FREQUENCY-AWARE SURROGATE MODELING WITH SMT KERNELS FOR ADVANCED DATA FORECASTING

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AeroBest 2025

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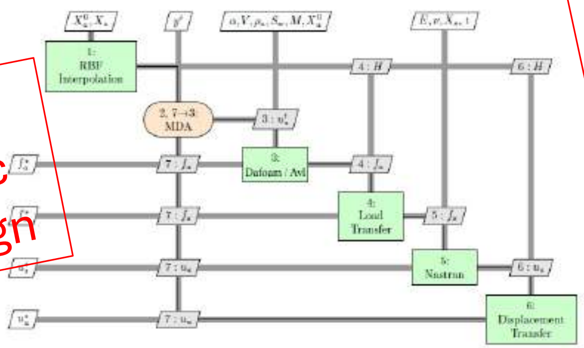
ICA

cnrs dépasser les frontières

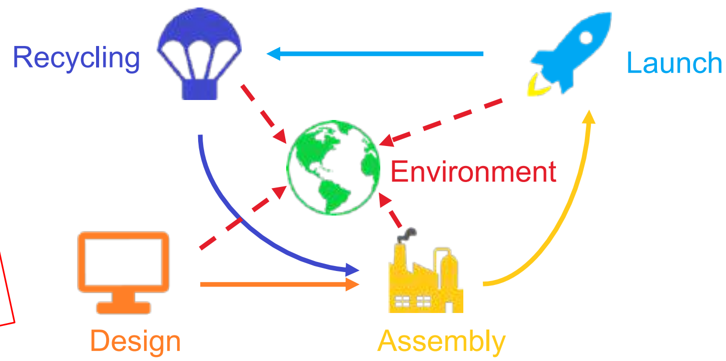
isae Institut Supérieur de l'Aéronautique et de l'Espace SUPAERO

Prof. J. Morlier

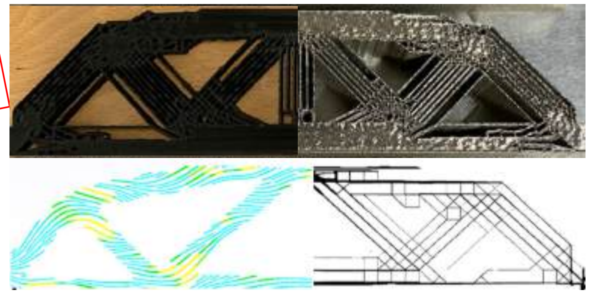
MDO for Aeroelastic Wing design



MDO for Aerospace systems Including LCA : = EcoOptimization



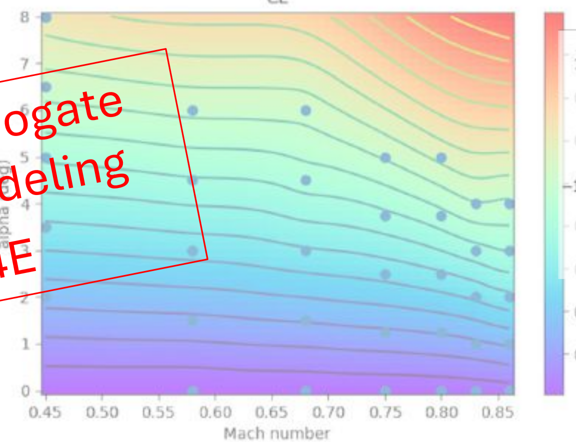
Digital fabrication

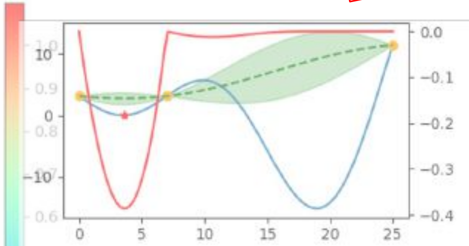


https://github.com/SMTorg/SMT

Surrogate modeling

AI4E





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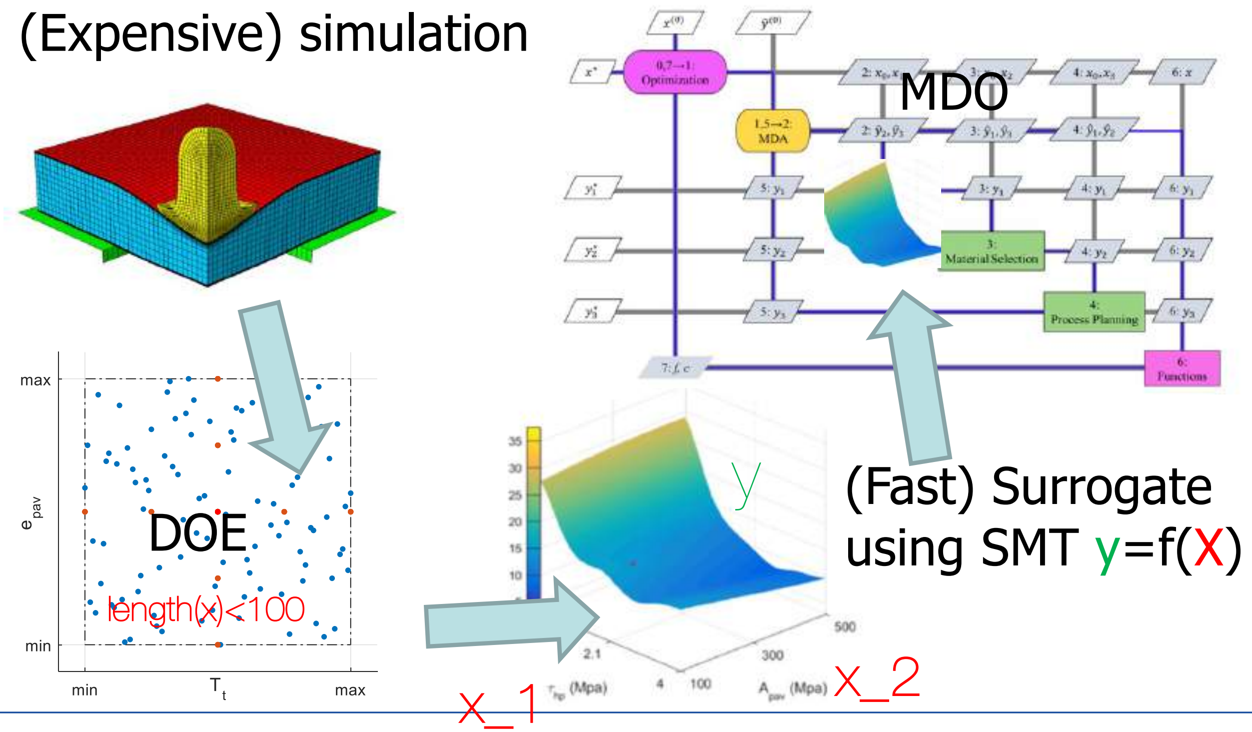
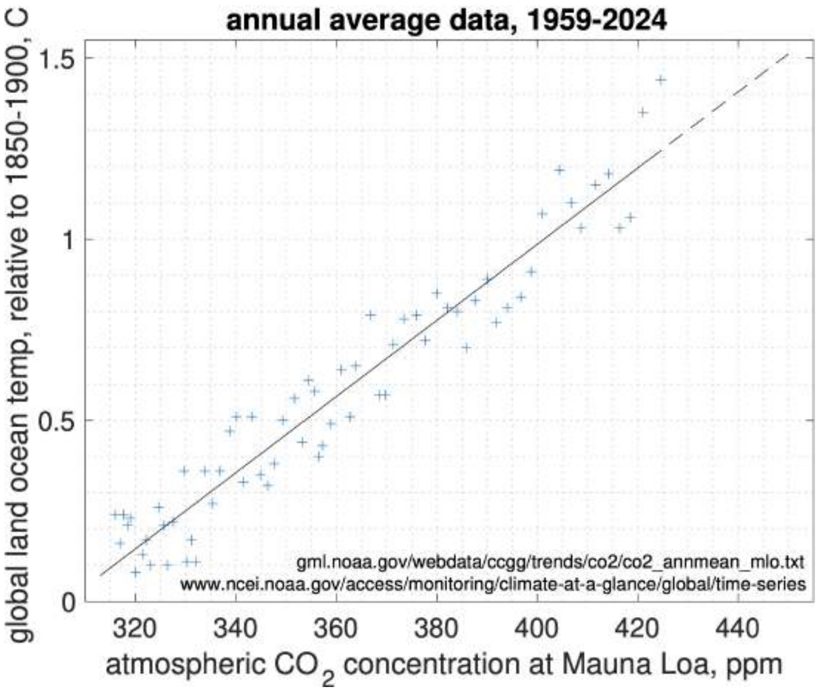
What is Surrogate Modeling ?

