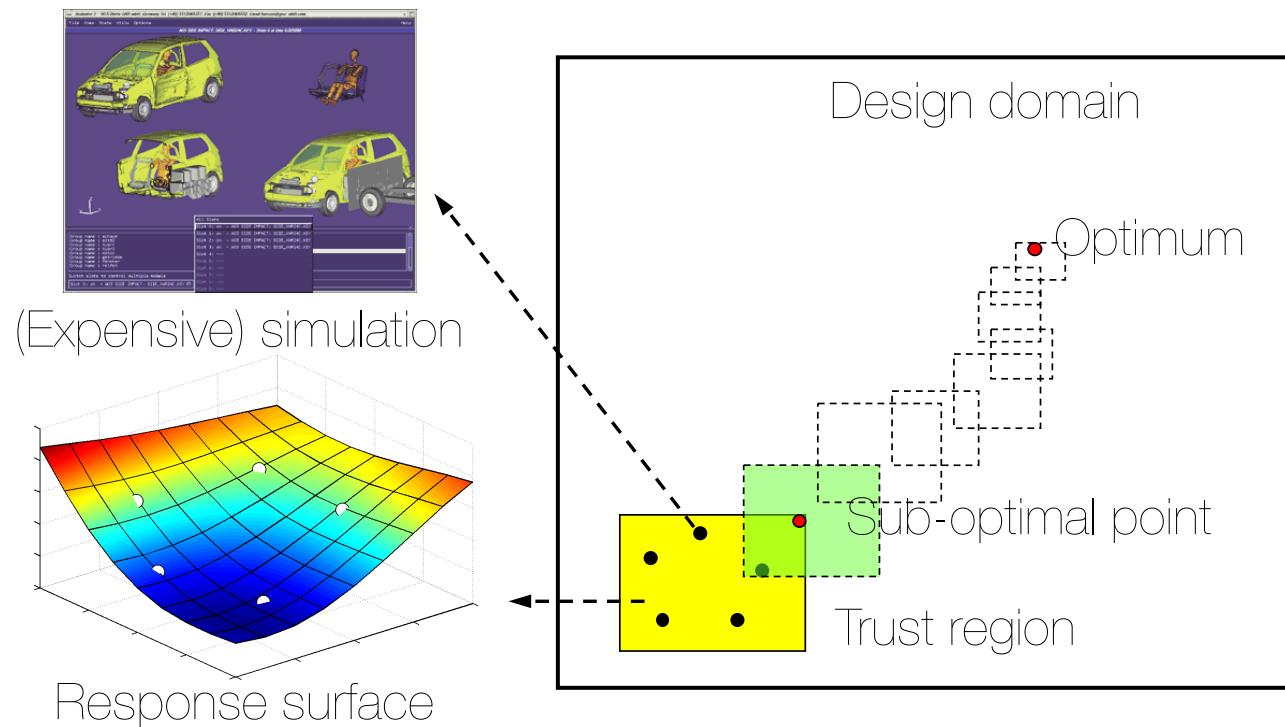
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<http://extrapolated-art.com>

Surrogate



Surrogate Based Optimization by Trust Region



Surrogate Models

- A surrogate model of a function is an approximation of the function that is **much** less costly to evaluate
- The surrogate model can then be used to help direct the search for the optimum of the real objective function

Fitting Surrogate Models

- Given a set of design points and function evaluations,

$$X = \{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(m)}\} \quad \mathbf{y} = \{y^{(1)}, y^{(2)}, \dots, y^{(m)}\}$$

- Find the model parameters which minimize error

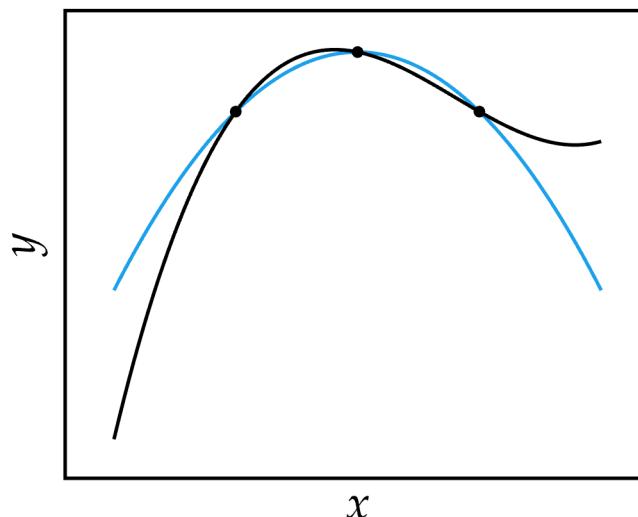
$$\underset{\theta}{\text{minimize}} \quad \|\mathbf{y} - \hat{\mathbf{y}}\|_p$$

$$\hat{\mathbf{y}} = \{\hat{f}_{\theta}(\mathbf{x}^{(1)}), \hat{f}_{\theta}(\mathbf{x}^{(2)}), \dots, \hat{f}_{\theta}(\mathbf{x}^{(m)})\}$$

- This optimization problem is called regression

Fitting Surrogate Models

- Example: approximating f with a quadratic function



- design points
- surrogate model
- true objective function

Basis Functions

- Any surrogate model represented as a linear combination of basis functions can be fit using regression

$$\underset{\boldsymbol{\theta}}{\text{minimize}} \quad \|\mathbf{y} - \mathbf{B}\boldsymbol{\theta}\|_2^2 \quad \boldsymbol{\theta} = \mathbf{B}^+\mathbf{y}$$

<code>inv(B)</code>	<code>linalg.inv(B)</code>	inverse of square 2D array B
<code>pinv(B)</code>	<code>linalg.pinv(B)</code>	pseudo-inverse of 2D array B
<code>y\B</code>	<code>linalg.solve(y, B)</code> if a is square; <code>linalg.lstsq(y, B)</code> otherwise	solution of $\mathbf{B}\boldsymbol{\theta} = \mathbf{y}$ for $\boldsymbol{\theta}$

Basis Functions: Polynomials

- A simple 1-D polynomial model of degree k has the form

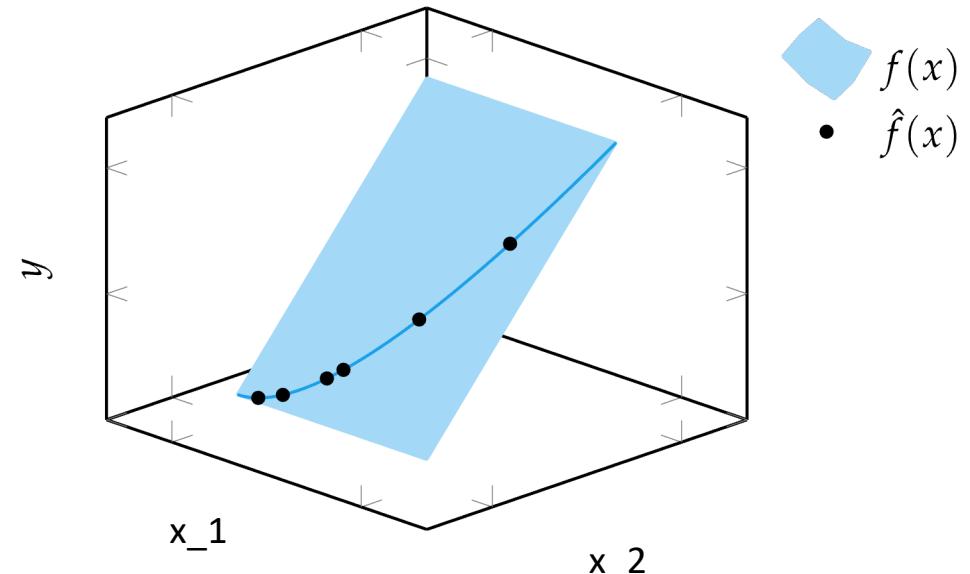
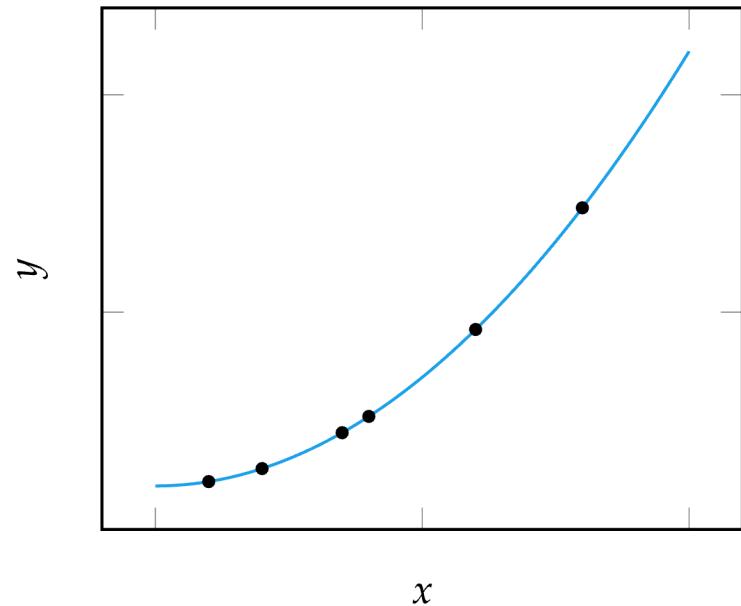
$$\hat{f}(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \cdots + \theta_k x^k = \sum_{i=0}^k \theta_i x^i$$

- In 2-D, the basis function has the form

$$b_{ij}(\mathbf{x}) = x_1^i x_2^j \text{ for } i, j \in \{0, \dots, k\}, \quad i + j \leq k$$

Basis Functions: Polynomials

- Polynomial surrogate models are fit with linear regression, so in a sufficiently high-dimensional space, each polynomial model is always linear



Model Selection

- After a model is fit to data, its quality still must be evaluated
- Data used to fit a model is called **training data**
- Models are compared based on generalization error which is the predictive error on data not in the training set

Model Selection

- One way to quantify generalization error is as the expected squared error of predictions

$$\epsilon_{\text{gen}} = \mathbb{E}_{\mathbf{x} \sim \mathcal{X}} \left[(f(\mathbf{x}) - \hat{f}(\mathbf{x}))^2 \right]$$

- Since this requires knowledge of the original function value at unknown points, it can be tempting to estimate generalization error using training error, which is the mean squared error (MSE) of the model compared to the training data

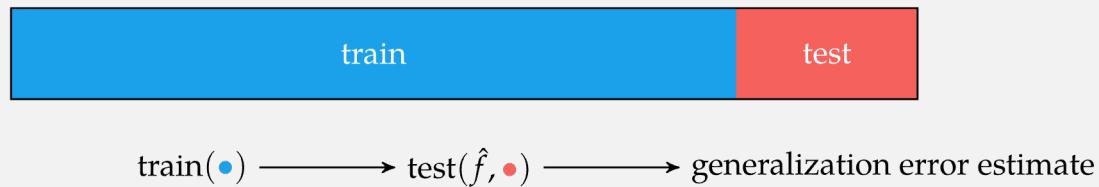
$$\epsilon_{\text{train}} = \frac{1}{m} \sum_{i=1}^m (f(\mathbf{x}^{(i)}) - \hat{f}(\mathbf{x}^{(i)}))^2$$

- Models with low training error can still perform poorly outside of the regions containing training data

Model Selection: Holdout

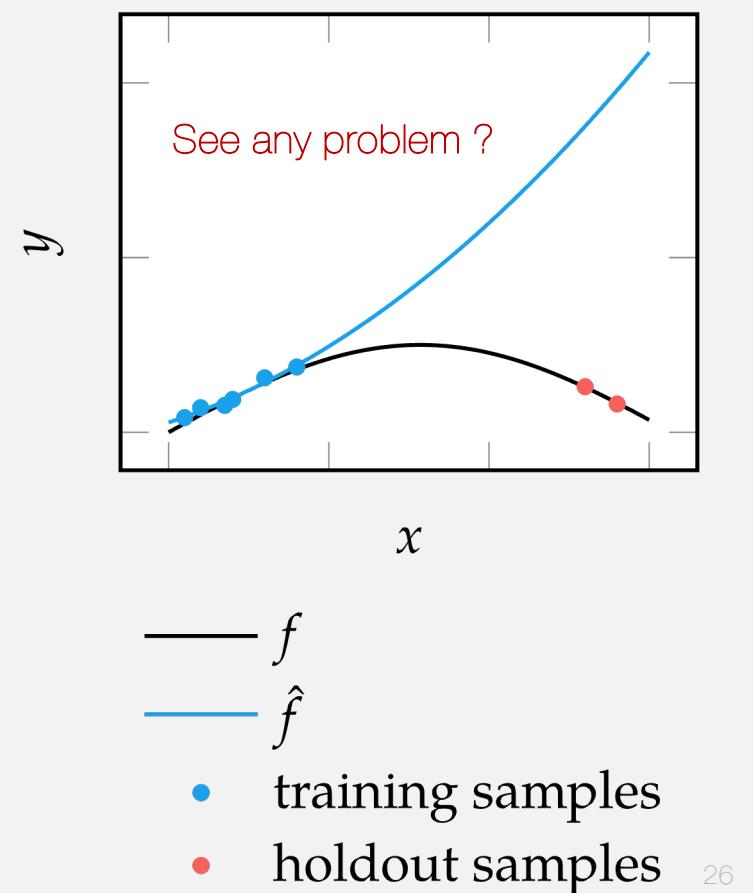
- The holdout method estimates generalization error by partitioning available data into a test set and a training set.
- Data from the test set is used to fit the model, and data from the training set is used to estimate generalization error.
- The model designer must decide how to partition the data into these two sets:
 - If training set is too small, the model will be poor
 - If training set is too large, the generalization error estimate will be poor
- In random subsampling, the holdout method is applied multiple times with randomly selected test-train partitions, with the generalization error averaged over all runs

Model Selection: Holdout



$$\epsilon_{\text{holdout}} = \frac{1}{h} \sum_{(\mathbf{x}, y) \in \mathcal{D}_h} (y - \hat{f}(\mathbf{x}))^2$$

SM311 - GP vs NN



Model Selection: Cross Validation

- Data can be more efficiently utilized for training and validation using k -fold cross validation
 - The original dataset is randomly partitioned into k subsets
 - At the i th iteration, the i th partition is selected as the holdout set
 - The remaining $k - 1$ partitions are used as the training set to generate a model and compute the i th generalization error μ_i
 - The k values of μ are used to compute a mean and standard deviation

Model Selection: Cross Validation



train() \longrightarrow test(\hat{f} ,) \longrightarrow generalization error estimate

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train() \longrightarrow test(\hat{f} ,) \longrightarrow generalization error estimate

train() \longrightarrow test(\hat{f} ,) \longrightarrow generalization error estimate

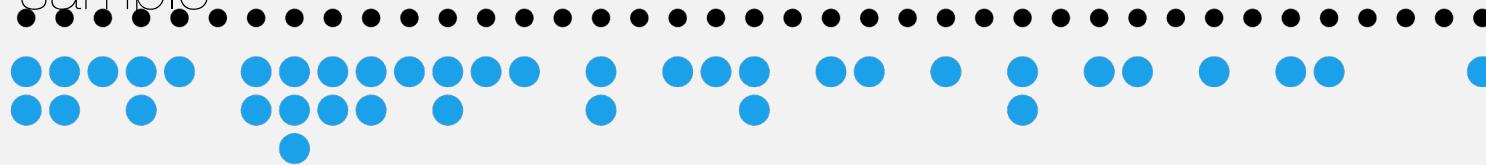
train() \longrightarrow test(\hat{f} ,) \longrightarrow generalization error estimate



generalization error μ and σ

Model Selection: Bootstrap

- The bootstrap method averages the generalization error by training on b bootstrap samples evaluated on the entire training set
- Each bootstrap sample is generated by randomly selecting m data points with replacement from a dataset of size m , meaning some data points can be selected multiple times in the same bootstrap sample