A. Forrester, A. Sobester, and A. Keane. "Engineering Design via Surrogate Modelling: A Practical Guide". Coll. John Wiley & Sons (2008).

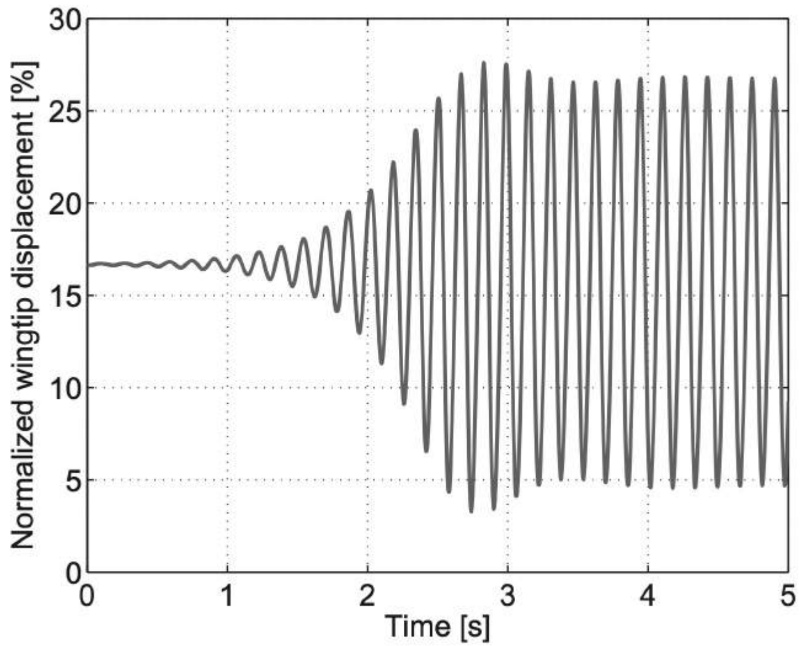


- A surrogate model of a function is an approximation of Expensive Computer simulation: It's a supervised learning process in AI.
- As the surrogate is less costly to evaluate it can be used as a "fast" code in a Multidisciplinary Design Optimization loop. [or do Uncertainty Quantification or do Bayesian Optimization etc…]

What's this ?



What is the link with flutter ?



→ Forecasting with GP (extrapolation)

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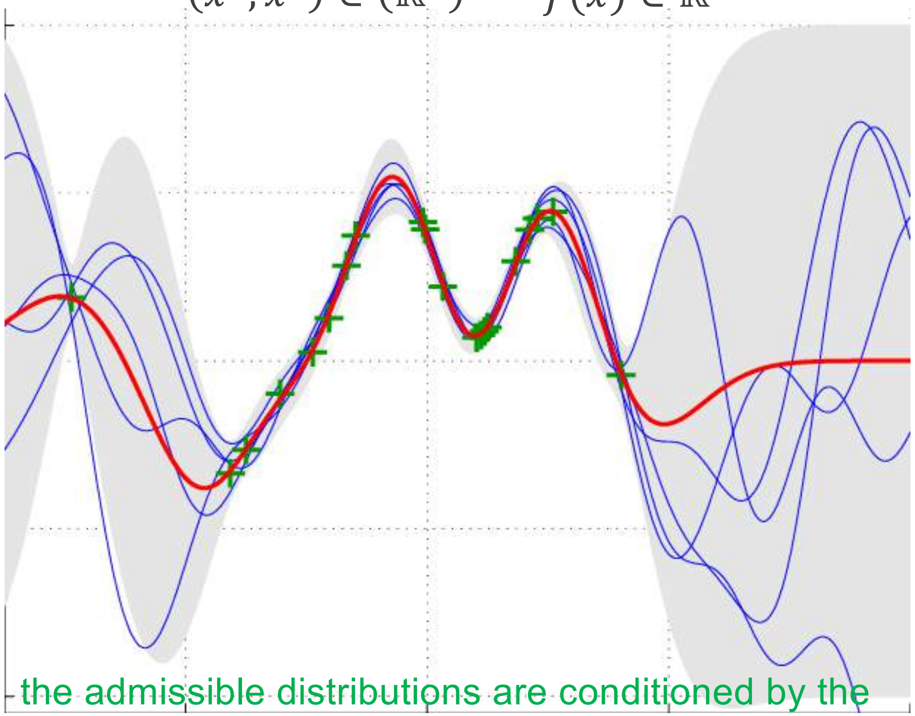
GP aka Kriging

$(x^r, x^s) \in (\mathbb{R}^n)^2 \qquad f(x) \in \mathbb{R}$



the admissible distributions are conditioned by the observations f(x^r)

A Gaussian process (GP) is characterized by:

- its trend
  $\mu(x^r) \in \mathbb{R}$
- its correlation kernel
  $\mathrm{k}(x^r, x^s) \in \mathbb{R}$

Learning database (observations x^r)

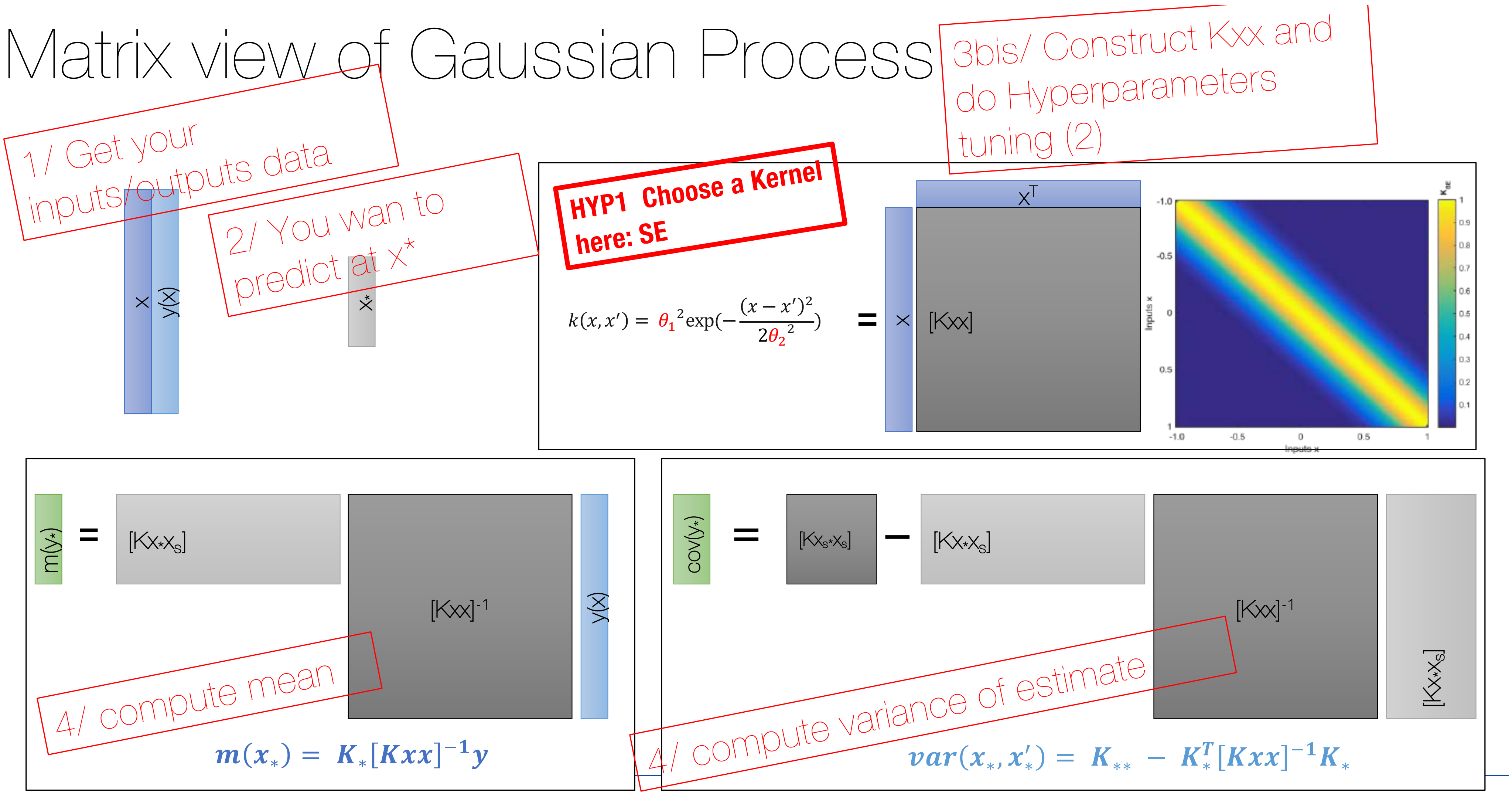
Samples from posterior distribution (1 realization)

Mean

Variance (CI at 99%)

$f\_approx(x) = \mathcal{N}(\hat{f}(\boldsymbol{x}), s^2(x))$

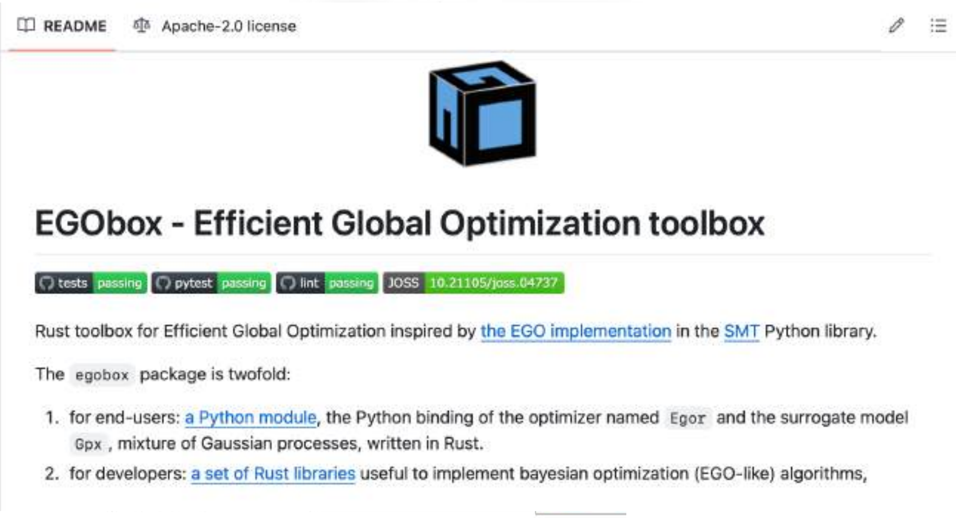
Matrix view of Gaussian Process



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

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

Not only SMT



README   Apache-2.0 license

EGObox - Efficient Global Optimization toolbox

tests passing | pytest passing | lint passing | JOSS 10.21105/joss.04737

Rust toolbox for Efficient Global Optimization inspired by the EGO implementation in the SMT Python library.

The `egobox` package is twofold:

1. for end-users: a Python module, the Python binding of the optimizer named `Egor` and the surrogate model `Gpx`, mixture of Gaussian processes, written in Rust.
2. for developers: a set of Rust libraries useful to implement bayesian optimization (EGO-like) algorithms,

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https://github.com/SMTorg/smt

https://github.com/relf/egobox

SMT 2.9.2

https://github.com/SMTorg/smt/tree/master/tutorial

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

Surrogate-based Optimization

- **Efficient Global Optimization: How to start?**
- **Bayesian Optimization - Efficient Global Optimization to solve expensive problems**
- **Bayesian Optimization with noisy data**

Multi-Fidelity Gaussian Process

- **With required nested sampling**
- **With noise**
- **Adaptative sampling**
- **Without nested sampling**

Proper Orthogonal Decomposition and Interpolation

- **PODI+I tutorial in SMT with global and local basis**
- **PODI+I application to airfoil design**

Kernel Engineering

- **Kernel engineering tutorial in SMT**
- **Kernel engineering application to aeroelasticity prediction**

Explainability and conformal prediction

- **Warning:** The explainability usage tutorial has been moved to SMTorg/smt-explainability

Other Gaussian Process Models and Sampling Methods

- **LHS sampling (initial and expanded)**
- **Gaussian Process Trajectory Sampling**
- **Noisy Gaussian Process**
- **Sparse Gaussian Process**
- **Cooperative Components Kriging**

Mixed-integer and mixed-hierarchical surrogate models

- **Warning:** The Design Space usage tutorial has been moved to SMTorg/smt-design-space-ext
- **Specific notebook associated to the SMT 2.0 Journal Paper (submitted) with a focus on mixed integer and mixed hierarchical surrogate models (continuous, discrete, categorical)**
- **Mixed-Integer Gaussian Process and Bayesian Optimization to solve unconstrained problems with mixed variables (continuous, discrete, categorical)**
- **Mixed-Integer Gaussian Process and Bayesian Optimization for Engineering application**

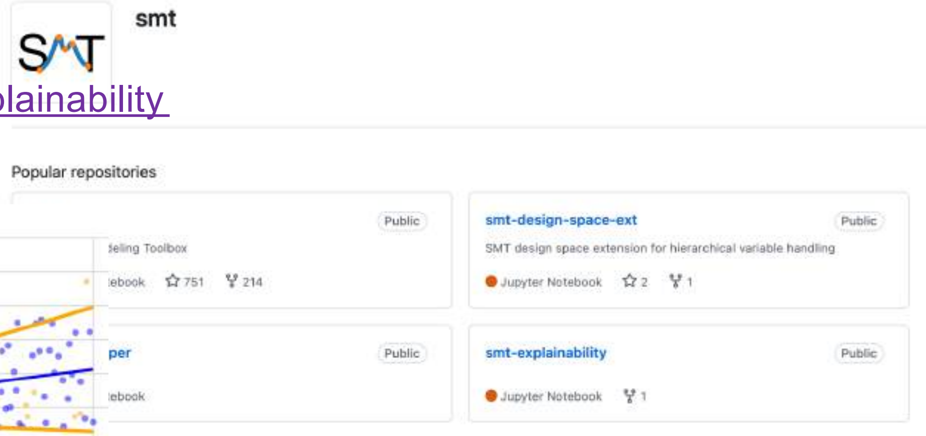
P. Saves, R. Lafage, N. Bartoli, Y. Diouane, J. Bussemaker, T. Lefebvre, J. Hwang, J. Morlier, J. Martins, **SMT 2.0: A Surrogate Modeling Toolbox with a focus on Hierarchical and Mixed Variables Gaussian Processes**, 2024, Advances in Engineering Software.

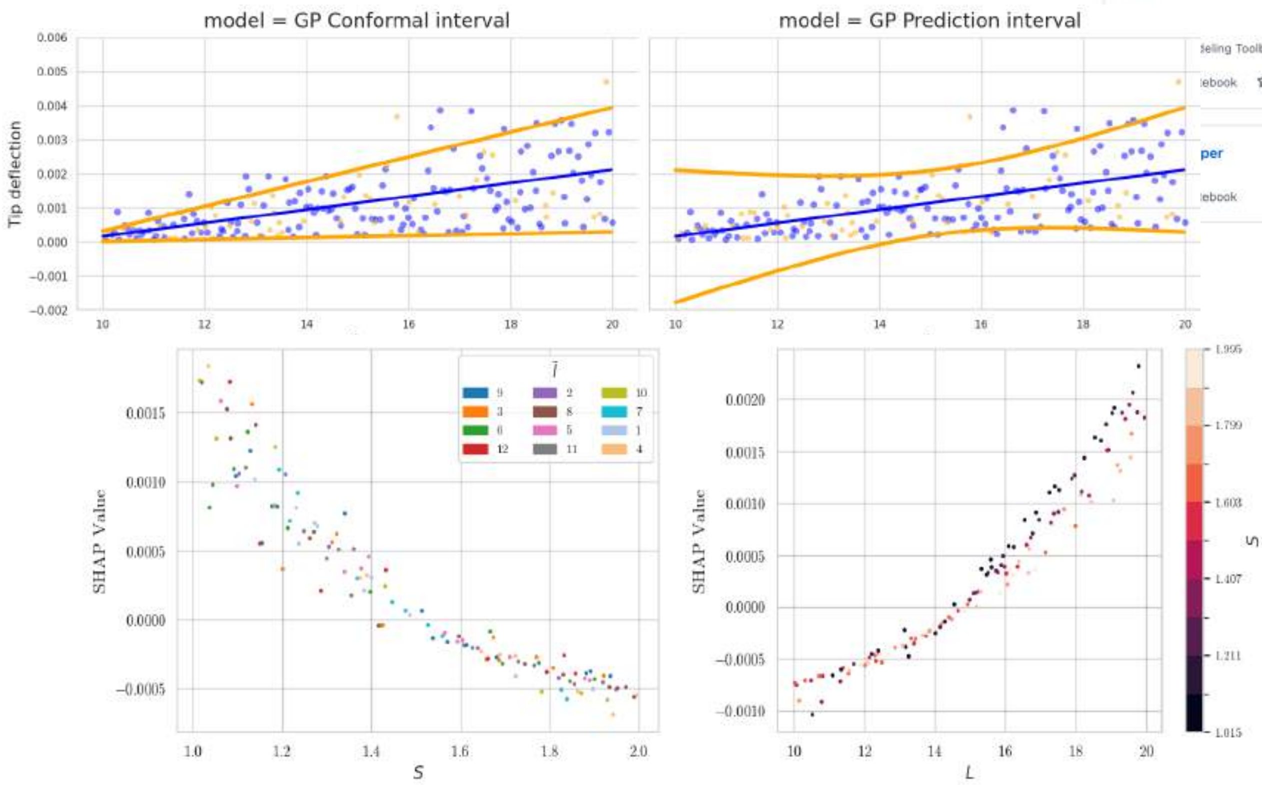
M.-A. Bouhlel, J. Hwang, N. Bartoli, R. Lafage, J. Morlier, J. Martins, **A Python surrogate modeling framework with derivatives**, 2019, Advances in Engineering Software.