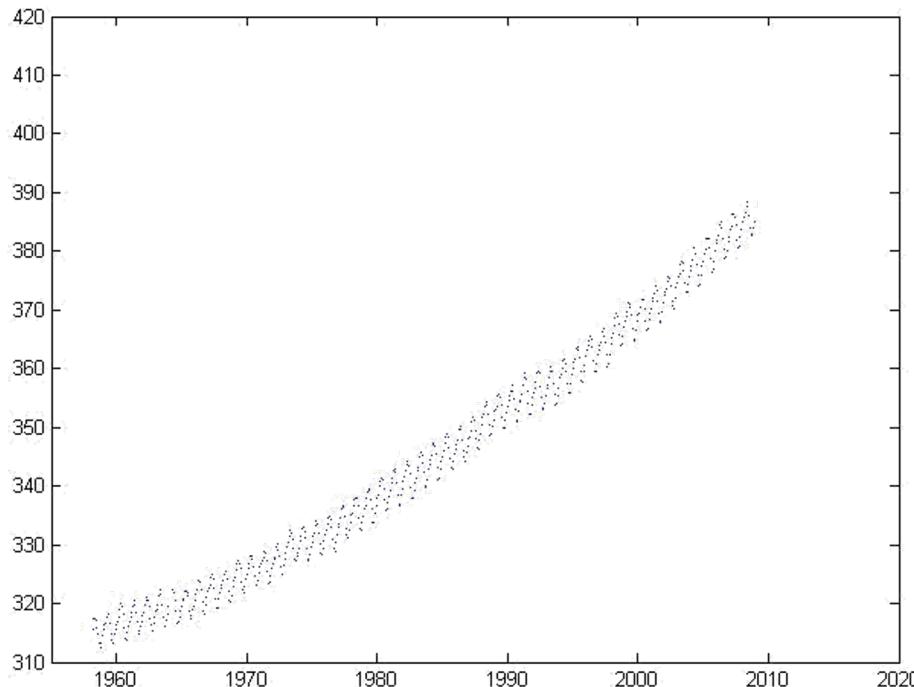


$\text{train}(\bullet) \longrightarrow \text{test}(\hat{f}, \bullet) \longrightarrow \text{generalization error estimate}$

Summary

- Surrogate models are function approximations that can be optimized instead of the true, potentially expensive objective function
- Many surrogate models can be represented using a linear combination of basis functions
- Model selection involves a bias-variance tradeoff between models with low complexity that cannot capture important trends and models with high complexity that overfit to noise
- Generalization error can be estimated using techniques such as holdout, k -fold cross validation, and the bootstrap

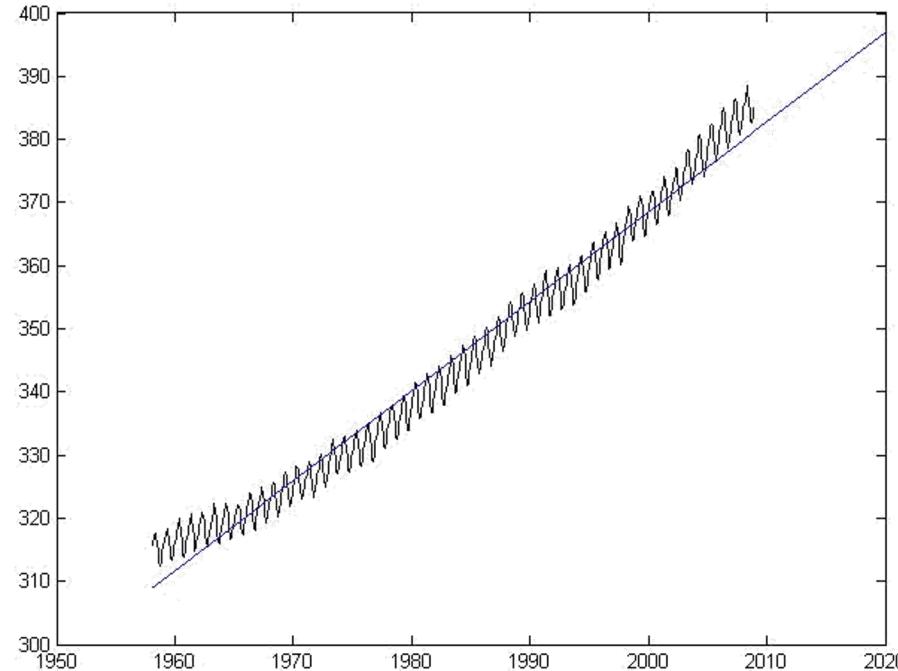
Limit of linear models for prediction



Month-wise data of CO₂ concentration in atmosphere at Hawaii

Image Source: <http://mlg.eng.cam.ac.uk/teaching/4f13/1314/>

Example – Linear Regression



Should we choose a **polynomial**?

What **degree** of polynomial should we choose? (overfitting)

For a given degree, what **parameters** of polynomial should we choose

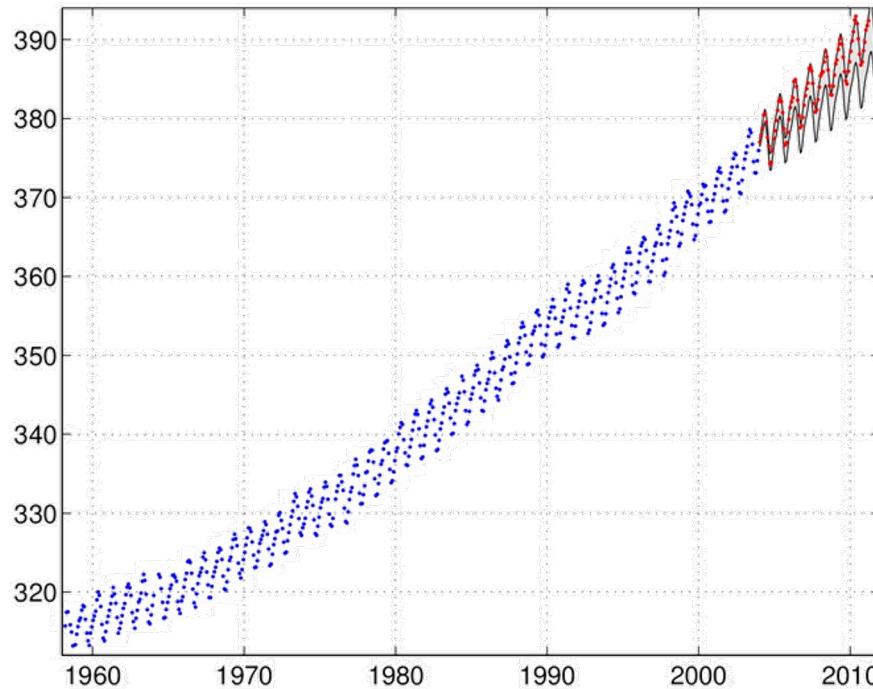
Image Source: <http://mlg.eng.cam.ac.uk/teaching/4f13/1314/>

Example – GP

https://www.pymc.io/projects/examples/en/latest/gaussian_processes/GP-MaunaLoa.html

<https://github.com/cs224/dev-meetup-gaussian-processes/tree/master>

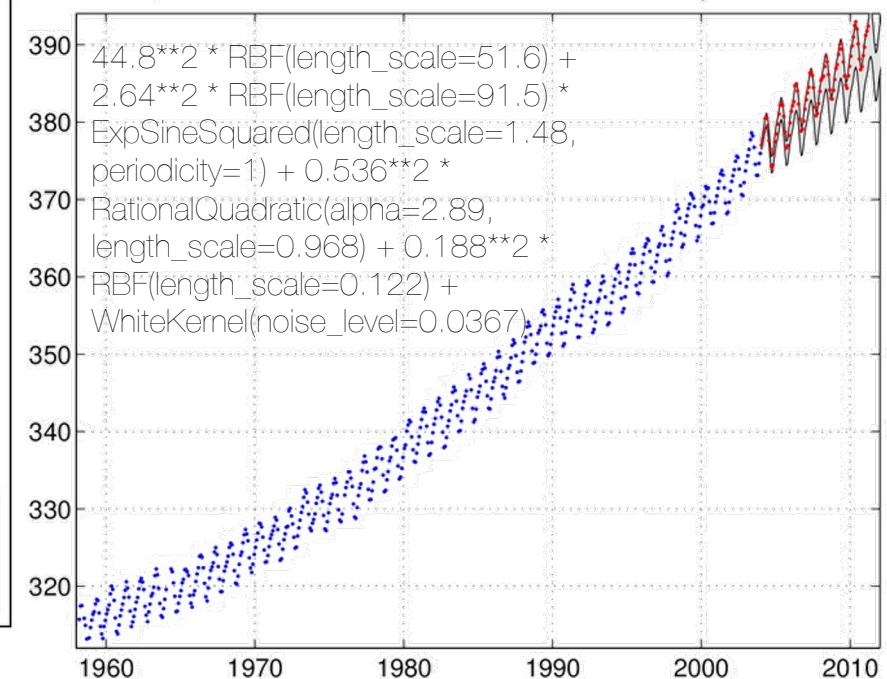
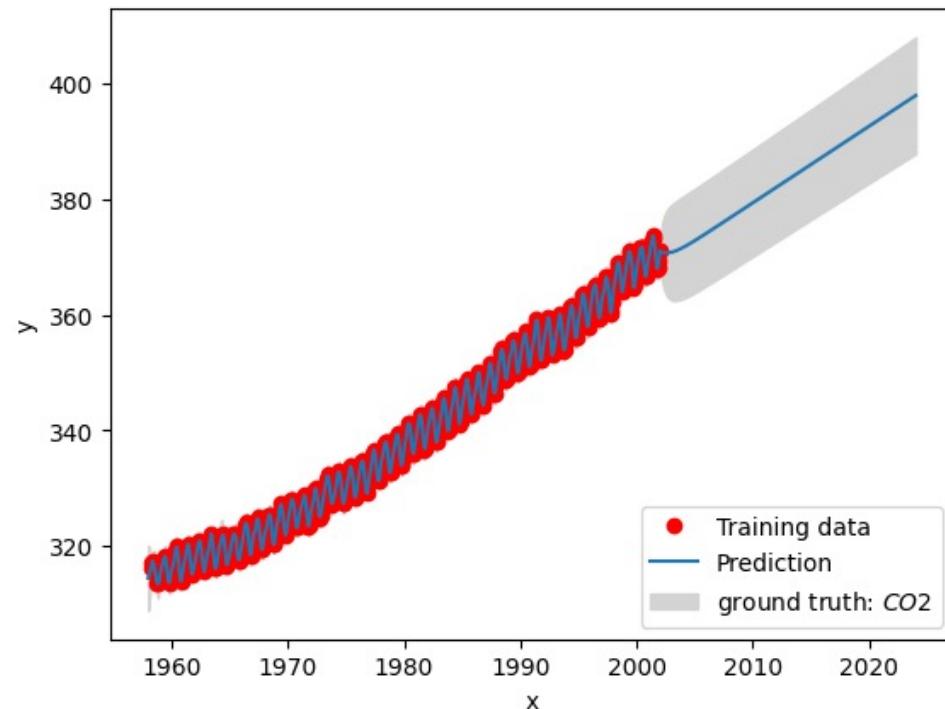
https://scikit-learn.org/stable/auto_examples/gaussian_process/plot_qpr_co2.html



Predicted variance after year 2005 in grey, real data-points in red

Image Source: <http://mlg.eng.cam.ac.uk/teaching/4f13/1314/>

Results



Qualitative claims such as "ML works OK for interpolation but doesn't work for extrapolation" are wrong.

<https://arxiv.org/abs/2110.0948>

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<https://www.cs.toronto.edu/~duvenaud/cookbook/>

https://scikit-learn.org/stable/auto_examples/gaussian_process/plot_gpr_co2.html

Probabilistic Surrogate Models

- It is often useful to quantify confidence in a surrogate model
- One approach is to use a probabilistic model that quantifies our confidence
- A common probabilistic model is the Gaussian process (or Kriging)

Gaussian Distribution



- Also called normal distribution
- Univariate Gaussian distribution is parameterized by mean μ and variance σ^2
- Multivariate Gaussian distribution is parameterized by mean vector μ and covariance matrix Σ
- Probability density at x is given by

$$\mathcal{N}(x | \mu, \Sigma) = (2\pi)^{-n/2} |\Sigma|^{-1/2} \exp\left(-\frac{1}{2} (x - \mu)^\top \Sigma^{-1} (x - \mu)\right)$$

mid ;

$\exp(\cdot) = e^{\cdot}$

Gaussian Distribution

- Sampling a value from a Gaussian is written as

$$\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

$$p(x_2 | x_1=3)$$

- Two jointly Gaussian random variables a and b are written as

$$\begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b \end{bmatrix}, \begin{bmatrix} \mathbf{A} & \mathbf{C} \\ \mathbf{C}^\top & \mathbf{B} \end{bmatrix}\right)$$

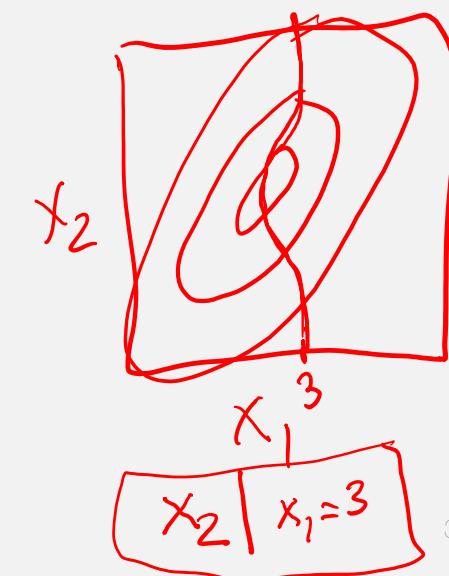
- Each variable's marginal distribution is written as

$$\mathbf{a} \sim \mathcal{N}(\boldsymbol{\mu}_a, \mathbf{A})$$

$$\mathbf{b} \sim \mathcal{N}(\boldsymbol{\mu}_b, \mathbf{B})$$

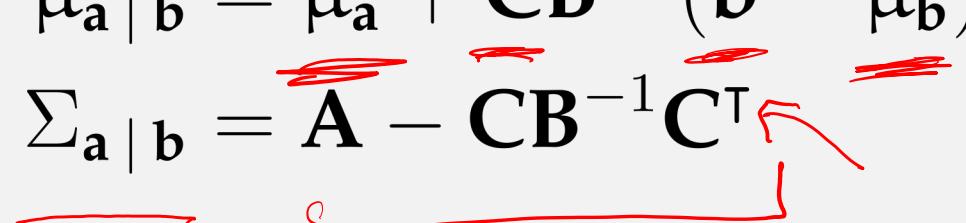
- A variable's conditional distribution is written as

$$\mathbf{a} | \mathbf{b} \sim \mathcal{N}(\boldsymbol{\mu}_{a|b}, \boldsymbol{\Sigma}_{a|b})$$

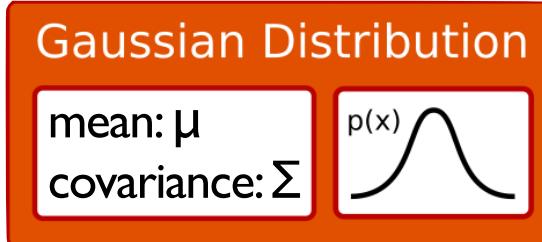


Gaussian Distribution

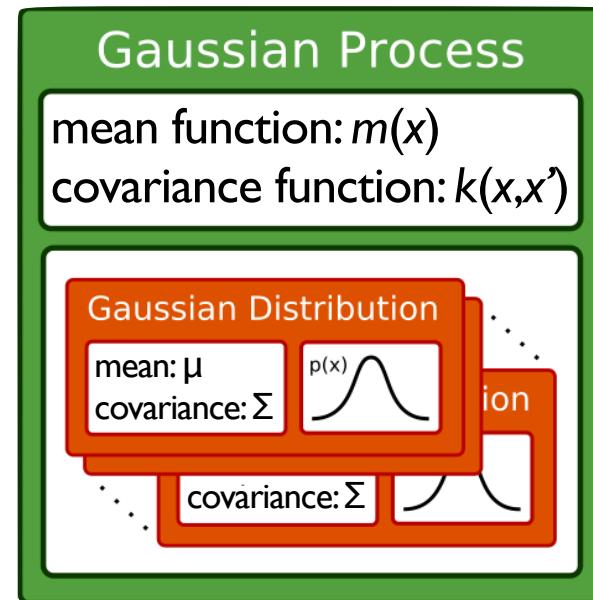
- Given the full set of parameters μ and Σ , the parameters for conditional distributions can be easily computed

$$\begin{aligned}\mu_{\mathbf{a} | \mathbf{b}} &= \mu_{\mathbf{a}} + \mathbf{C}\mathbf{B}^{-1}(\mathbf{b} - \mu_{\mathbf{b}}) \\ \Sigma_{\mathbf{a} | \mathbf{b}} &= \mathbf{A} - \mathbf{C}\mathbf{B}^{-1}\mathbf{C}^T\end{aligned}$$


GD versus GP



$$X \sim \mathcal{G}(\mu, \Sigma)$$



$$f = (f_1, \dots, f_n)^T \sim \mathcal{GP}(m(x), k(x, x'))$$

Gaussian Processes

- A Gaussian Process extends the idea of Gaussian distributions to functions

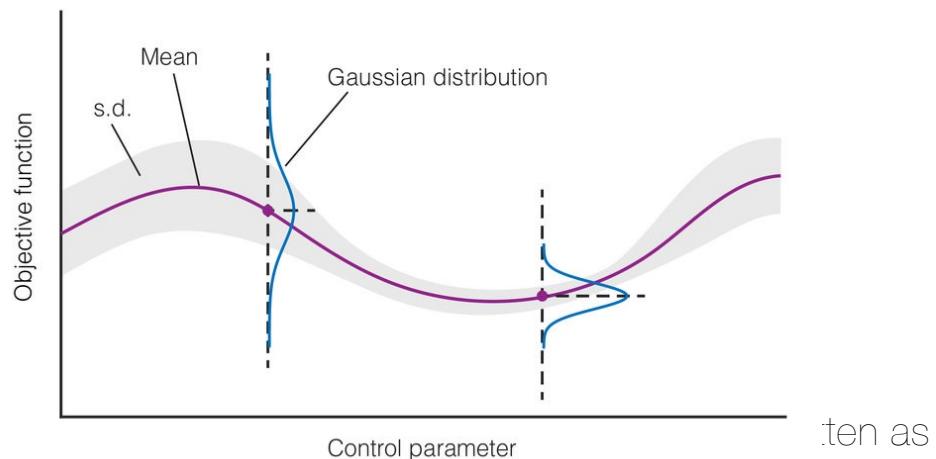
- For any finite set of points, the distribution is

$$k(x, x') = \varphi(x)^T \varphi(x')$$

$\varphi(x)$: a nonlinear feature space mapping

k is a symmetric function of its arguments so that

$$k(x, x') = k(x', x)$$



$$\begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} m(\mathbf{x}^{(1)}) \\ \vdots \\ m(\mathbf{x}^{(m)}) \end{bmatrix}, \begin{bmatrix} k(\mathbf{x}^{(1)}, \mathbf{x}^{(1)}) & \cdots & k(\mathbf{x}^{(1)}, \mathbf{x}^{(m)}) \\ \vdots & \ddots & \vdots \\ k(\mathbf{x}^{(m)}, \mathbf{x}^{(1)}) & \cdots & k(\mathbf{x}^{(m)}, \mathbf{x}^{(m)}) \end{bmatrix} \right)$$

Here, $m(x)$ is the mean function and $k(x, x')$ is the covariance function or kernel

Supervised learning + Normal distribution

— Soit $D = \{\mathbf{x}^i, y^i\}_{i=1}^N$ nos données et $\mathbf{x}_t^1 \dots \mathbf{x}_t^T$ les points que l'on veut inférer.
On a établit que (en simplifiant en fixant la moyenne à 0) :

$$p \left(\begin{pmatrix} y^1 \\ \vdots \\ y^N \\ y_t^1 \\ \vdots \\ y_t^T \end{pmatrix} \mid \mathbf{x}^1, \mathbf{x}^2, \dots, \mathbf{x}^N, \mathbf{x}_t^1, \dots, \mathbf{x}_t^T \right) \sim \mathcal{N}(0, \Sigma), \quad \Sigma = \begin{bmatrix} K & K_\star \\ K_\star^t & K_{**} \end{bmatrix}$$

Alors

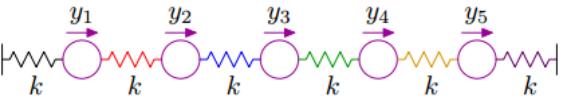
$$p(y_t^1 \dots y_t^T \mid \mathbf{y}, \mathbf{x}^1, \dots, \mathbf{x}_t^T) \sim \mathcal{N}(K_\star^t K^{-1} \mathbf{y}, K_{**} - K_\star^t K^{-1} K_\star)$$

Mais comment obtenir:

- K les covariances entre les points d'entraînement ?
- K_\star les covariances entre entraînement et test ?
- K_{**} les covariances entre test ?

[Processus Gaussien](#) , Cours 8, ML Master DAC , Nicolas Baskiotis

Quiz on the meaning of K

- Example: 
- Which is the covariance matrix, and which the inverse covariance?

$$\frac{k}{T} \begin{bmatrix} 2 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix} \quad \frac{T}{k} \begin{bmatrix} 0.83 & 0.67 & 0.50 & 0.33 & 0.17 \\ 0.67 & 1.33 & 1.00 & 0.67 & 0.33 \\ 0.50 & 1.00 & 1.50 & 1.00 & 0.50 \\ 0.33 & 0.67 & 1.00 & 1.33 & 0.67 \\ 0.17 & 0.33 & 0.50 & 0.67 & 0.83 \end{bmatrix}$$

<http://www.inference.org.uk/mackay/humble.pdf>

Matrice de covariance = Kernel !

Ce que l'on veut pour la matrice de covariance :

- qu'elle soit symétrique ! (i influence j comme j influence i)
- deux points "similaires" doivent avoir une corrélation forte : $\text{Cov}(\mathbf{x}^i, \mathbf{x}^j)$ grand
- deux points "dissimilaires" doivent avoir une corrélation faible : $\text{Cov}(\mathbf{x}^i, \mathbf{x}^j)$ petit
- qu'elle soit semi-défini positive
- $\text{Cov}(\mathbf{x}^i, \mathbf{x}^i)$ doit dénoté la variance en ce point

⇒ Très similaire à la notion de noyaux en SVM ! Autant utiliser une fonction noyau pour encoder la covariance ...

Covariances typiques :

- Squared Exponential : $K(\mathbf{x}^1, \mathbf{x}^2) = \sigma^2 e^{-\frac{1}{2}\left(\frac{\|\mathbf{x}^1 - \mathbf{x}^2\|^2}{\lambda}\right)}$
- Linéaire : $K(\mathbf{x}^1, \mathbf{x}^2) = \lambda + \langle \mathbf{x}^1, \mathbf{x}^2 \rangle$
- Periodic : $K(\mathbf{x}^1, \mathbf{x}^2) = \sigma^2 e^{-\frac{2\sin^2\left(\frac{\|\mathbf{x}^1 - \mathbf{x}^2\|}{2}\right)}{\lambda^2}}$

Sometimes people express probabilistic models in terms of energy functions that are minimized in the most probable configuration. For example, in regression with cubic splines, a regularizer is defined which describes the energy that a steel ruler would have if bent into the shape of the curve.

Such models usually have the form:

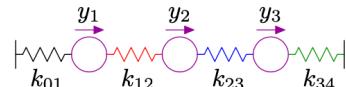
$$P(\mathbf{y}) = \frac{1}{Z} e^{-\frac{E(\mathbf{y})}{T}}, \quad (29)$$

and in simple cases, the energy $E(\mathbf{y})$ may be a quadratic function of \mathbf{y} , such as

$$E(\mathbf{y}) = - \sum_{i < j} J_{ij} y_i y_j + \sum_i a_i y_i^2 \quad (30)$$

If so, then the distribution is a Gaussian (just like (1)), and the ‘couplings’ J_{ij} are minus the coefficients in the *inverse* covariance matrix.

As a simple example, consider a set of three masses coupled by springs, and subjected to thermal perturbations.



THREE MASSES, FOUR SPRINGS

The equilibrium positions are $(y_1, y_2, y_3, y_4) = (0, 0, 0, 0)$, and the spring constants are k_{ij} . The extension of the second spring is $y_2 - y_1$. The energy of this system is

$$\begin{aligned} E(\mathbf{y}) &= \frac{1}{2} k_{01} y_1^2 + \frac{1}{2} k_{12} (y_2 - y_1)^2 + \frac{1}{2} k_{23} (y_3 - y_2)^2 + \frac{1}{2} k_{34} y_3^2 \\ &= \frac{1}{2} \begin{bmatrix} y_1 & y_2 & y_3 \end{bmatrix} \begin{bmatrix} k_{01} + k_{12} & -k_{12} & 0 \\ -k_{12} & k_{12} + k_{23} & -k_{23} \\ 0 & -k_{23} & k_{23} + k_{34} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \end{aligned}$$

So at temperature T , the probability distribution of the displacements is Gaussian with inverse covariance matrix

$$\frac{1}{T} \begin{bmatrix} k_{01} + k_{12} & -k_{12} & 0 \\ -k_{12} & k_{12} + k_{23} & -k_{23} \\ 0 & -k_{23} & k_{23} + k_{34} \end{bmatrix} \quad (31)$$

Notice that there are 0 entries between displacements y_1 and y_3 , the two masses that are not directly coupled by a spring.

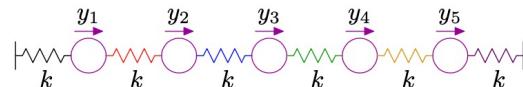


Figure 1. FIVE MASSES, SIX SPRINGS

So inverse covariance matrices are sometimes very sparse. If we have five masses in a row connected by identical springs k for example, then

$$\mathbf{K}^{-1} = \frac{k}{T} \begin{bmatrix} 2 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix}. \quad (32)$$

But this sparsity doesn't carry over to the covariance matrix, which is

$$\mathbf{K} = \frac{T}{k} \begin{bmatrix} 0.83 & 0.67 & 0.50 & 0.33 & 0.17 \\ 0.67 & 1.33 & 1.00 & 0.67 & 0.33 \\ 0.50 & 1.00 & 1.50 & 1.00 & 0.50 \\ 0.33 & 0.67 & 1.00 & 1.33 & 0.67 \\ 0.17 & 0.33 & 0.50 & 0.67 & 0.83 \end{bmatrix}. \quad (33)$$

Et si on introduit du bruit ?

Bruit additif gaussien

- On observe $y^i = f(\mathbf{x}^i) + \epsilon_i$, avec ϵ_i indépendant et suivant $\mathcal{N}(0, \sigma^2)$
- La covariance est changée en $\hat{\Sigma}$:

$$\hat{\Sigma}_{ij} = \mathbb{E}[(f(\mathbf{x}^i) + \epsilon_i)(f(\mathbf{x}^j) + \epsilon_j)] = \mathbb{E}[f(\mathbf{x}^i)f(\mathbf{x}^j)] + \mathbb{E}[f(\mathbf{x}^j)]\mathbb{E}[\epsilon_i] + \mathbb{E}[f(\mathbf{x}^i)]\mathbb{E}[\epsilon_j] + \mathbb{E}[\epsilon_i\epsilon_j]$$

- Pour $i \neq j$, $\mathbb{E}[\epsilon_i] = 0$, $\mathbb{E}[\epsilon_i\epsilon_j] = \mathbb{E}[\epsilon_i]\mathbb{E}[\epsilon_j] = 0$

$$\hat{\Sigma}_{ij} = \mathbb{E}[f(\mathbf{x}^i)f(\mathbf{x}^j)] = \Sigma_{ij}$$

- Pour $i = j$, $\mathbb{E}[\epsilon_i] = 0$, $\mathbb{E}[\epsilon_i^2] = \sigma^2$

$$\hat{\Sigma}_{ii} = \mathbb{E}[f(\mathbf{x}^i)f(\mathbf{x}^i)] + \mathbb{E}[\epsilon_i^2] = \Sigma_{ii} + \sigma^2$$

- Donc $\hat{\Sigma} = \Sigma + \sigma^2 \mathbf{I}$

Formule de la régression GP dans le cas général

$$p(y_t^1 \dots y_t^T | \mathbf{y}, \mathbf{x}^1, \dots \mathbf{x}_t^T) \sim \mathcal{N}(K_\star^t(K + \sigma^2 \mathbf{I})^{-1} \mathbf{y}, K_{\star\star} - K_\star^t(K + \sigma^2 \mathbf{I})^{-1} K_\star)$$

⇒ Régression à noyaux !

- Mais avec l'information sur l'incertitude liée à la prédiction !

Définition

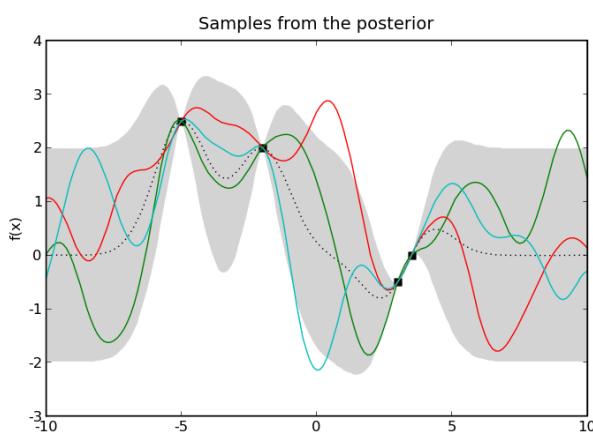
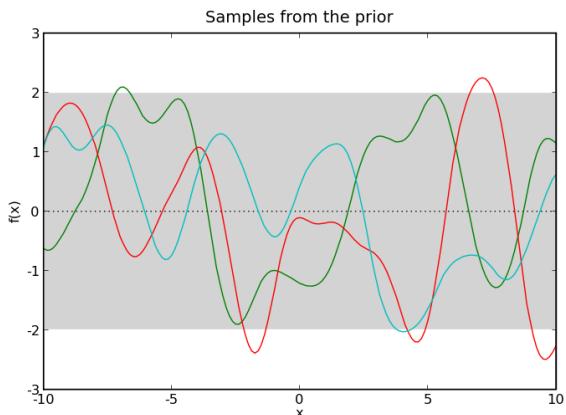
- La fonction f dont on cherche la prédiction est vue comme une collection de points f (les mesures en différents points) potentiellement infinie.
- Un processus gaussien est une collection de variables aléatoires (potentiellement infinie) tels que la distribution jointe de tout sous-ensemble de ces variables est une gaussienne multivariée :

$$f \sim GP(\mu, k)$$

avec $\mu(\mathbf{x})$ et $k(\mathbf{x}^1, \mathbf{x}^2)$ sont les fonctions de moyenne et de covariance.