Lafage, R. (2022). **egobox, a Rust toolbox for efficient global optimization**. *Journal of Open Source Software*, *7*(78), 4737.

Not only SMT

https://github.com/SMTorg/smt-explainability





P. Saves, R. Lafage, N. Bartoli, Y. Diouane, J. Bussemaker, T. Lefebvre, J. Hwang, J. Morlier, J. Martins, **SMT 2.0: A Surrogate Modeling Toolbox with a focus on Hierarchical and Mixed Variables Gaussian Processes**, 2024, Advances in Engineering Software.

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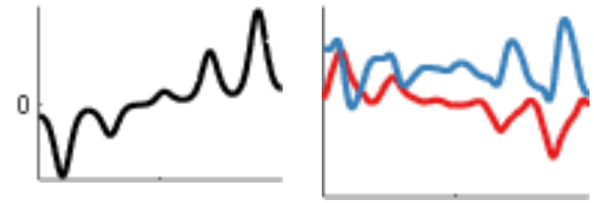
Combining kernels

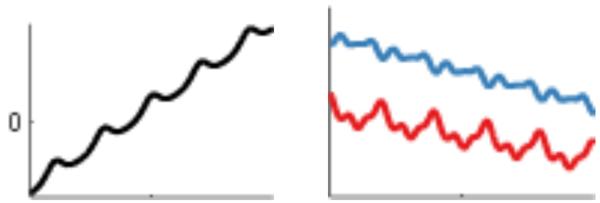
Linear times Periodic



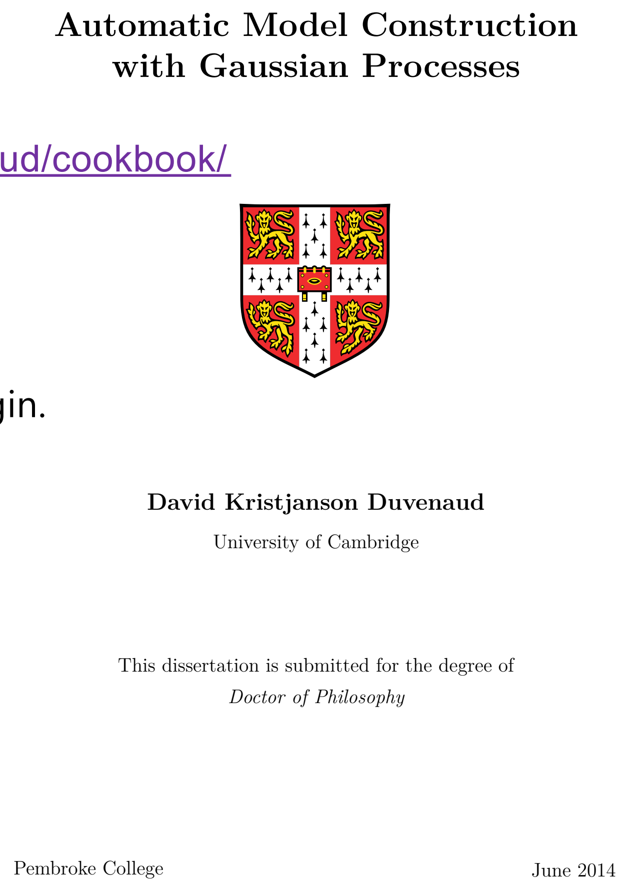
https://pyro.ai/examples/gp.html
https://www.cs.toronto.edu/~duvenaud/cookbook/
https://github.com/jkfitzsimons/

A linear kernel times a periodic results in functions
which are periodic with increasing amplitude as we move away from the origin.

Linear plus Periodic



A linear kernel plus a periodic results in functions
which are periodic with increasing mean as we move away from the origin.


Automatic Model Construction
with Gaussian Processes

David Kristjanson Duvenaud

University of Cambridge

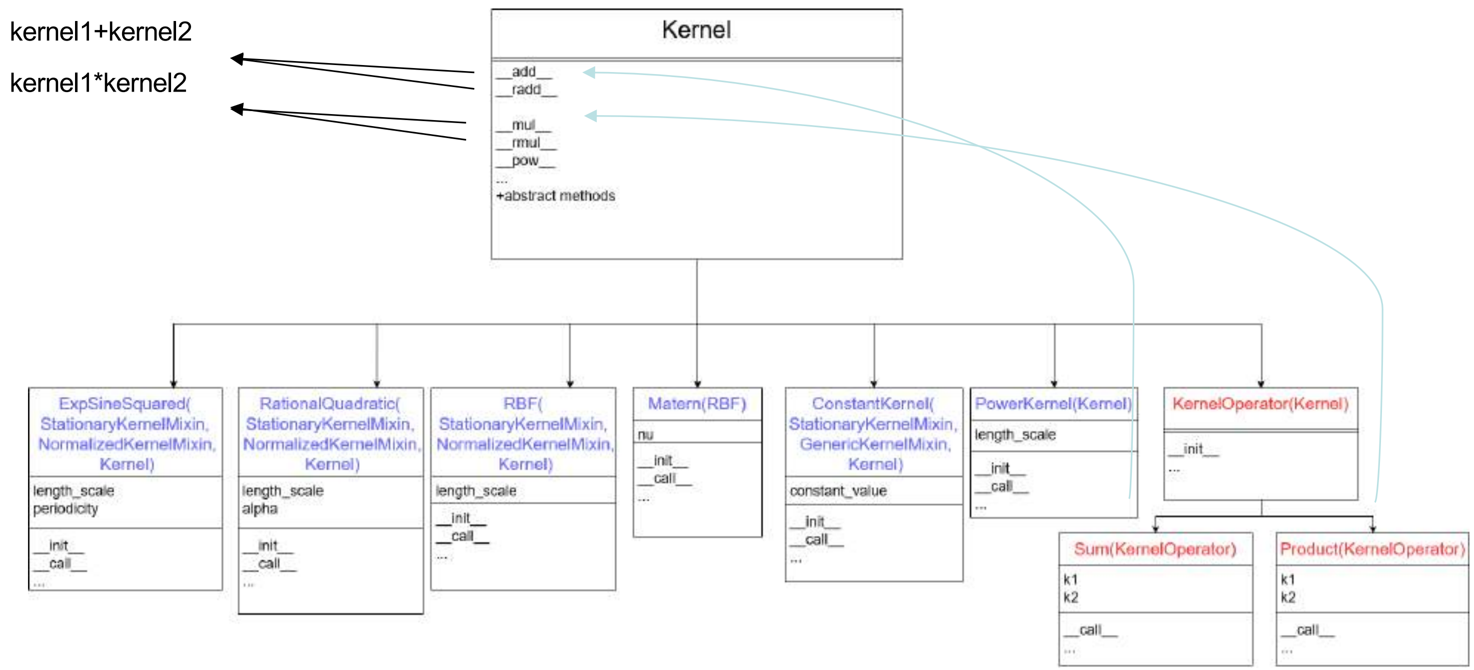
This dissertation is submitted for the degree of
Doctor of Philosophy

Pembroke College

June 2014

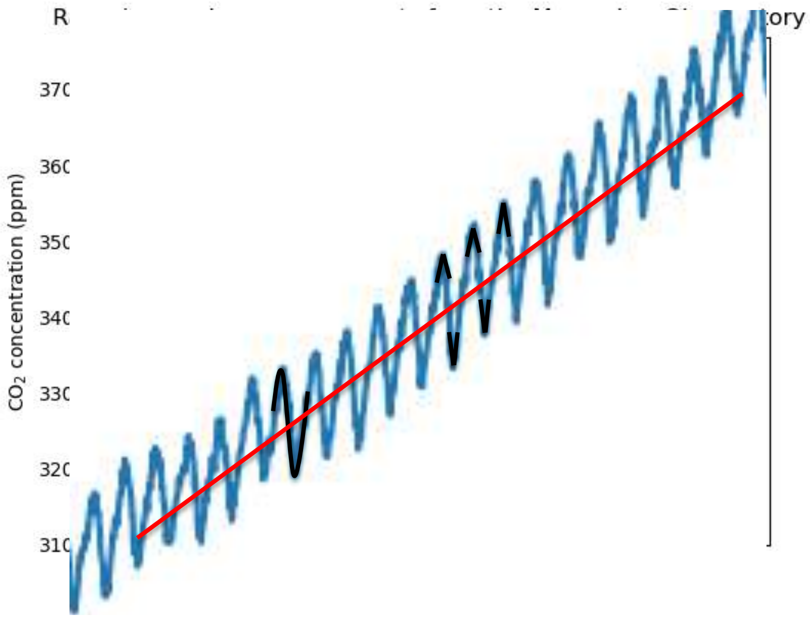
Modeling periodic data with periodic kernel

New architecture for kernels in SMT



Modeling periodic data with periodic kernel

Simple dataset: Mauna Loa CO2 concentration measurements

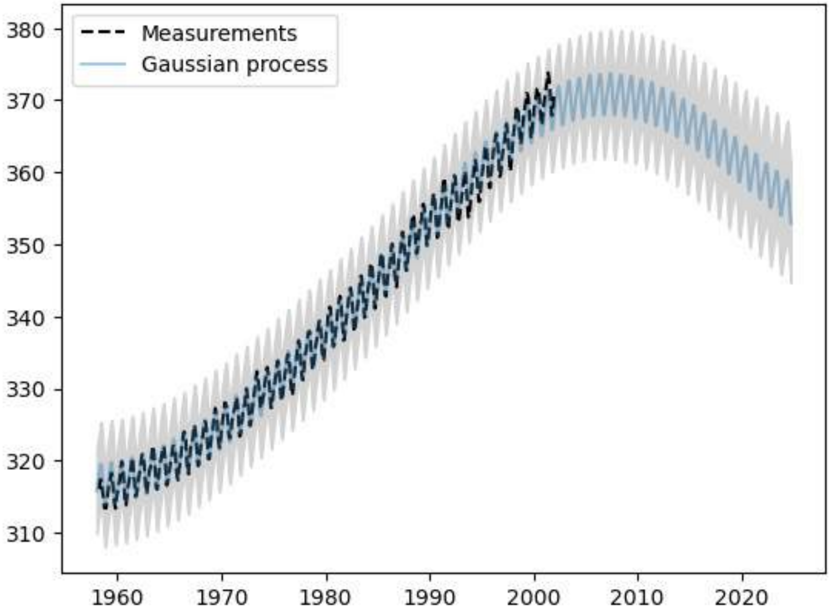


Goal: Interpolate data correctly and use periodicity to extrapolate

Rasmussen, Carl Edward. “Gaussian processes in machine learning.” Summer school on machine learning. Springer, Berlin, Heidelberg, 2003.
Keeling, C. D., Bacastow, R. B., Bainbridge, A. E., Ekdahl Jr, C. A., Guenther, P. R., Waterman, L. S., & Chin, J. F. (1976). Atmospheric carbon dioxide variations at Mauna Loa observatory, Hawaii. Tellus, 28(6), 538-551.
Beck, E.-G. (2008). 50 Years of Continuous Measurement of CO2 on Mauna Loa. *Energy & Environment*,

Validation (Mauna Loa observation)

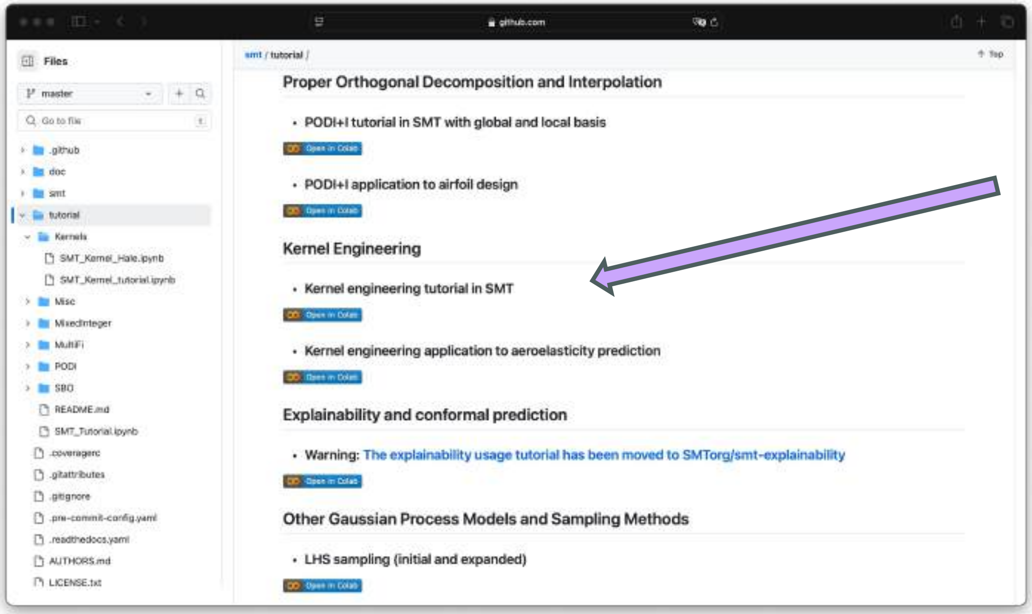
Kernel = squared exponential*periodic kernel +squared exponential



poor extrapolation and interpolation

Tutorial (Mauna Loa observation)

https://github.com/SMTorg/smt/tree/master/tutorial



θ_0

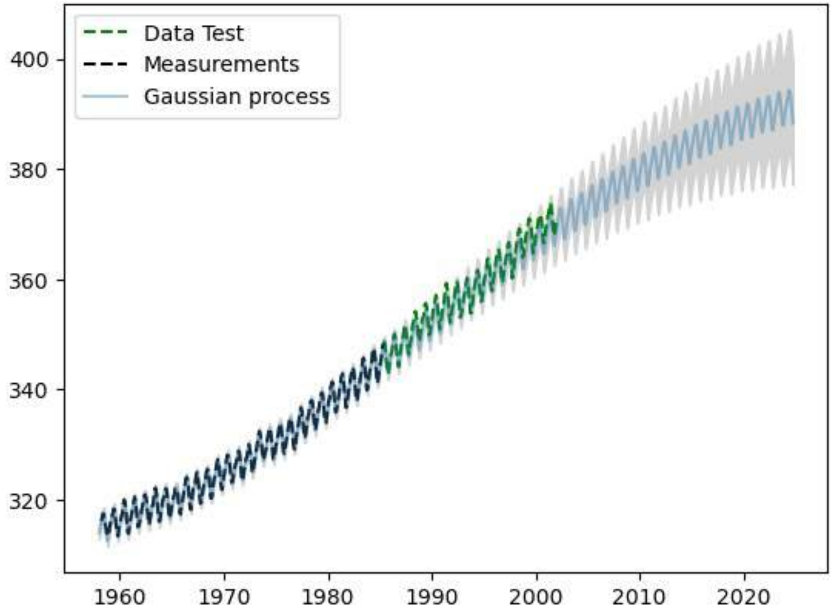
```
…
k=RBF([0.01])+Period([0.01,0.01])*RBF([0.01])+Rat_quad([0.01,0.01])

from smt.surrogate_models import KRG
sm=KRG(corr=k, hyper_opt="Cobyla",n_start=50)
sm.set_training_values(X, y)
sm.train()
…
```

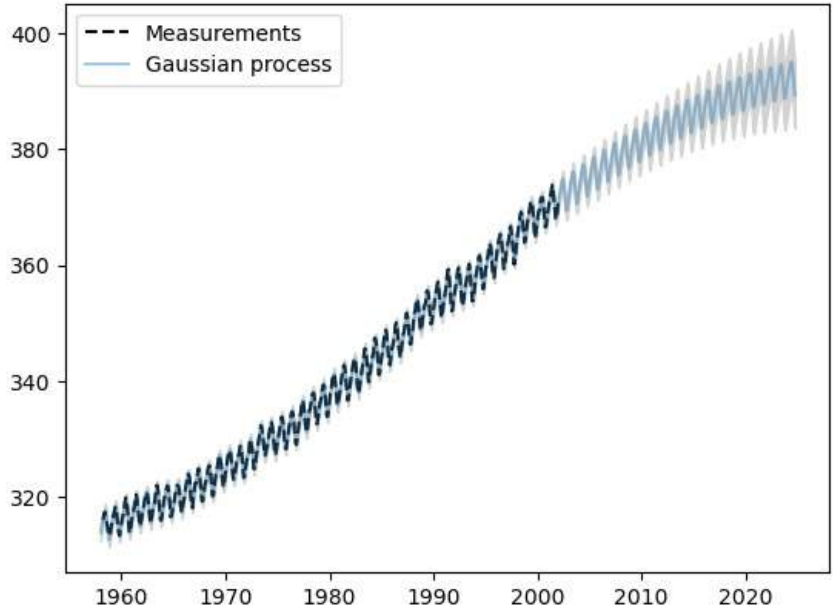
θ^* is found, then predict mean and variance for test

Validation (Mauna Loa observation)

Kernel = squared exponential*periodic kernel +squared exponential + rational quadratic



Kernel = squared exponential + squared exponential * periodic kernel + rational quadratic + squared exponential +whitenoise



Similar results as scikit-learn with a simpler kernel. Successful regression and good extrapolation.