- On cherche à estimer la distribution $P(f_t | \mathbf{x}_t, D)$ en utilisant un prior GP : $P(f | \mathbf{x}) \sim \mathcal{N}(\mu, \Sigma)$ et en le conditionnant par les données d'entraînement D afin de modéliser la distribution jointe f des points d'entraînement et f_t , les points de test.

- The covariance function defines how smoothly the (latent) function f varies from a given x .
- The data points “anchor” the function f at specific x locations.



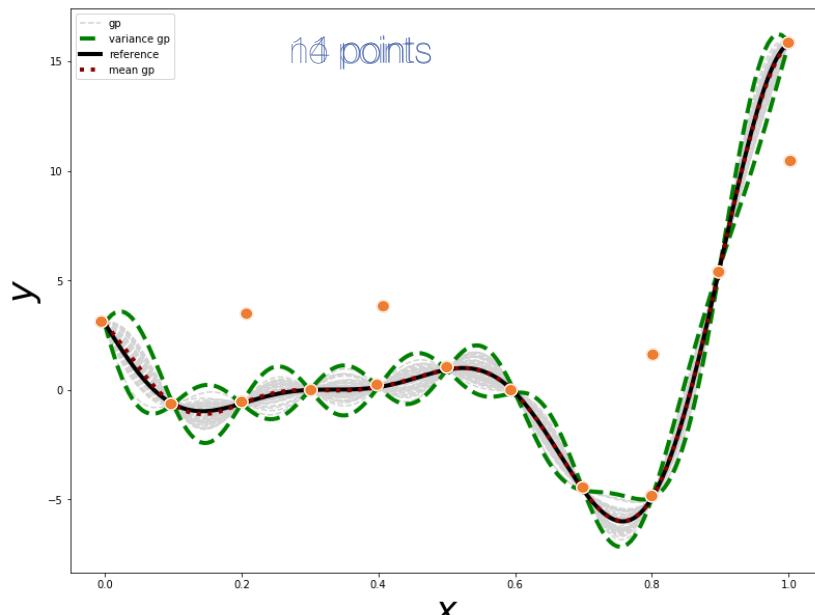
Main steps to build a surrogate model

1. Black box to replace by a surrogate model

$$y(x^{(i)}) = f(x^{(i)}) \text{ with } x^{(i)} \in \mathbb{R}^d$$

where f is the model (expensive, free-derivative, noise-free) such as CFD code or FEM code

Gaussian process or Kriging model

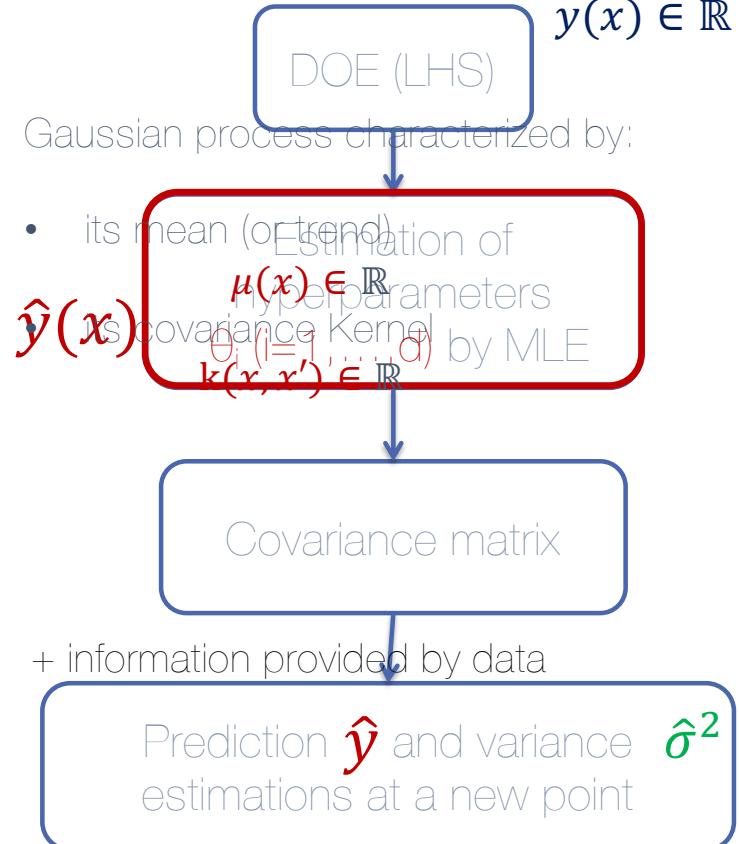


- Hyperparameters tuning (99% of time not the uncertainties in these estimates)
- Number of hyperparameters increases with the dimension d (number of design variables)
- Curse of dimensionality

D. G. Krige, A statistical approach to some basic mine valuation problems on the Witwatersrand, 1951, Journal of the Southern African Institute of Mining and Metallurgy.

$$x \in \mathbb{R}^d$$

$$y(x) \in \mathbb{R}$$



$$\mu_{\mathbf{a} \mid \mathbf{b}} = \mu_{\mathbf{a}} + \mathbf{C}\mathbf{B}^{-1}(\mathbf{b} - \mu_{\mathbf{b}})$$

$$\Sigma_{\mathbf{a} \mid \mathbf{b}} = \mathbf{A} - \mathbf{C}\mathbf{B}^{-1}\mathbf{C}^T$$

Prediction

- The predicted values can be found using the conditional distribution

$$\hat{\mathbf{y}} \mid \mathbf{y} \sim \mathcal{N} \left(\underbrace{\mathbf{m}(X^*) + \mathbf{K}(X^*, X)\mathbf{K}(X, X)^{-1}(\mathbf{y} - \mathbf{m}(X))}_{\text{mean}}, \underbrace{\mathbf{K}(X^*, X^*) - \mathbf{K}(X^*, X)\mathbf{K}(X, X)^{-1}\mathbf{K}(X, X^*)}_{\text{covariance}} \right)$$

using the conditional distribution formulas previously presented

- The predicted mean and variance of $\hat{\mathbf{y}}$ is

$$\begin{aligned} \hat{\mu}(\mathbf{x}) &= m(\mathbf{x}) + \mathbf{K}(\mathbf{x}, X)\mathbf{K}(X, X)^{-1}(\mathbf{y} - \mathbf{m}(X)) \\ &= m(\mathbf{x}) + \theta^T \mathbf{K}(X, \mathbf{x}) \\ \hat{\nu}(\mathbf{x}) &= \mathbf{K}(\mathbf{x}, \mathbf{x}) - \mathbf{K}(\mathbf{x}, X)\mathbf{K}(X, X)^{-1}\mathbf{K}(X, \mathbf{x}) \end{aligned}$$

Matrix view of Gaussian Process

1/ Get your inputs/outputs data

$$\begin{bmatrix} x \\ y(x) \end{bmatrix}$$

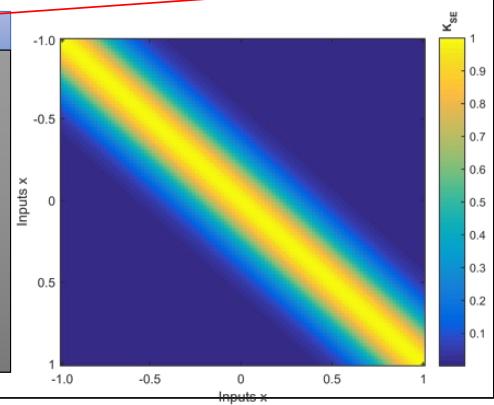
2/ You wan to predict at x^*

$$\begin{bmatrix} x^* \end{bmatrix}$$

$$k(x, x') = \theta_1^2 \exp\left(-\frac{(x - x')^2}{2\theta_2^2}\right)$$

3/ Choose a Kernel/Construct K_{xx} and Hyperparameters tuning

$$= \begin{bmatrix} x^T \\ K_{xx} \end{bmatrix}$$



$$m(y^*) = [K_{x^*x_S}] \begin{bmatrix} [K_{xx}]^{-1} \\ y(x) \end{bmatrix}$$

4/ compute mean

$$m(x^*) = K_* [K_{xx}]^{-1} y$$

$$\text{cov}(y^*) = [K_{x_S x_S}] - [K_{x^* x_S}] \begin{bmatrix} [K_{xx}]^{-1} \\ [K_{x^* x_S}] \end{bmatrix}$$

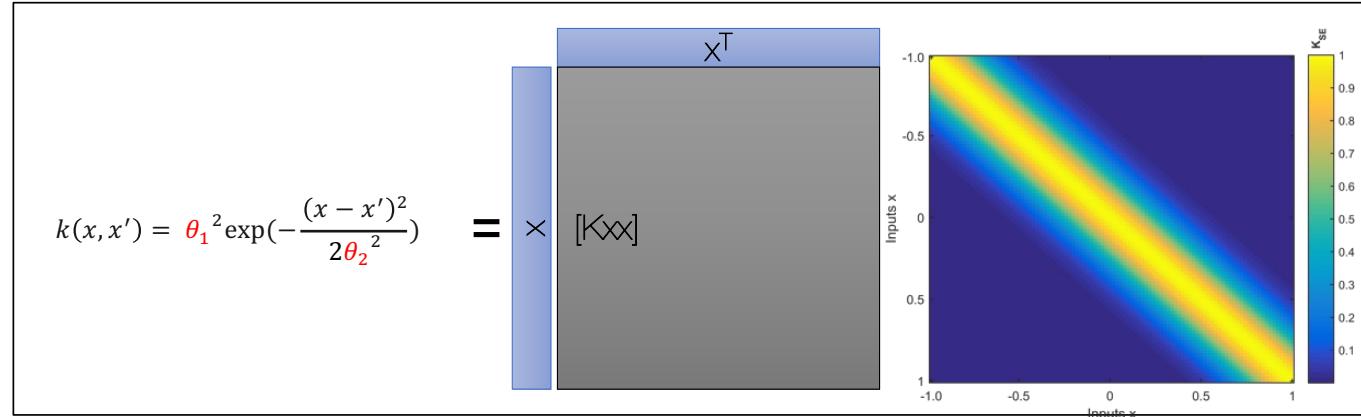
4/ compute variance of estimate

$$\text{var}(x^*, x'^*) = K_{**} - K_*^T [K_{xx}]^{-1} K_*$$

Matrix view of Gaussian Process

$$\begin{bmatrix} \times \\ \times \end{bmatrix} \begin{bmatrix} y(x) \end{bmatrix}$$

$$*\;$$



$$m(y^*) = [K_{x^*x_s}] \begin{bmatrix} [K_{xx}]^{-1} \\ y(x) \end{bmatrix}$$

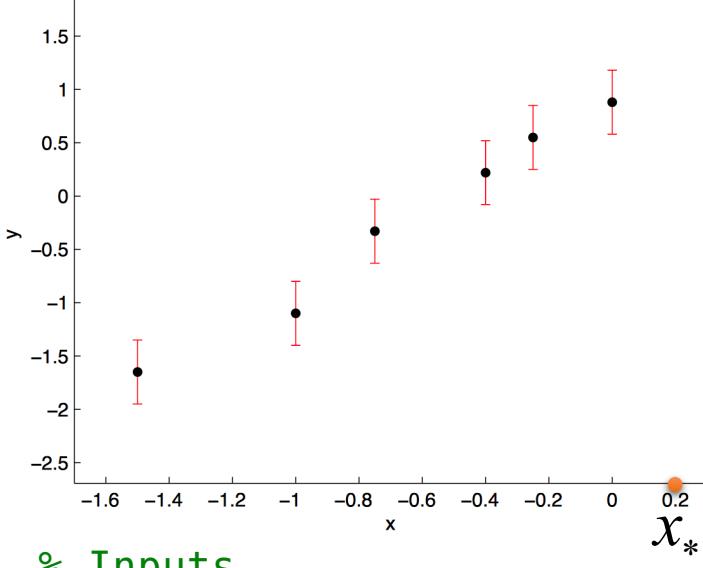
posterior_mean = covXXs @ np.linalg.inv(covXX_noisy) @ y

$$\text{cov}(y^*) = [K_{x_s x_s}] - [K_{x^* x_s}] \begin{bmatrix} [K_{xx}]^{-1} \\ [K_{x^* x_s}] \end{bmatrix}$$

posterior_cov = covXsXs - covXXs @ np.linalg.inv(covXX_noisy) @

Example

Gaussian Processes for Regression A Quick Introduction, M.Ebden, August 2008.



$$k(x, x') = \sigma_f^2 \exp\left[-\frac{(x - x')^2}{2l^2}\right] + \sigma_n \delta(x, x') \quad \delta(x, x') = \begin{cases} 1, & x = x' \\ 0, & x \neq x' \end{cases}$$

$$K = \begin{bmatrix} k(x_1, x_1) & k(x_1, x_2) & \cdots & k(x_1, x_n) \\ k(x_2, x_1) & k(x_2, x_2) & \cdots & k(x_2, x_n) \\ \vdots & \vdots & \ddots & \vdots \\ k(x_n, x_1) & k(x_n, x_2) & \cdots & k(x_n, x_n) \end{bmatrix} \quad \% \text{ Taille } 6*6$$

$$K_* = [k(x_*, x_1) \quad k(x_*, x_2) \quad \cdots \quad k(x_*, x_n)] \quad K_{**} = k(x_*, x_*)$$

$$\begin{bmatrix} \mathbf{y} \\ y_* \end{bmatrix} \sim \mathcal{N} \left(\mathbf{0}, \begin{bmatrix} K & K_*^T \\ K_* & K_{**} \end{bmatrix} \right)$$

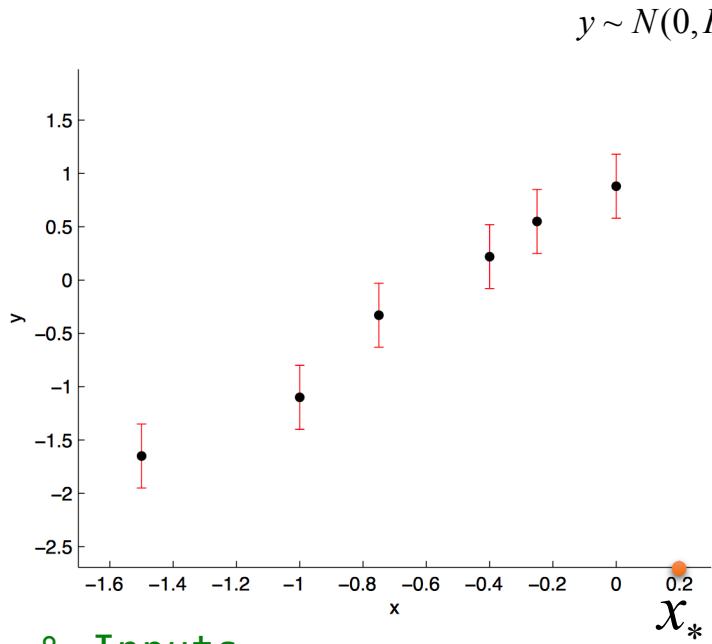
$$y_* | \mathbf{y} \sim \mathcal{N}(K_* K^{-1} \mathbf{y}, K_{**} - K_* K^{-1} K_*^T)$$

$$\bar{y}_* = K_* K^{-1} \mathbf{y} \quad \text{var}(y_*) = K_{**} - K_* K^{-1} K_*^T$$

(0.20, ?)