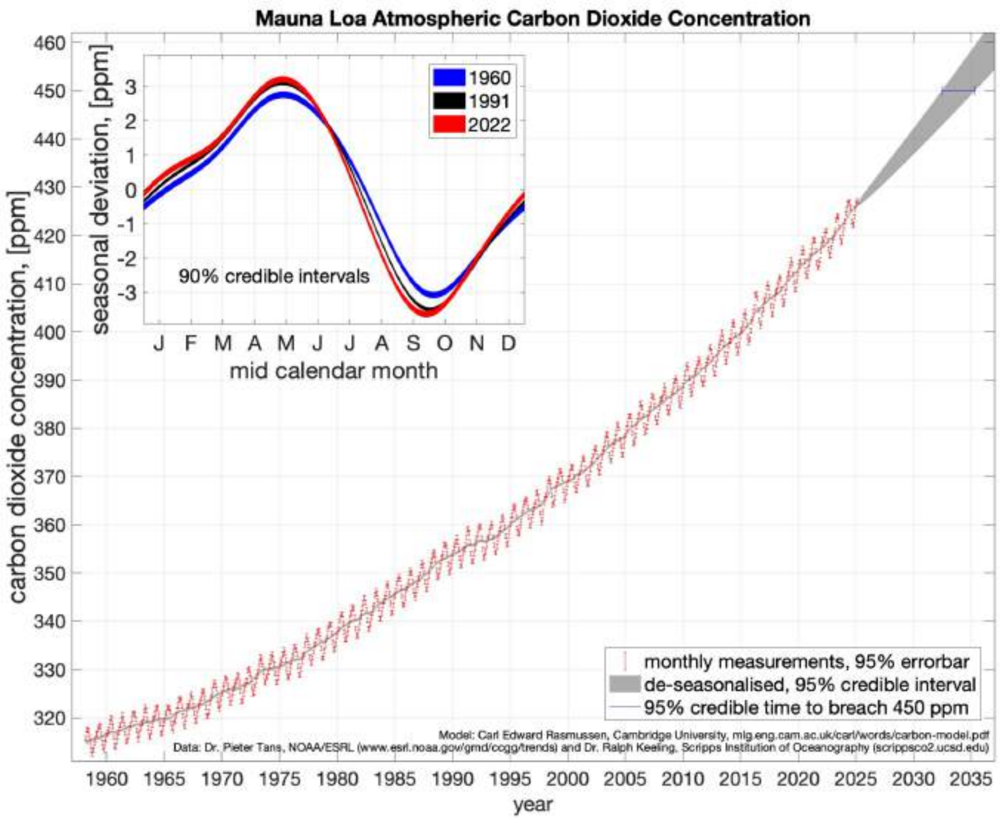
https://scikit-learn.org/stable/auto_examples/gaussian_process/plot_gpr_co2.html

D. Duvenaud (2014). "The Kernel Cookbook: Advice on Covariance functions". https://www.cs.toronto.edu/~duvenaud/cookbook/

Scikit-learn: Machine Learning in Python, Pedregosa *et al.*, JMLR 12, pp. 2825-2830, 2011

Want more details…
Ask Carl !

https://mlg.eng.cam.ac.uk/carl/climate/onepointfive.html#co2-model-details



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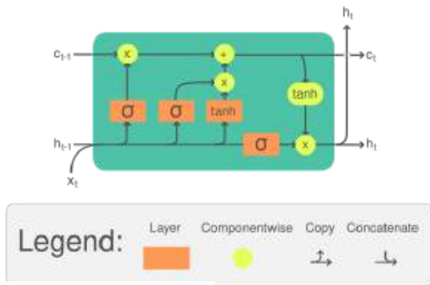
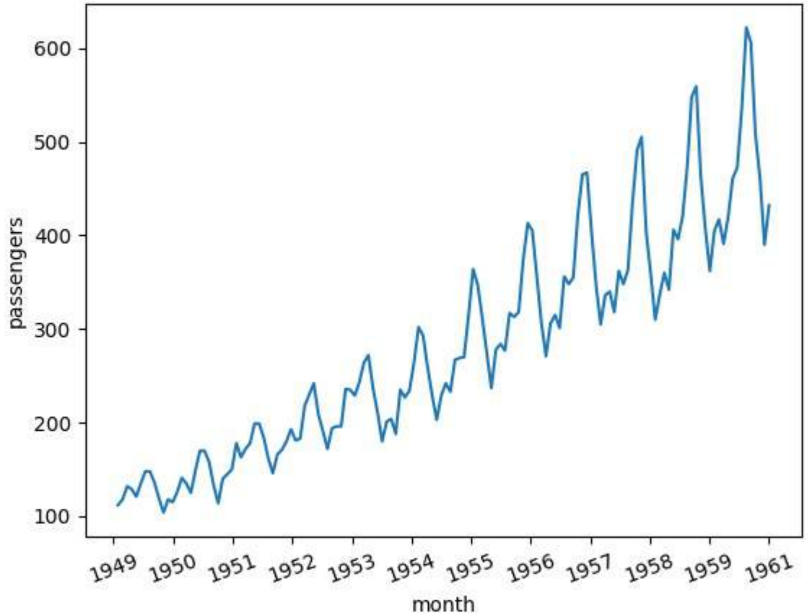
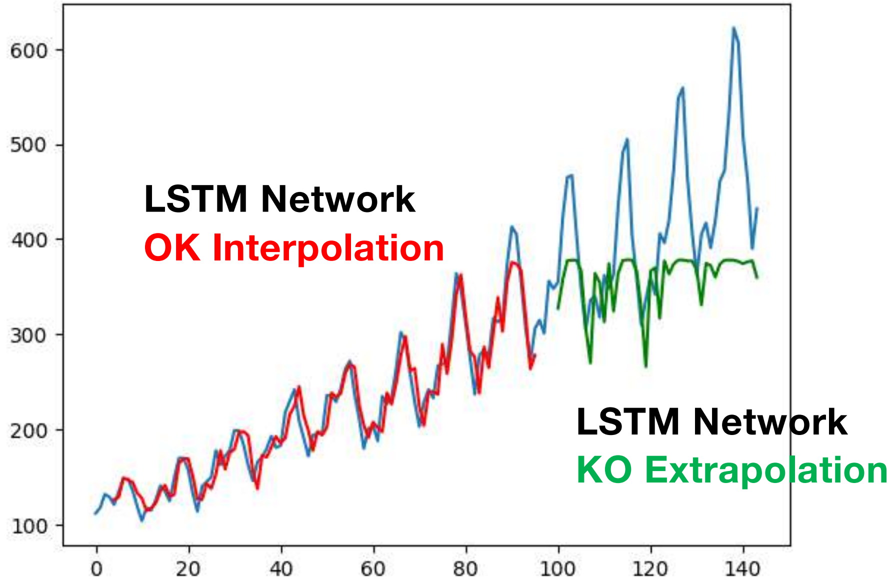
Test case 1 (international airline passengers)



International airline passengers

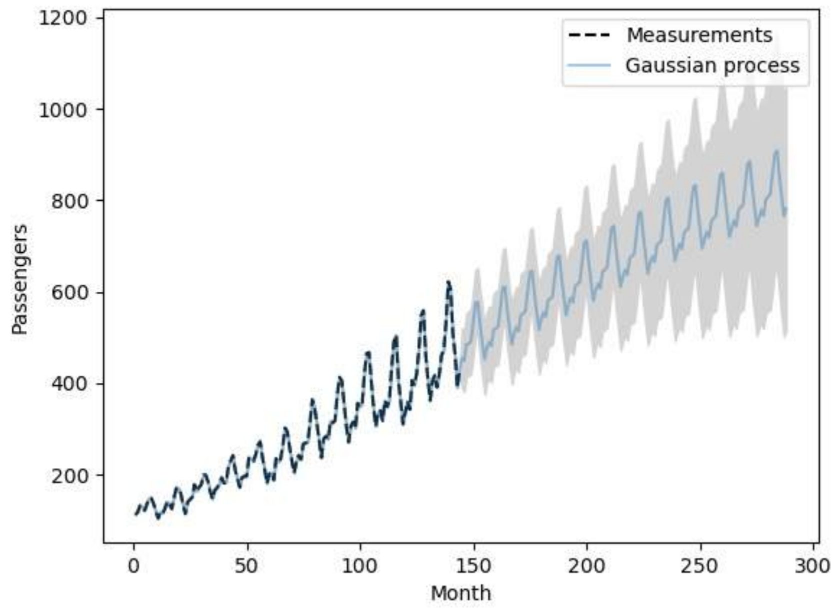




https://machinelearningmastery.com/lstm-for-time-series-prediction-in-pytorch/

Test Case 1 (international airline passengers)

Kernel = squared exponential*periodic kernel
+squared exponential + rational quadratic



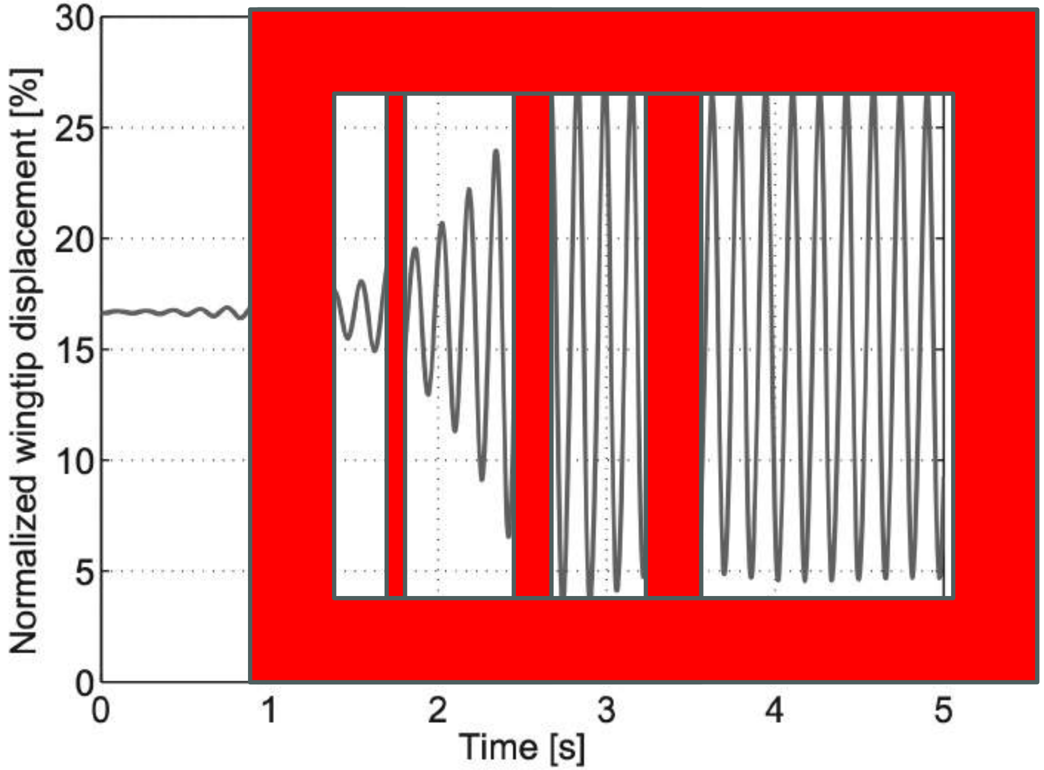
GP with good kernel

OK Extrapolation

NEED TO INFERE THE KERNEL?

Test case 2 Flutter detection

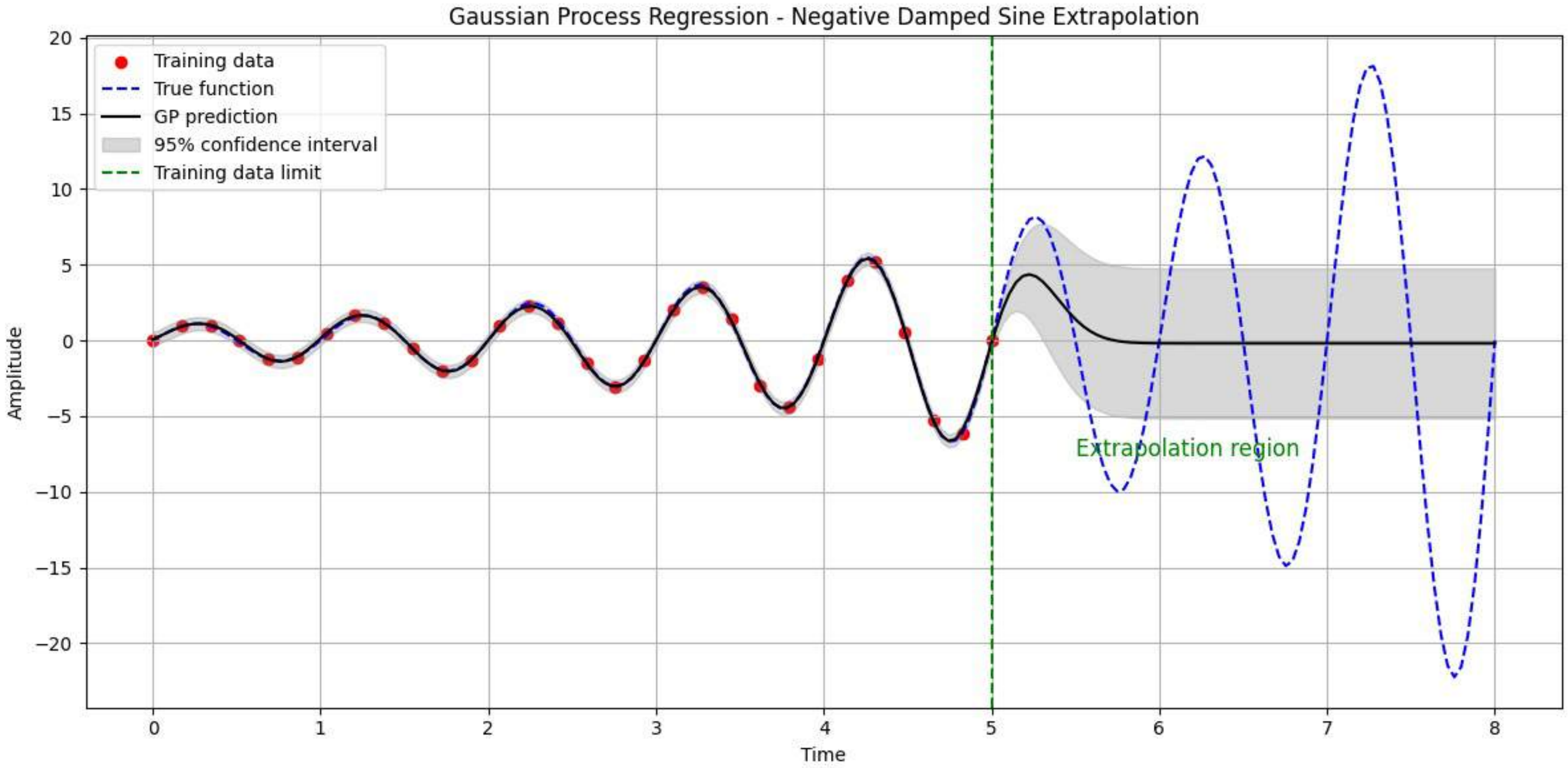
Preliminary Results:
Need time signals
Find best kernels for different extrapolation rates



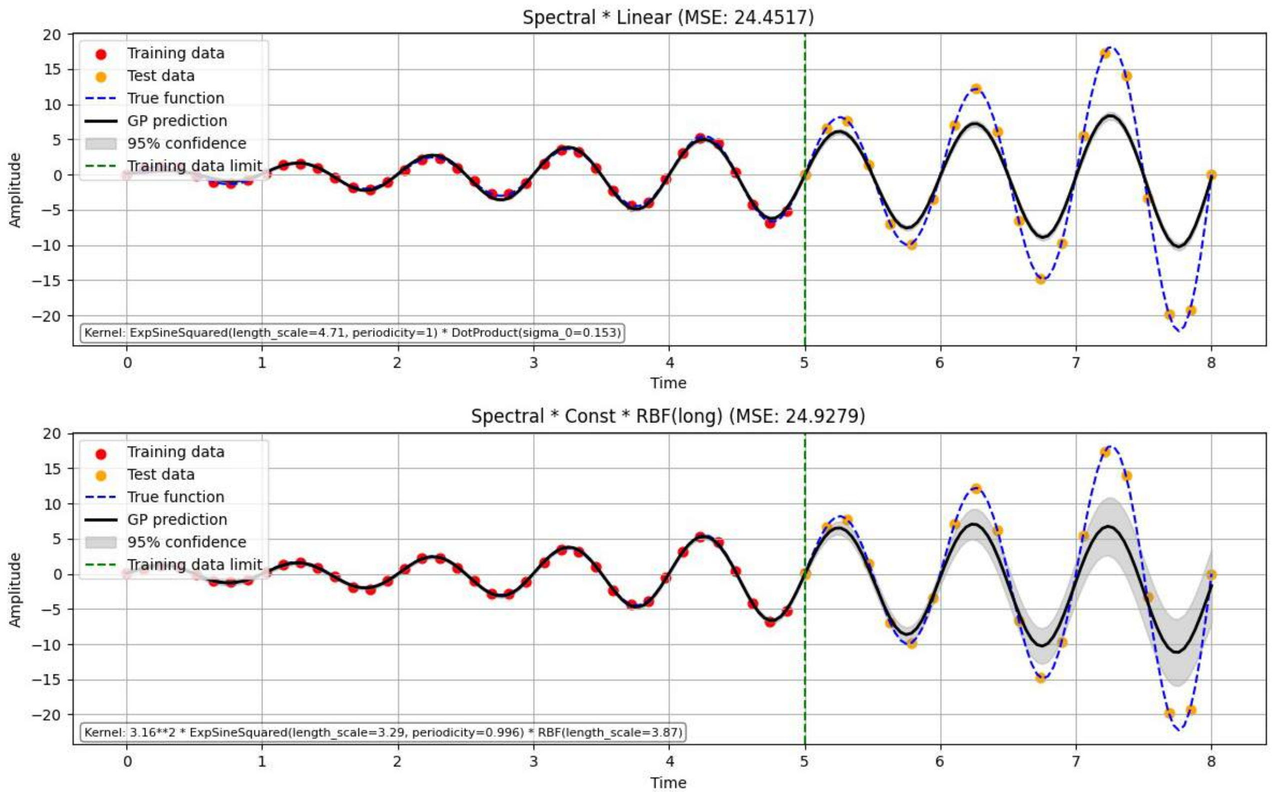
Su, W., & Cesnik, C. E. (2010). Nonlinear aeroelasticity of a very flexible blended-wing-body aircraft. *Journal of Aircraft*, *47*(5), 1539-1553.