Example

Gaussian Processes for Regression A Quick Introduction, M.Ebden, August 2008.



```
% Inputs
X = [-1.5 -1 -.75 -.4 -.25 0]';
% Outputs
y = [-1.6 -1.10 -.4 .2 0.6 1]';
```

(0.20, ?)

$$y \sim N(0, K)$$

$$k(x, x') = \sigma_f^2 \exp\left[-\frac{(x - x')^2}{2l^2}\right] + \sigma_n \delta(x, x') \quad \delta(x, x') = \begin{cases} 1, & x = x' \\ 0, & x \neq x' \end{cases}$$

Code

```
from scipy.spatial.distance import cdist

def rbf_kernel(x1, x2, varSigma, lengthscale):
    if x2 is None:
        d = cdist(x1, x1)
    else:
        d = cdist(x1, x2)

    K = varSigma*np.exp(-np.power(d, 2)/lengthscale)

    return K
```

Code

```
def lin_kernel(x1, x2, varSigma):
    if x2 is None:
        return varSigma*x1.dot(x1.T)
    else:
        return varSigma*x1.dot(x2.T)

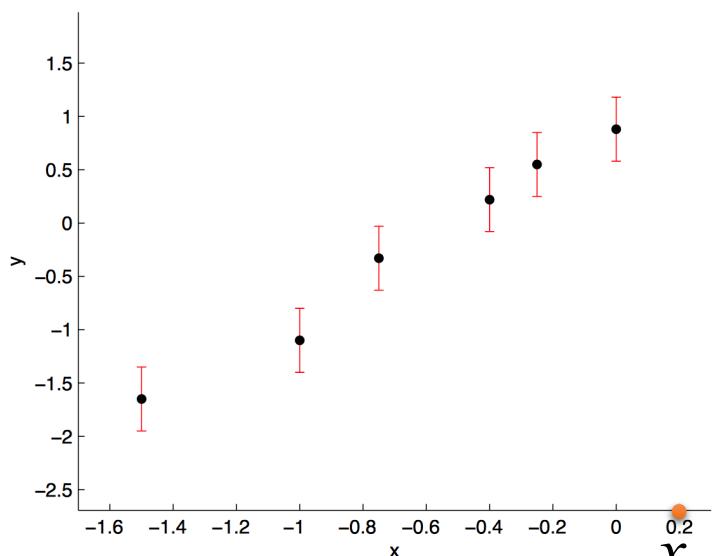
def white_kernel(x1, x2, varSigma):
    if x2 is None:
        return varSigma*np.eye(x1.shape[0])
    else:
        return np.zeros(x1.shape[0], x2.shape[0])

def periodic_kernel(x1, x2, varSigma, period, lengthScale):
    if x2 is None:
        d = cdist(x1, x1)
    else:
        d = cdist(x1, x2)

    return varSigma*np.exp(-(2*np.sin((np.pi/period)*d)**2)/lengthScale**2)
```

Example

Gaussian Processes for Regression A Quick Introduction, M.Ebden, August 2008.



```
% Inputs
X = [-1.5 -1 -.75 -.4 -.25 0]';
% Outputs
y = [-1.6 -1.10 -.4 .2 0.6 1]';
```

(0.20, ?)

Code

```
def gp_prediction(x1, y1, xstar, lengthScale, varSigma, noise):

    k_starX = rbf_kernel(xstar,x1,lengthScale,varSigma,noise)
    k_xx = rbf_kernel(x1, None, lengthScale, varSigma, noise)
    k_starstar = rbf_kernel(xstar,None,lengthScale,varSigma,noise)

    mu = k_starX.dot(np.linalg.inv(k_xx)).dot(y1)
    var = k_starstar - (k_starX).dot(np.linalg.inv(k_xx)).dot(k_starX.T)

    return mu, var, xstar
```

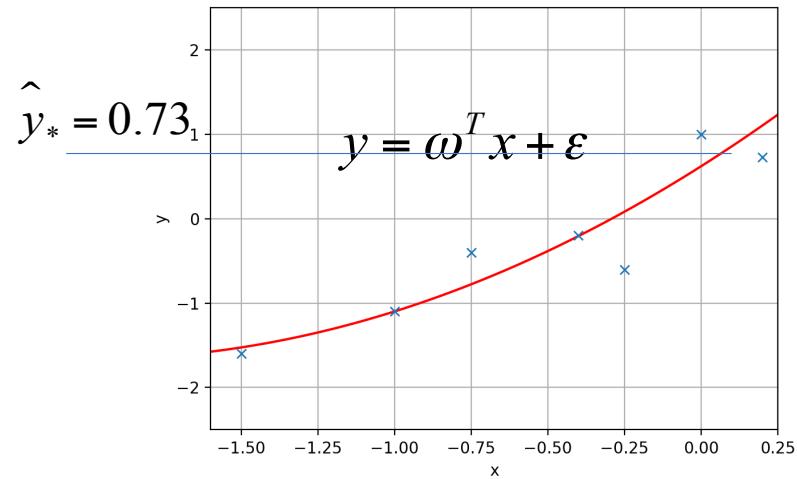
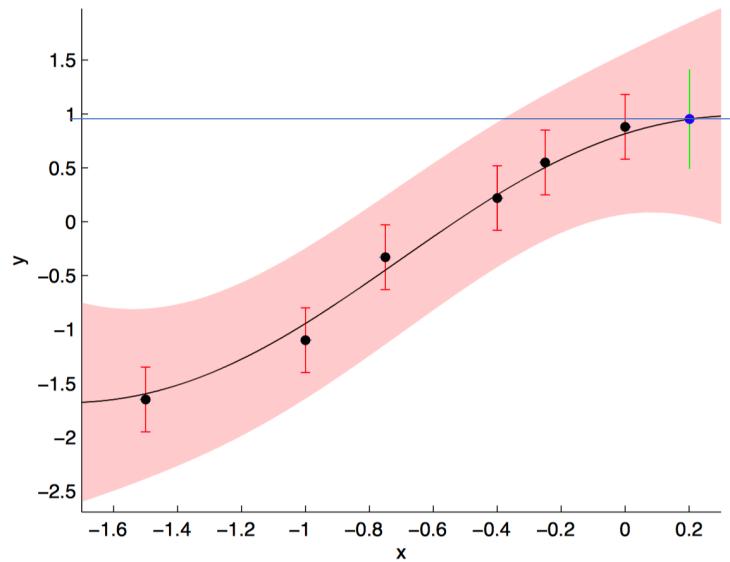
$$K_* = [k(x_*, x_1) \quad k(x_*, x_2) \quad \cdots \quad k(x_*, x_n)] \quad K_{**} = k(x_*, x_*)$$

$$\begin{bmatrix} \mathbf{y} \\ y_* \end{bmatrix} \sim \mathcal{N} \left(\mathbf{0}, \begin{bmatrix} K & K_*^T \\ K_* & K_{**} \end{bmatrix} \right)$$

$$y_* | \mathbf{y} \sim \mathcal{N}(K_* K^{-1} \mathbf{y}, K_{**} - K_* K^{-1} K_*^T)$$

$$\bar{y}_* = K_* K^{-1} \mathbf{y} \quad \text{var}(y_*) = K_{**} - K_* K^{-1} K_*^T$$

Numerical values



$$\sigma_n = 0.3$$

$$K = \begin{bmatrix} 1.70 & 1.42 & 1.21 & 0.87 & 0.72 & 0.51 \\ 1.42 & 1.70 & 1.56 & 1.34 & 1.21 & 0.97 \\ 1.21 & 1.56 & 1.70 & 1.51 & 1.42 & 1.21 \\ 0.87 & 1.34 & 1.51 & 1.70 & 1.59 & 1.48 \\ 0.72 & 1.21 & 1.42 & 1.59 & 1.70 & 1.56 \\ 0.51 & 0.97 & 1.21 & 1.48 & 1.56 & 1.70 \end{bmatrix}$$

$$K_{**} = 1.70 \quad K_* = [0.38 \quad 0.79 \quad 1.03 \quad 1.35 \quad 1.46 \quad 1.58]$$

$$\bar{y}_* = 0.95 \quad \text{var}(y_*) = 0.21$$

How to start?

Use Google's Colab (no installation required, but times out if idle):

1. go to **<https://colab.research.google.com>**
2. login
3. File > Open notebook
4. click on Github (no need to login or authorize anything)
5. paste the git link: **https://github.com/jomorlier/IA_CNRS_ICA**
6. click search and then click on the notebook

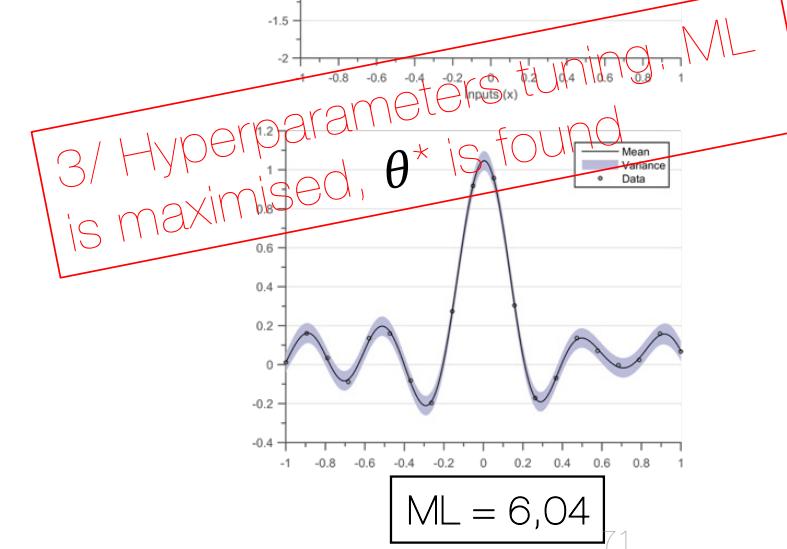
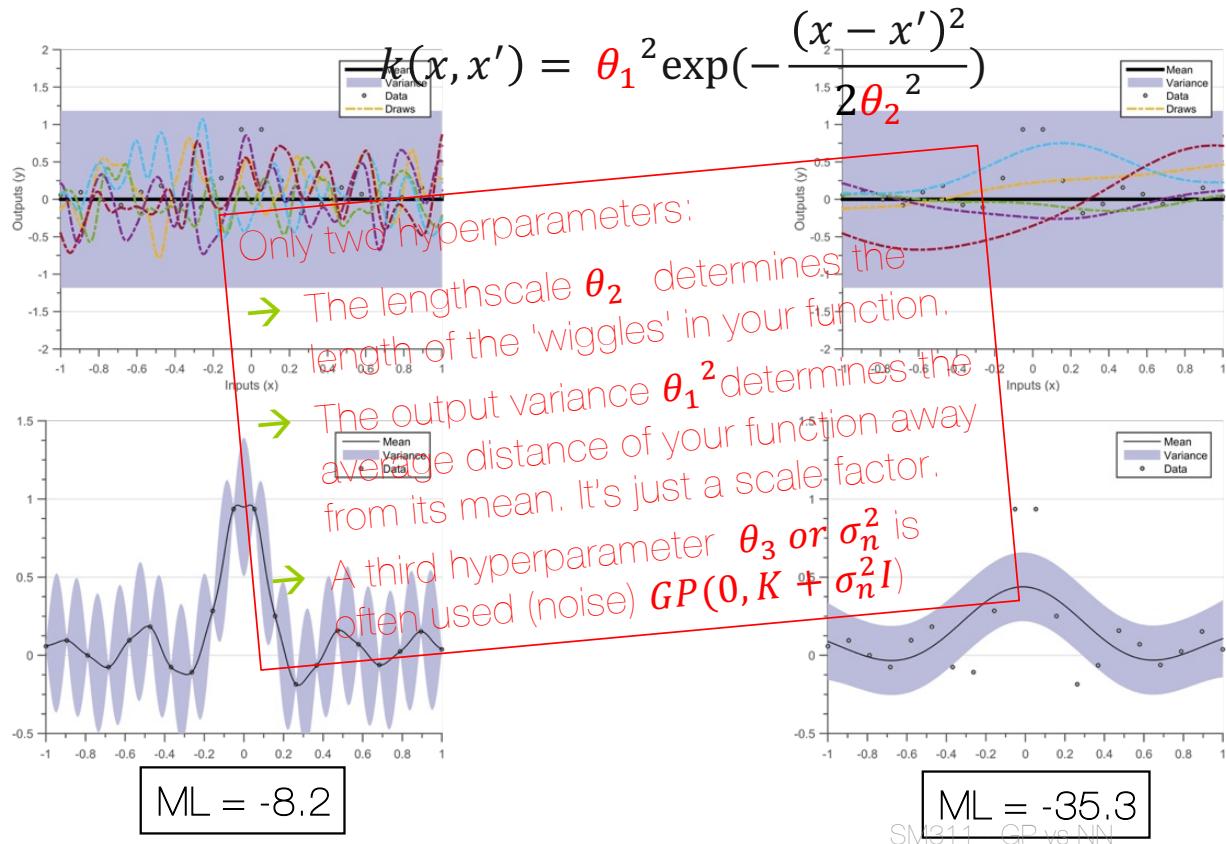
Part 1. Régression par processus gaussiens

Part 2. processus gaussiens versus réseaux de neurones

Optimizing Marginal Likelihood (ML)

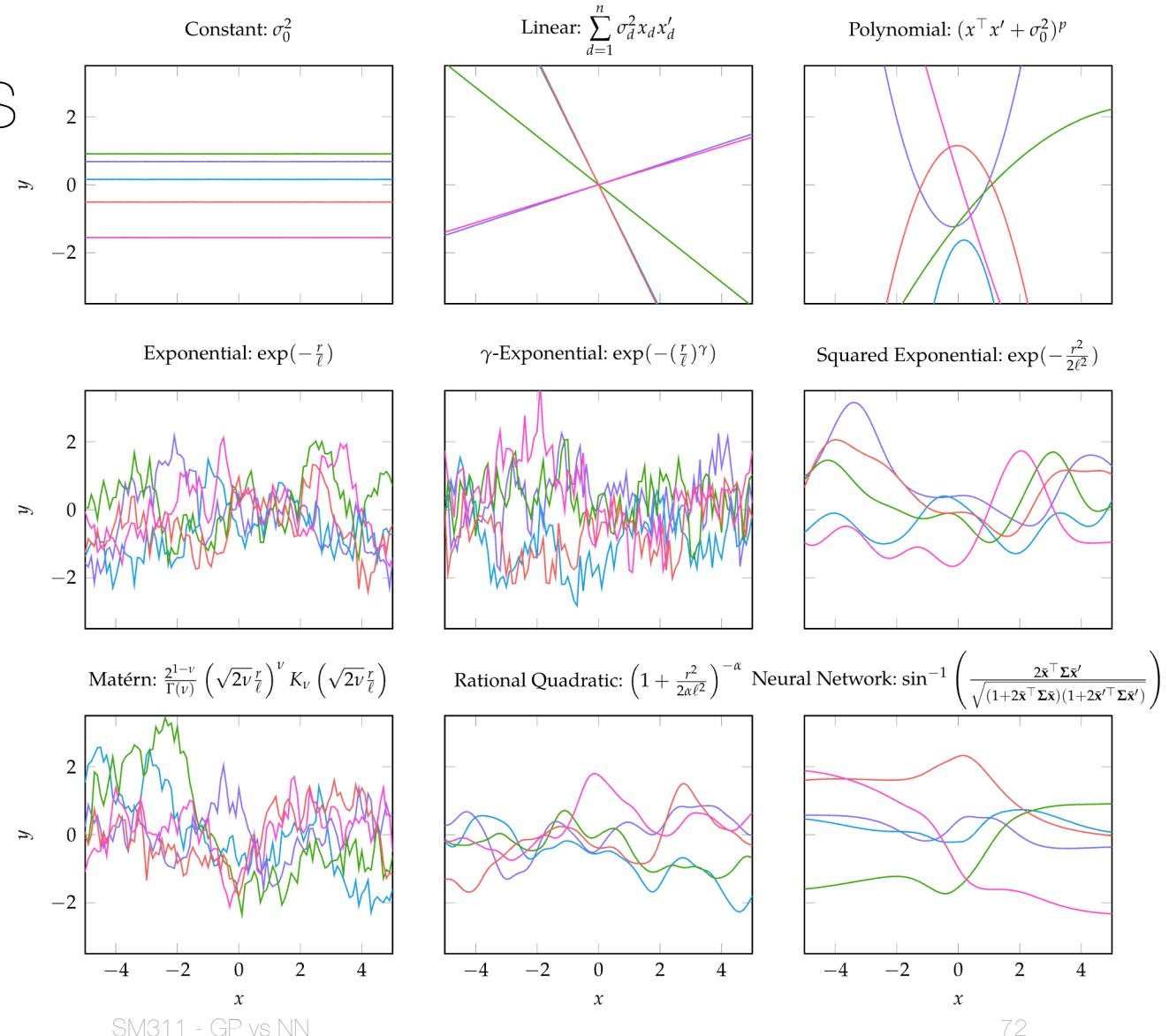
$$\text{ML} = \log(p(y|X, \theta)) = -\frac{1}{2} y^T K^{-1} y - \frac{1}{2} \log|K| - \frac{n}{2} \log(2\pi)$$