Play with Negative damped sine

i.e. Simplify flutter :) without Kernel combination



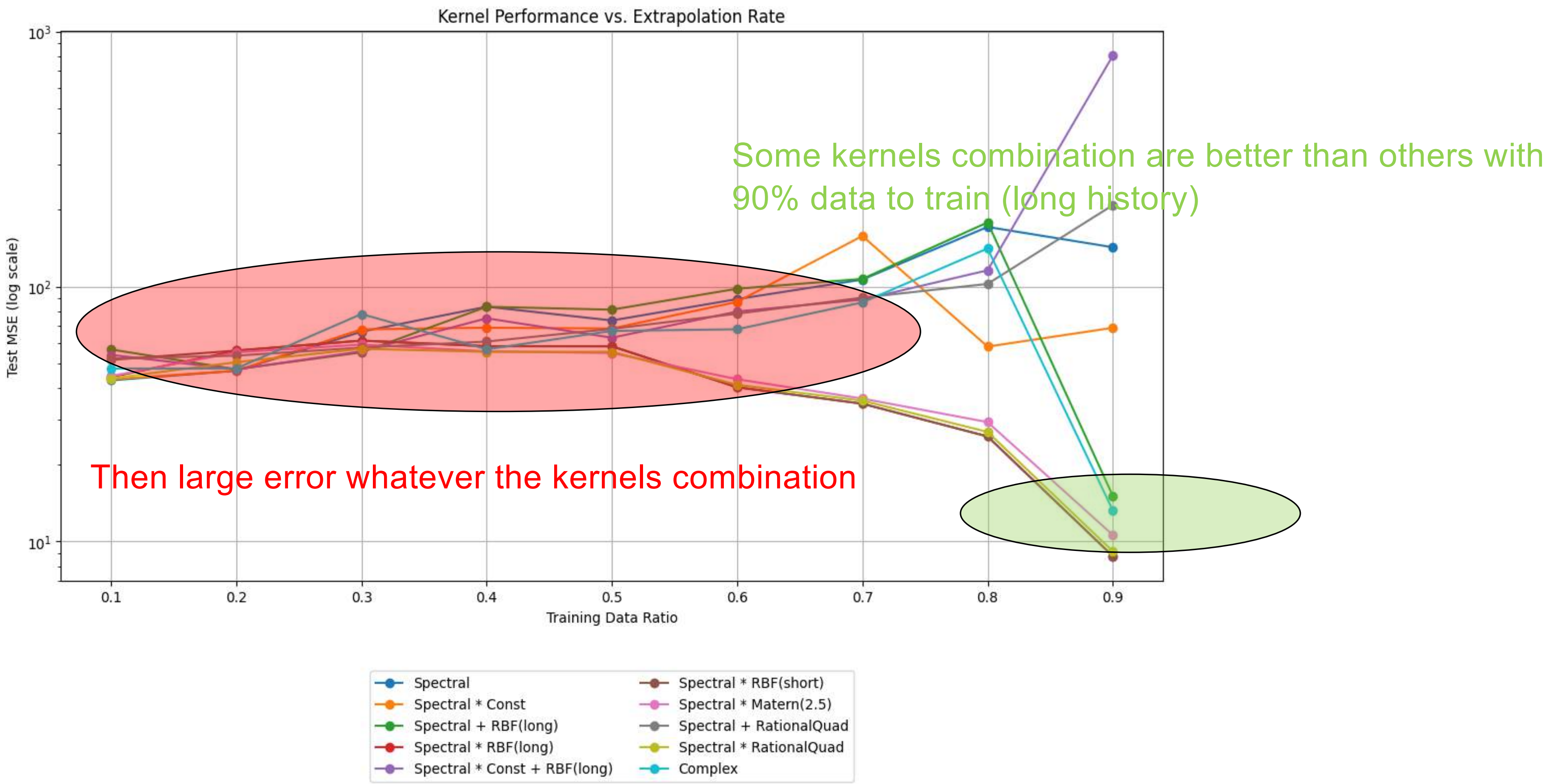
Simplify flutter :) with Kernels combination



Enumeration of Kernels combination is not the solution
Especially for different extrapolation rate (Train/test)

How to tune a flutter detection algorithm with few real time data ? (Train:= long history / test := new short length data)

Simplify flutter :) with Kernels combination



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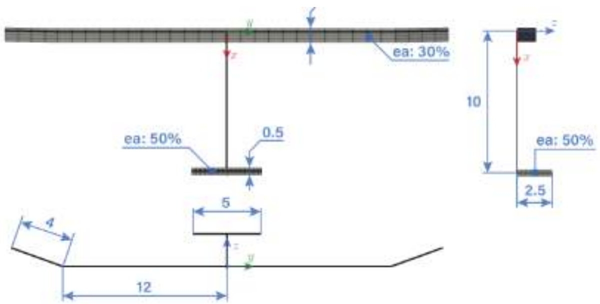
Conclusions and Perspectives

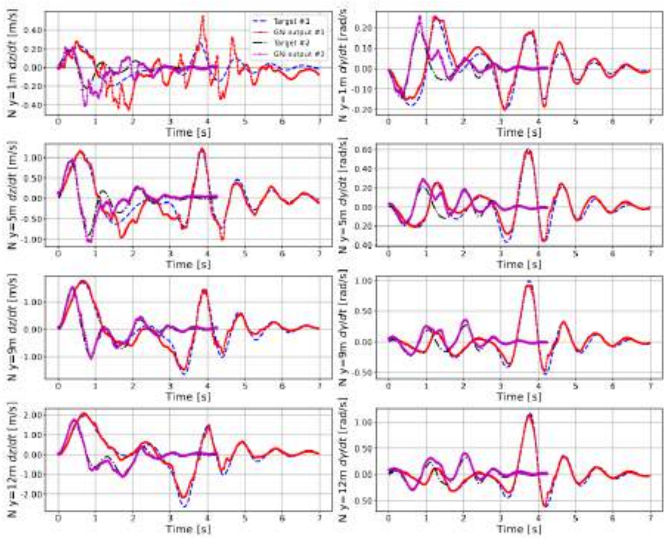


- Developed new kernels to increase extrapolation results quality

- New architecture for kernels in SMT
  - Chain rule to compute gradients (specificity of SMT)
  - Allow user-defined kernels so we can create more complex kernel

- Work in progress :
  - Adding more classical kernels and combination
  - Symbolic regression for avoiding enumeration
  - Gradient computing using jax

David Duvenaud (2014). "The Kernel Cookbook: Advice on Covariance functions". https://www.cs.toronto.edu/~duvenaud/cookbook/
Hensman, J., Durrande, N. and Solin, A. "Variational Fourier features for Gaussian processes." Journal of Machine Learning Research
(1) A. Wilson and R. Adams. "Gaussian process kernels for pattern discovery and extrapolation", International Conference on Machine Learning (2013)
Cranmer, M., Sanchez Gonzalez, A., Battaglia, P., Xu, R., Cranmer, K., Spergel, D., & Ho, S. (2020). Discovering symbolic models from deep learning with inductive biases. Advances in neural information processing systems, 33, 17429-17442.
Fernandez, L. F. T. (2024). *Controllability-aware multidisciplinary design optimization of small vertical take-off and landing vehicles*(Doctoral dissertation, Ecole Nationale Aviation Civile).



- Perspectives :
  - Application to HALE data https://imperialcollegelondon.github.io/sharpy/
  - Combine kernels combination with dimension reduction technique

Thank you for your attention!

European Workshop on MDO for Industrial Applications in Aeronautics - Toulouse, France, 3 – 5 June 2025

https://tinyurl.com/EWMDO2025

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