- It is a combination of **data-fit term**, a **complexity penalty** term and a **normalization term**



Gaussian Processes

- Examples of the same Gaussian process with different kernel functions

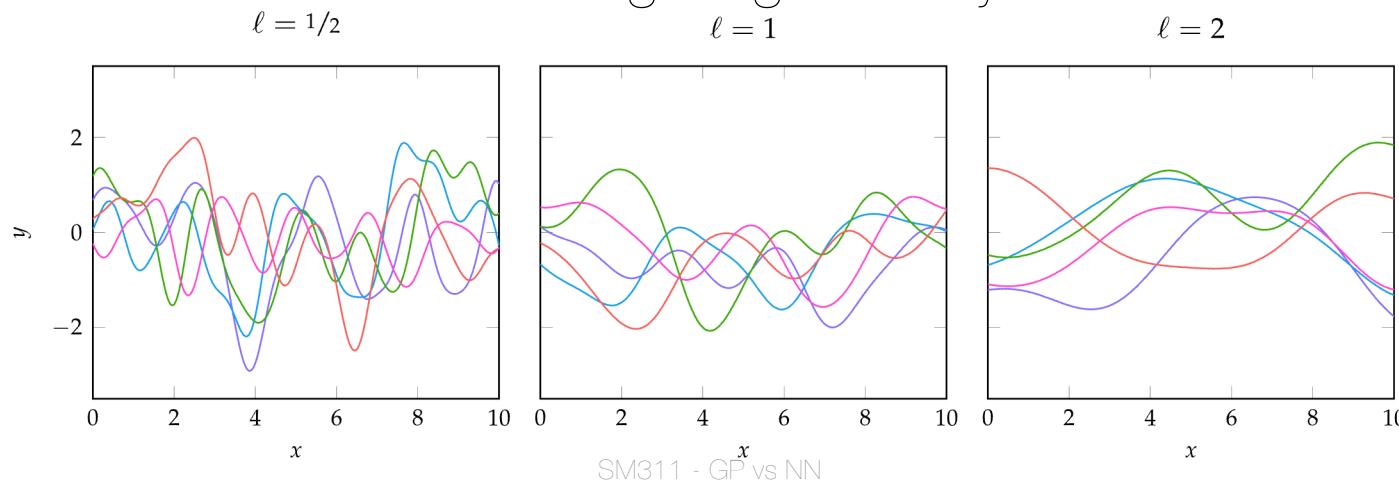


Gaussian Processes

- A common kernel function is the squared exponential kernel

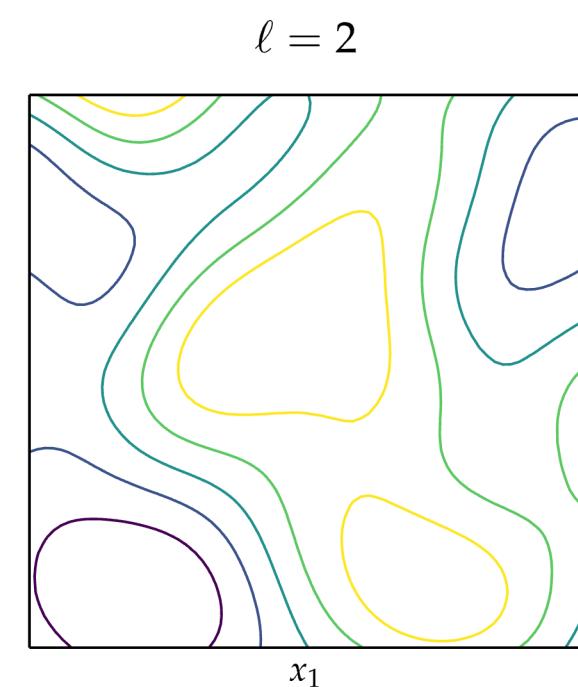
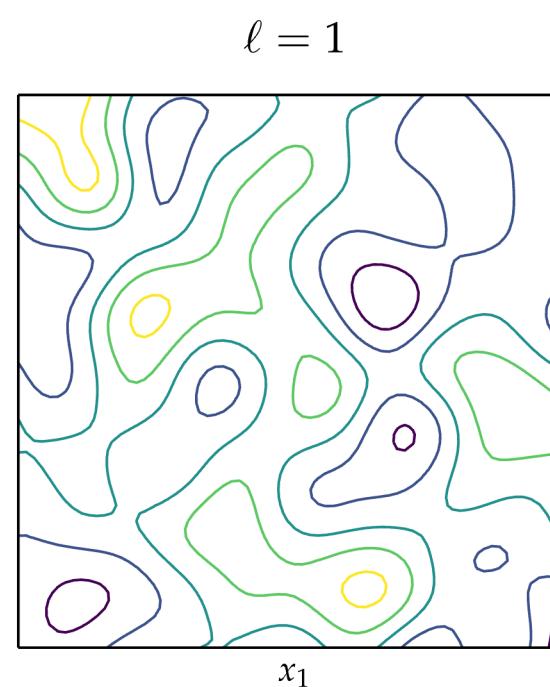
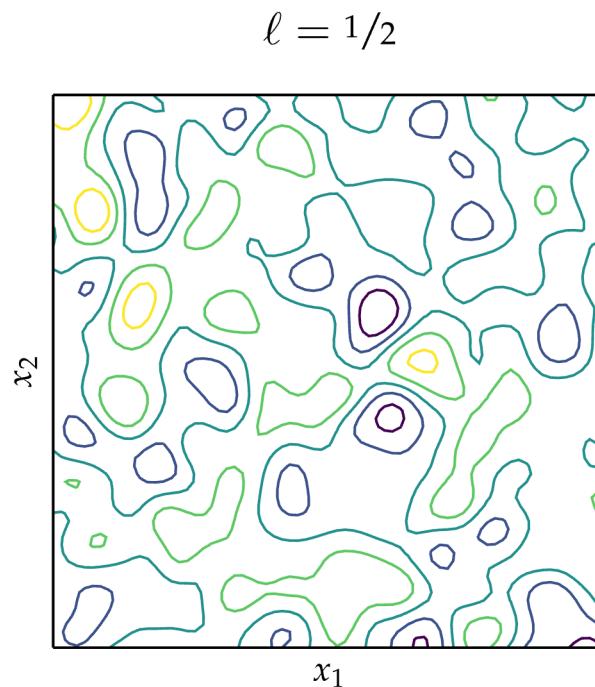
$$k(x, x') = \exp\left(-\frac{(x - x')^2}{2\ell^2}\right)$$

where ℓ is the characteristic length-scale, which is the distance required for the function to change significantly



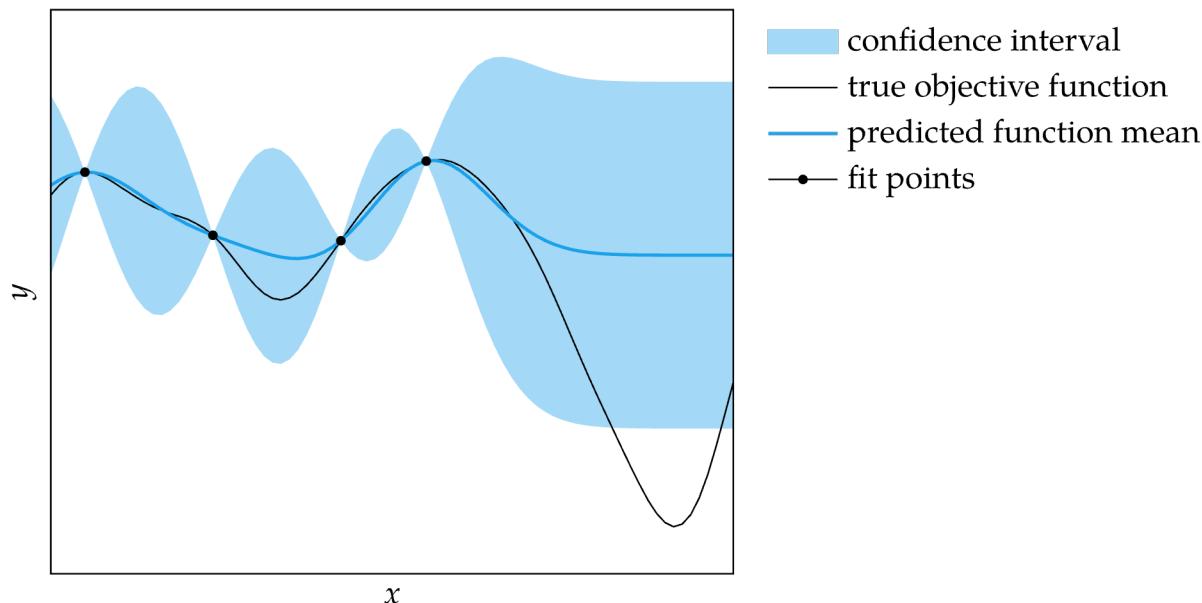
Gaussian Processes

- Example of multivariate Gaussian with squared-exponential kernel at different length scales



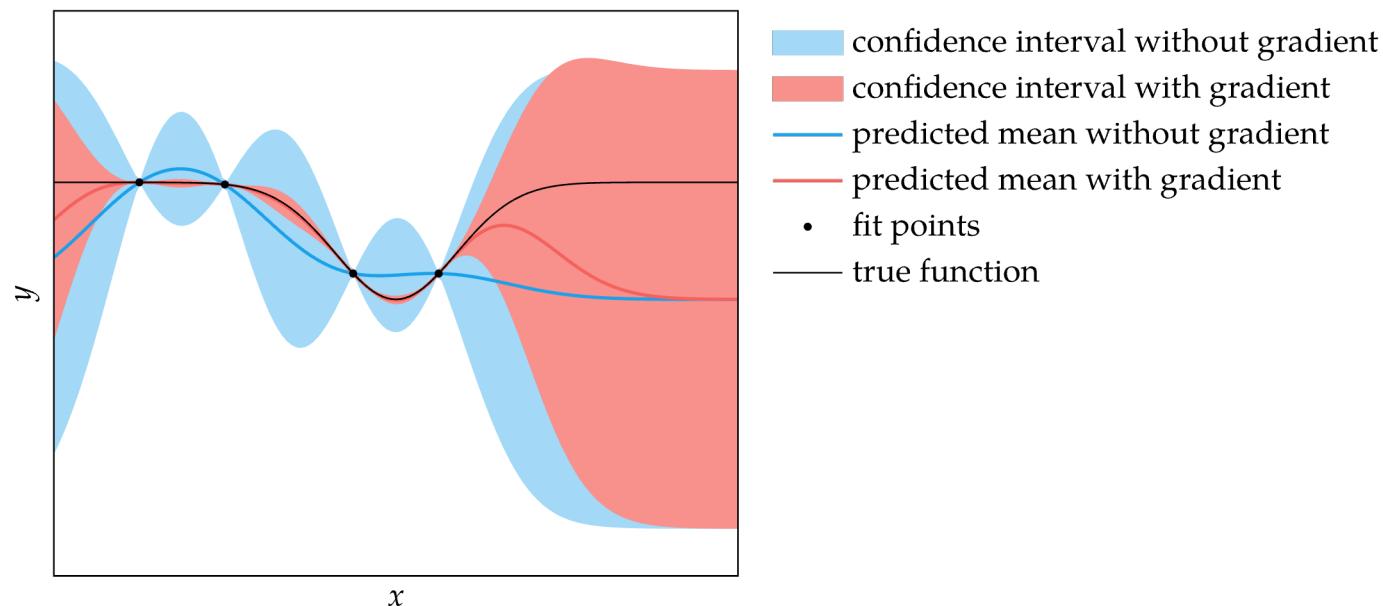
Prediction

- Using variance to compute standard deviation, the predicted mean and standard deviation can be computed at any point
- This enables calculation of the 95% confidence region



Gradient Measurements

- If function gradient evaluations can be made as well, the process can be extended to include gradient predictions for higher prediction fidelity



Summary

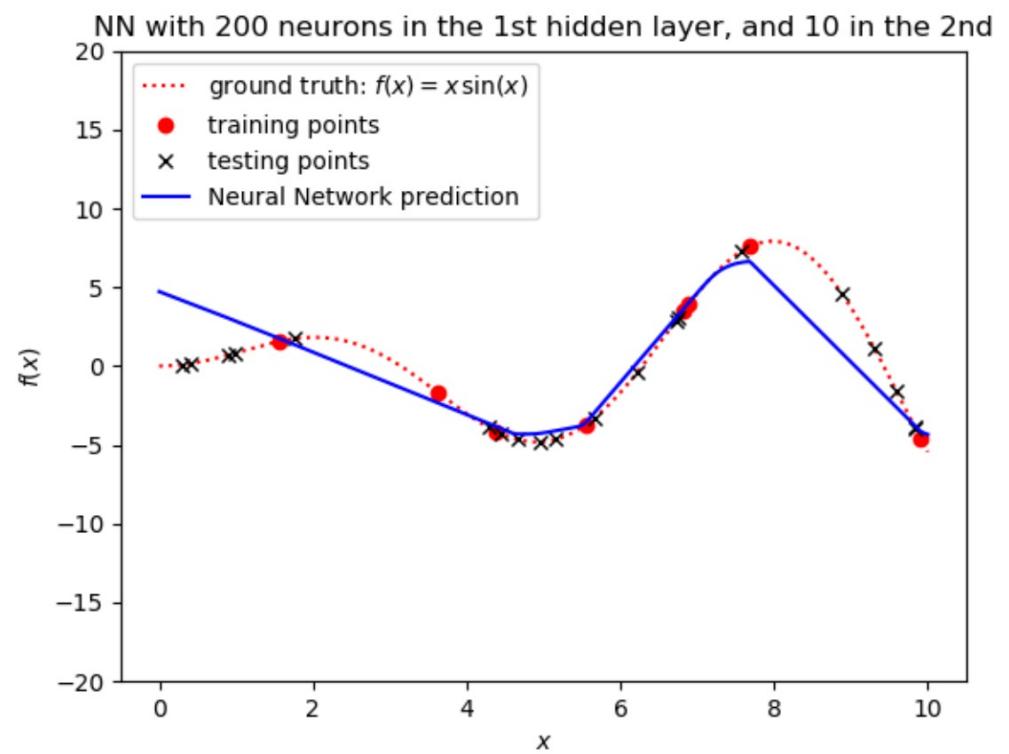
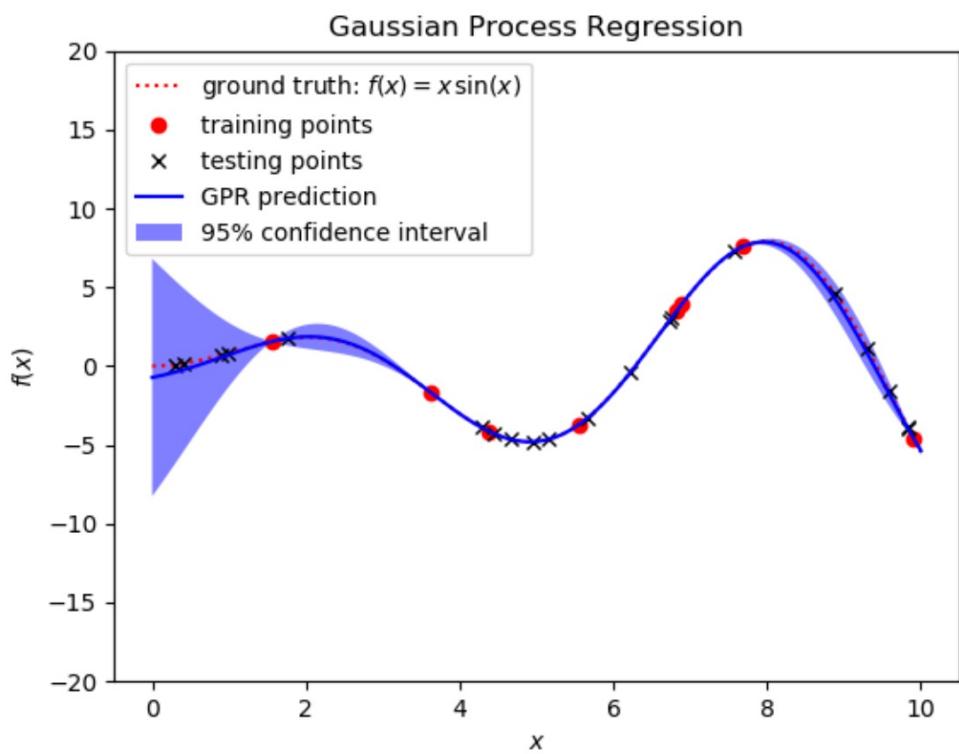
- Gaussian processes are probability distributions over functions
- The choice of kernel affects the smoothness of the functions sampled from a Gaussian process
- The multivariate normal distribution has analytic conditional and marginal distributions
- We can compute the mean and standard deviation of our prediction of an objective function at a particular design point given a set of past evaluations

Choosing an ML algorithm

- Training involves finding this vast amount of weights such that they fit the data accordingly. Neural networks are very simple algorithms, so they are extremely scalable (they can easily deal with millions of data points).
- Gaussian Processes (GPs): a Bayesian or probabilistic ML algorithm, meaning that it predicts the response as well as the uncertainty. This algorithm has outstanding regression capabilities and, in general, is easy to train. Unfortunately, this algorithm is poorly scalable, so it is limited to small datasets (approximately 10,000 points).

GP vs NN

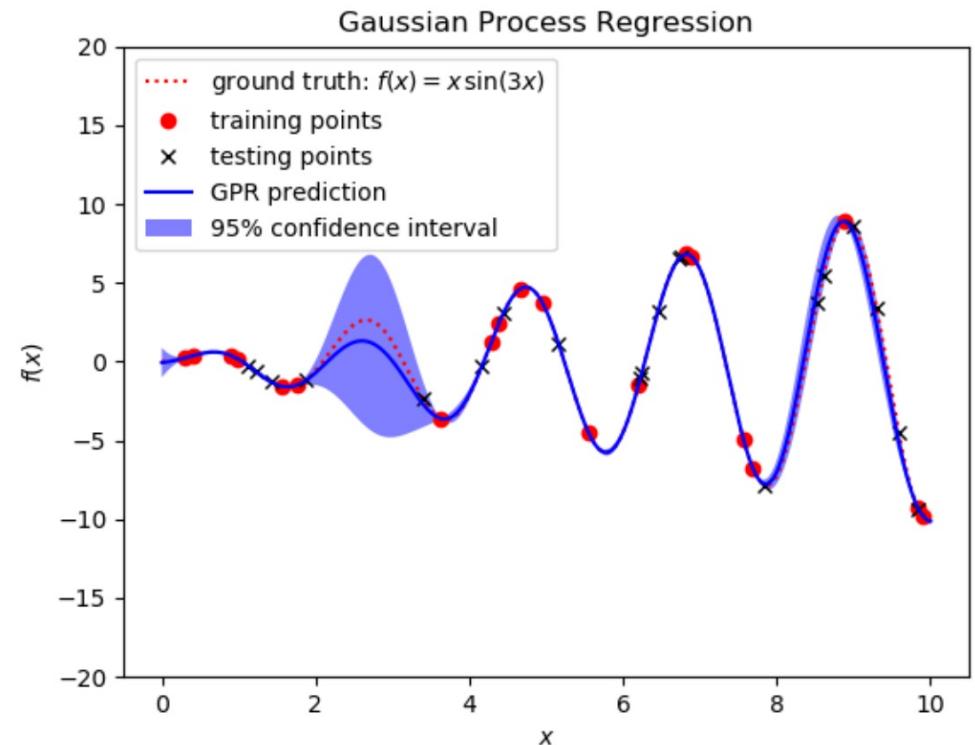
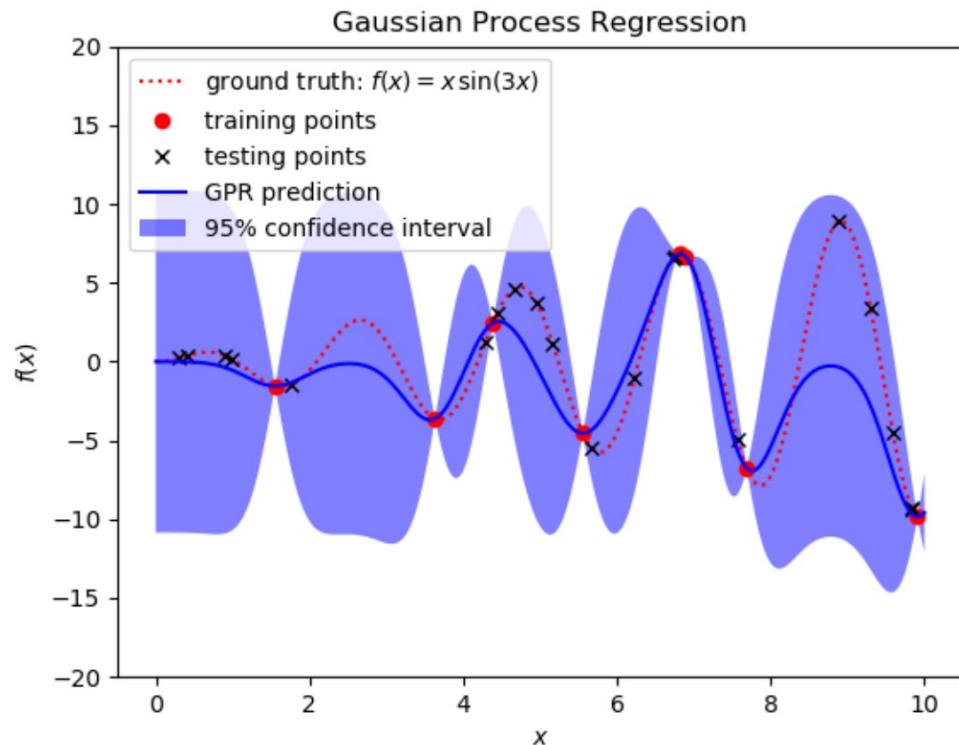
As can be observed, GPs provide an excellent approximation of the function $x^*\sin(x)$ even when using only 8 points, and they also quantify the uncertainty away from the training data.



Do we know a priori if there are "enough" training points?

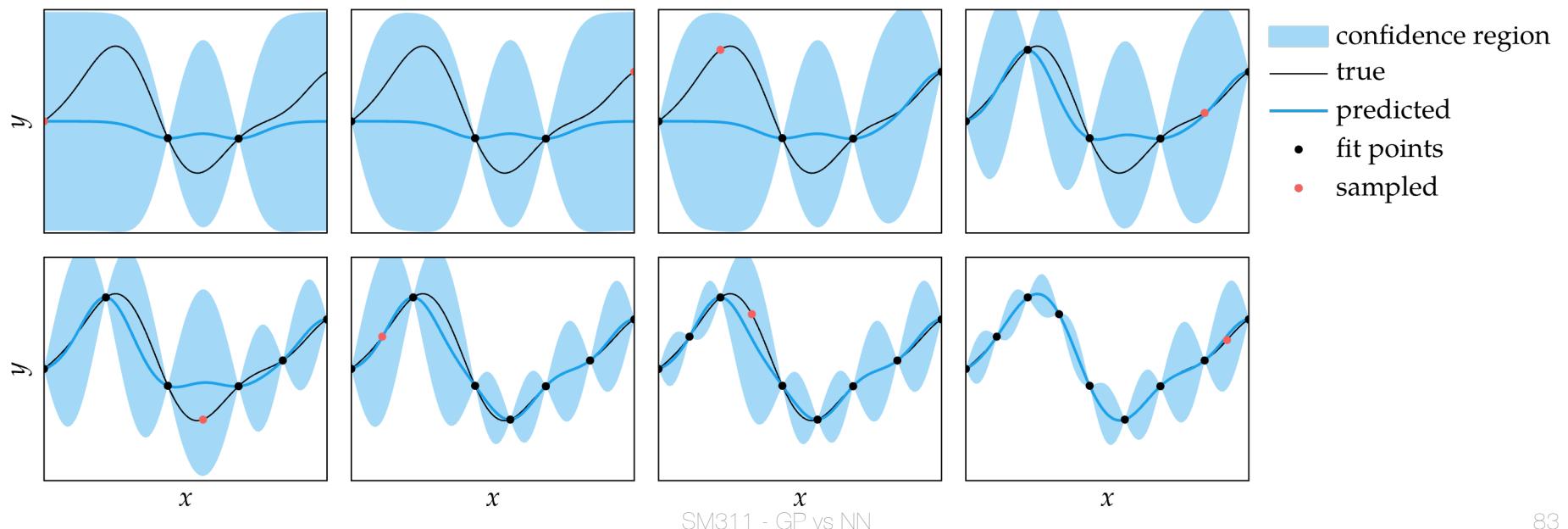
we have enough training data by iteratively assessing the error of our approximation against the test data.

In practice, the training data size may need to be very large when our problem has many input variables due to the curse of dimensionality: every additional input variable causes an exponential growth of the volume that needs to be sampled.



Error-Based Exploration

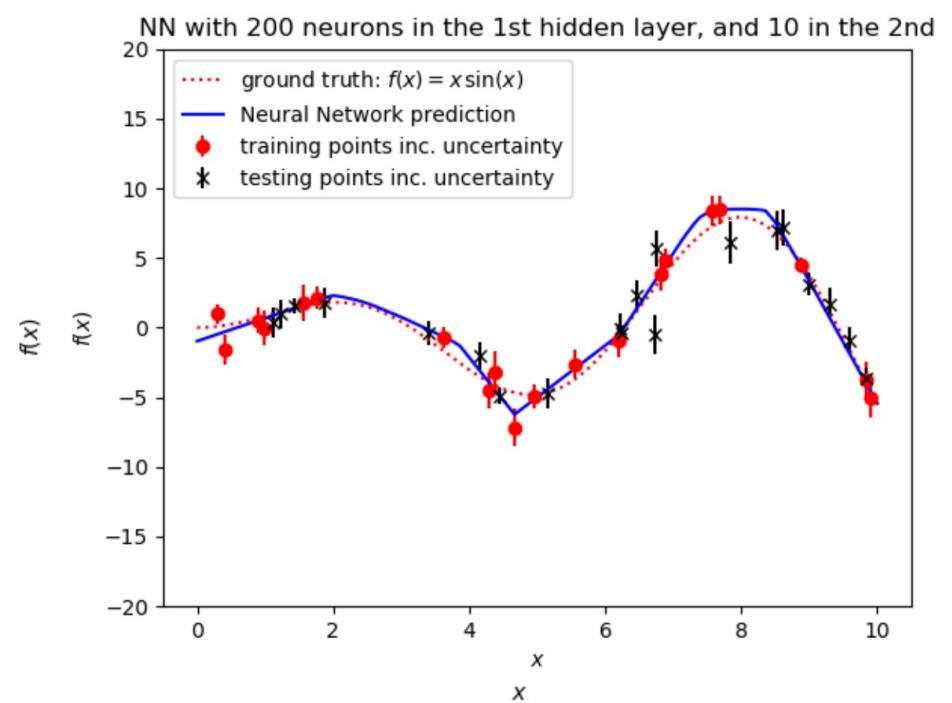
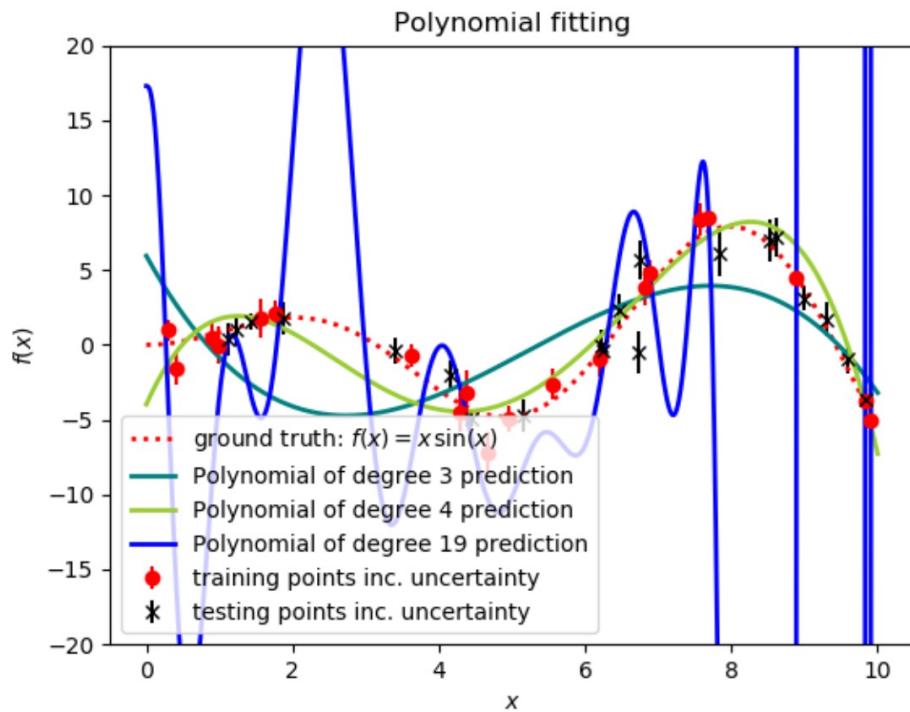
- Focuses exclusively on exploration
- For Gaussian processes, error-based exploration simply minimizes the maximum standard deviation within a specified domain



SM311 - GP vs NN

What happens if my data is noisy or uncertain?

Noisy datasets are very common in Engineering. Data coming from experiments is often dependent on environmental fluctuations, material defects, etc. Note even with simulations : structures undergoing buckling depend on the geometric imperfections considered in the model.

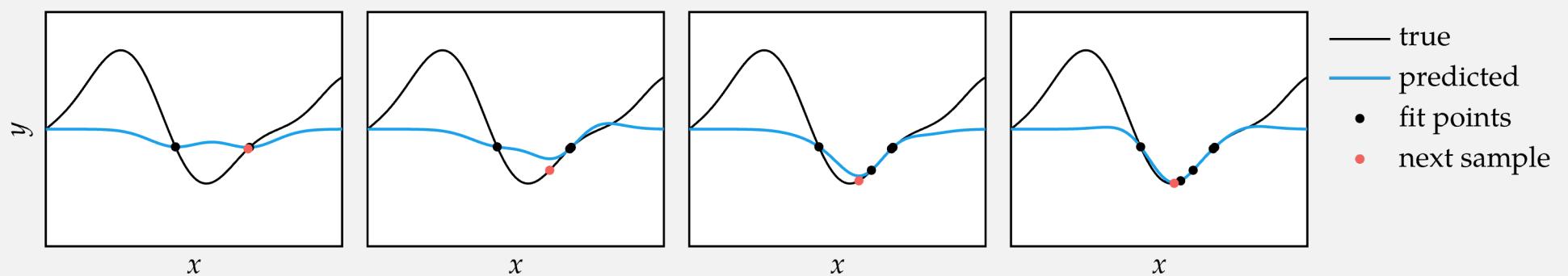


Surrogate Optimization

- Given a surrogate model with both prediction and confidence parameters, an optimization procedure must balance the search for the expected optimal point and decreasing uncertainty
- In other words, the optimization algorithm must balance exploitation with exploration

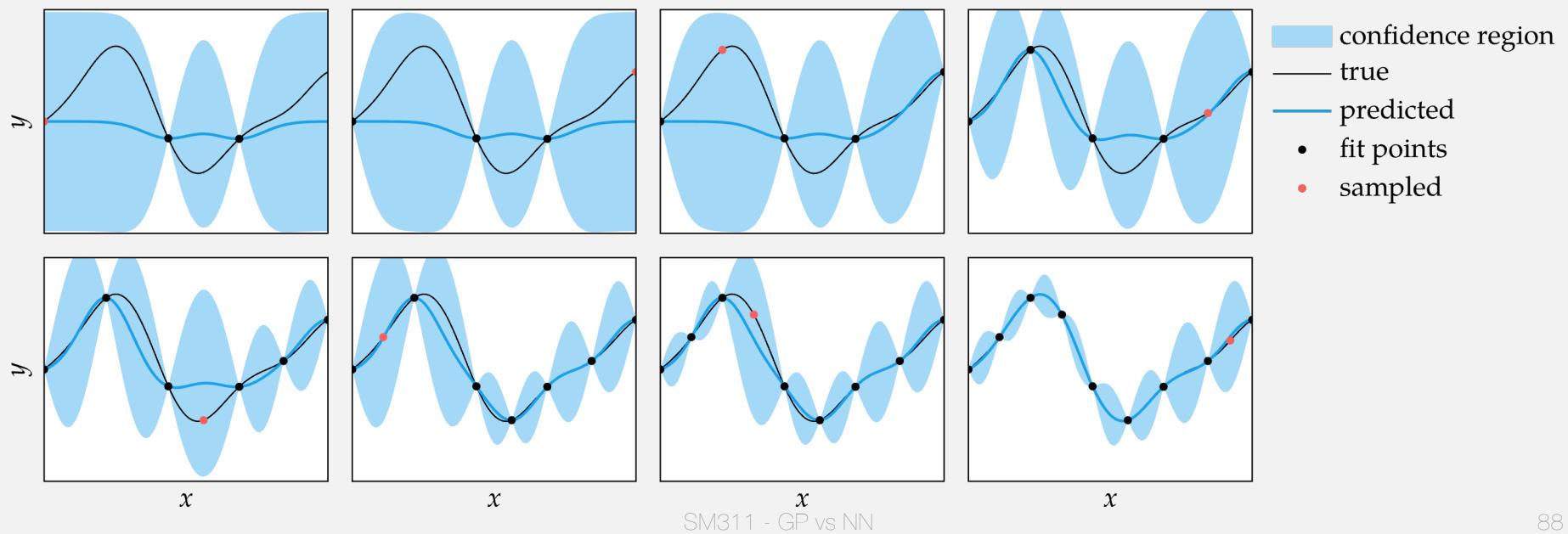
Prediction-Based Exploration

- Focuses exclusively on exploitation, also called greedy approach
- When using a Gaussian process surrogate model, prediction-based exploration simply optimizes over the mean function and ignores uncertainty



Error-Based Exploration

- Focuses exclusively on exploration
- For Gaussian processes, error-based exploration simply minimizes the maximum standard deviation within a specified domain

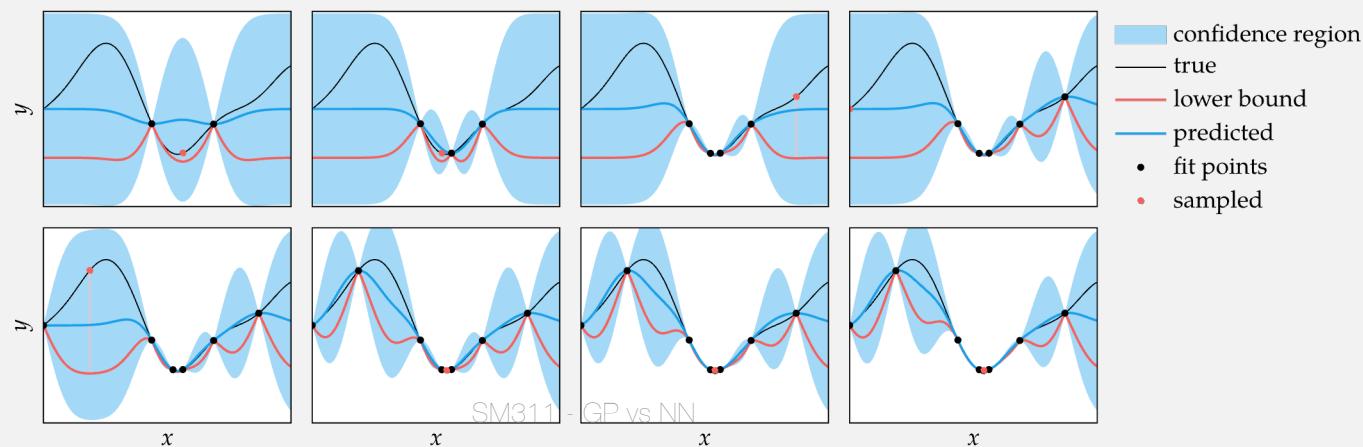


Lower Confidence Bound Exploration

- Tradeoff between exploration and exploitation
- The next sample minimizes the lower confidence bound of the objective function

$$LB(\mathbf{x}) = \hat{\mu}(\mathbf{x}) - \alpha\hat{\sigma}(\mathbf{x})$$

where $\alpha \geq 0$ is the tradeoff parameter



Probability of Improvement Exploration

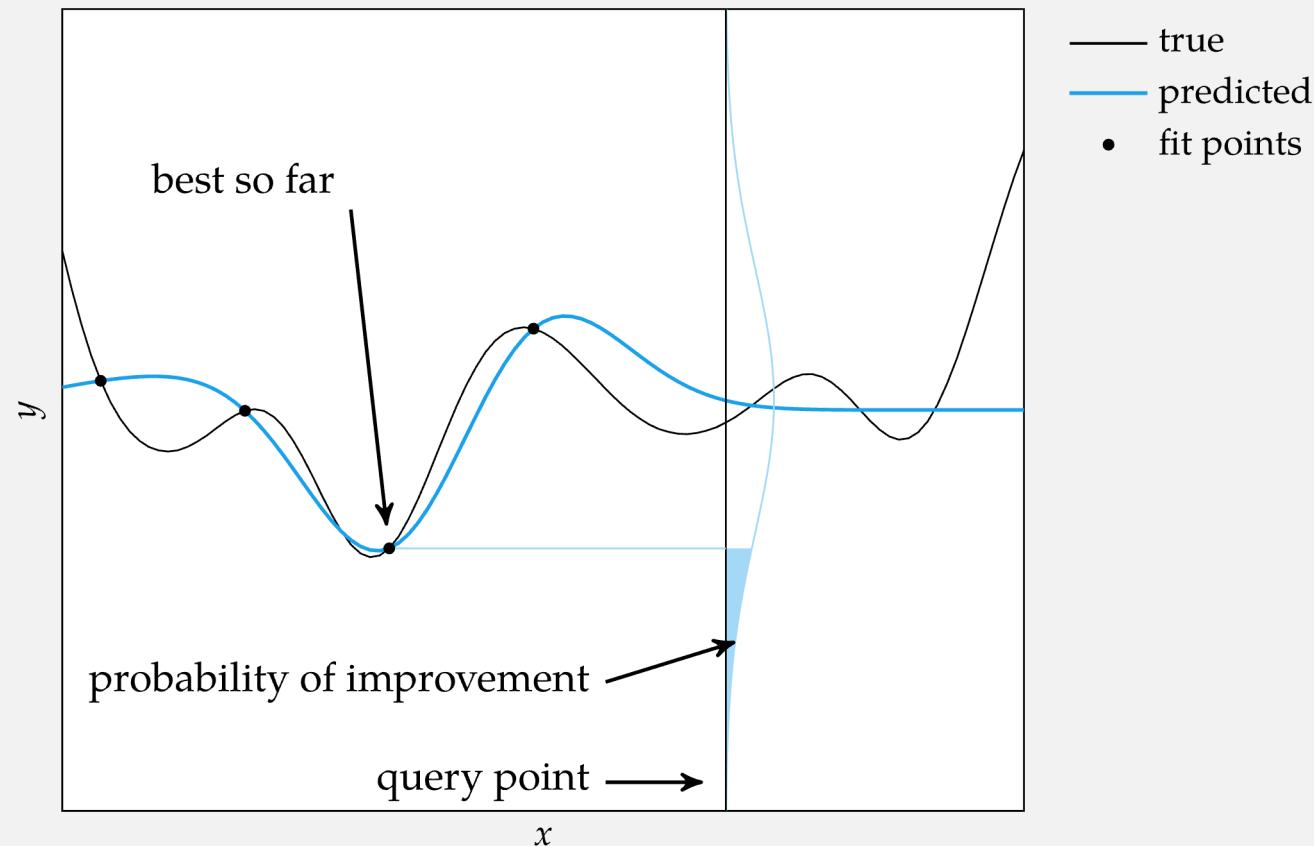
- Searches at the location with the highest probability of improvement
- Improvement is defined as

$$I(y) = \begin{cases} y_{\min} - y & \text{if } y < y_{\min} \\ 0 & \text{otherwise} \end{cases}$$

- The probability of improvement is defined as

$$\begin{aligned} P(y < y_{\min}) &= \int_{-\infty}^{y_{\min}} \mathcal{N}(y | \hat{\mu}, \hat{\sigma}) dy \\ &= \Phi\left(\frac{y_{\min} - \hat{\mu}}{\hat{\sigma}}\right) \end{aligned}$$

Probability of Improvement Exploration

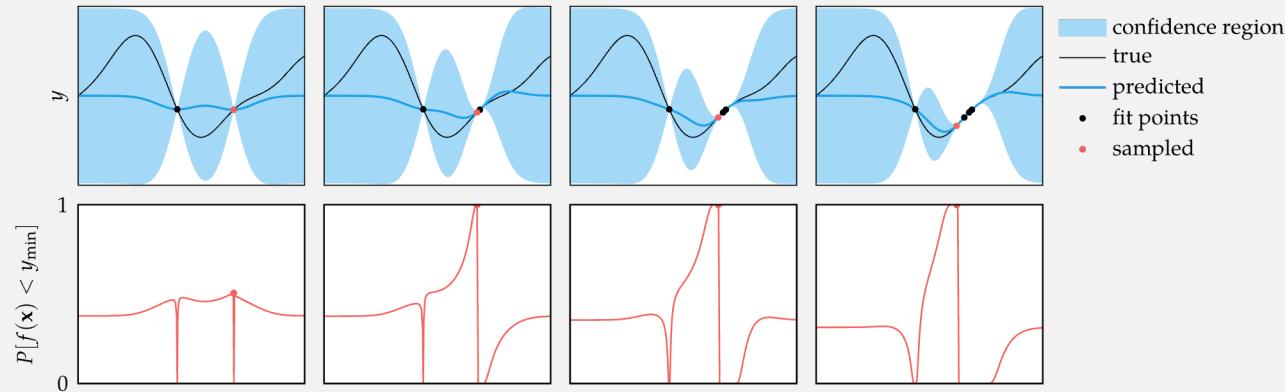


Expected Improvement Exploration

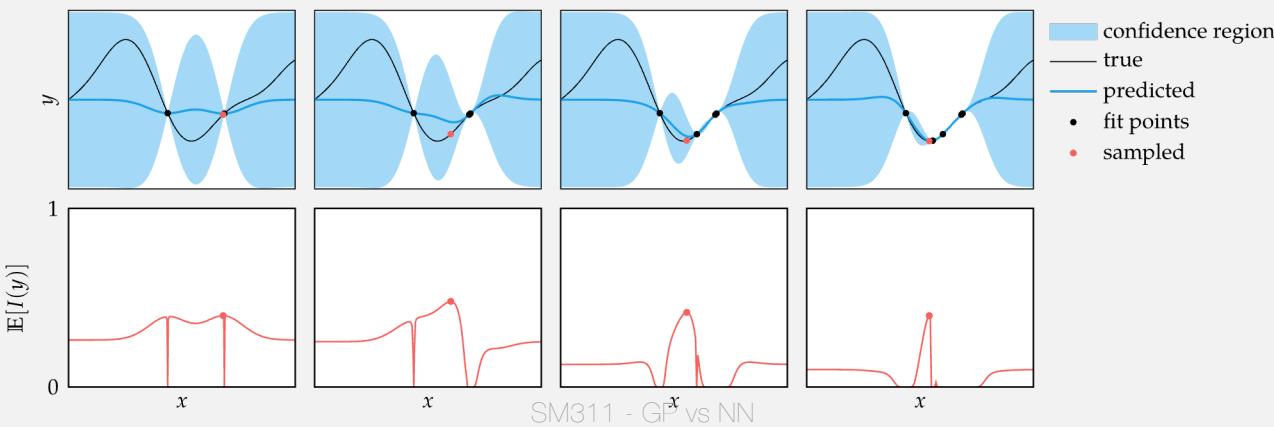
- While probability of improvement exploration seeks to ensure some expected improvement at each step, expected improvement exploration seeks to maximize expected improvement at each step

Expected Improvement Exploration

Probability of Improvement Exploration



Expected Improvement Exploration



Summary

- Gaussian processes can be used to guide the optimization process using a variety of strategies that use estimates of quantities such as the lower confidence bound, probability of improvement, and expected improvement
- Some problems do not allow for the evaluation of unsafe designs, in which case we can use safe exploration strategies that rely on Gaussian processes

To finish Complementary materials online

CHALLENGE # deeper understanding

<https://thegradient.pub/gaussian-process-not-quite-for-dummies/>

<https://www.cs.toronto.edu/~duvenaud/cookbook/>

<https://distill.pub/2019/visual-exploration-gaussian-processes/>

<https://sandipanweb.wordpress.com/2020/12/08/gaussian-process-regression-with-python/>

To conclude

1. If you are interested in AI4E please join us on linkedin.
2. Have a look to SMT tutorials:
<https://github.com/SMTorg/smt/tree/master/tutorial#readme>
3. Contact: joseph.morlier@isae-supraero.fr

SMT Tutorial (linear, quadratic, gaussian process, ...)

 Open in Colab

Noisy Gaussian process

 Open in Colab

Multi-Fidelity Gaussian Process (with or without noise)

 Open in Colab

LHS sampling

 Open in Colab

Gaussian Process Trajectory Sampling

 Open in Colab

Bayesian Optimization - Efficient Global Optimization to solve unconstrained problems

 Open in Colab

Mixed-Integer Gaussian Process and Bayesian Optimization to solve unconstrained problems with mixed variables (continuous, discrete, categorical)

 Open in Colab