

Incorporating prior knowledge into Gaussian Process regression: with applications to aerospace engineering

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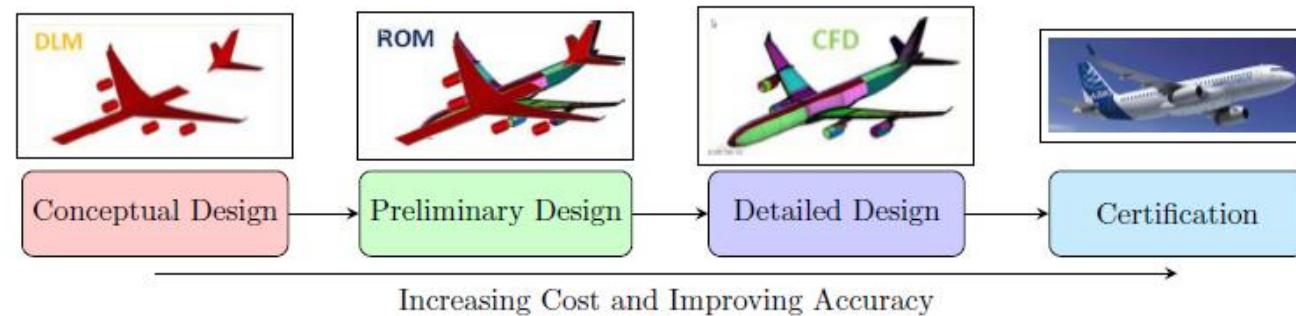


AIRBUS



Motivation and Objectives

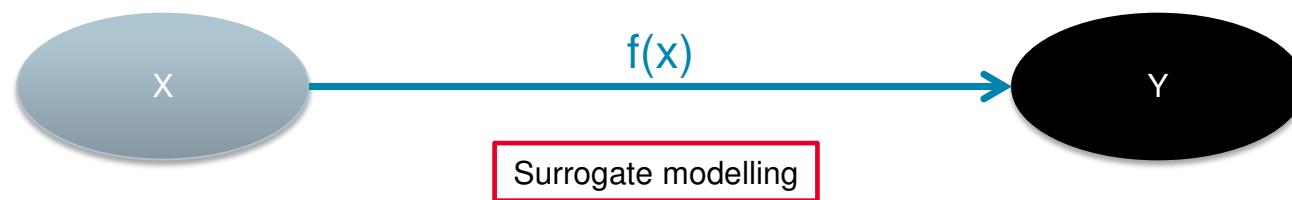
Motivation



Time	Few seconds	Few minutes	Few hours	Few days
Cost	N/A	N/A	10k euros	Millions euros

Find a quicker, cheaper and accurate representation

Objective of the PhD



- Engineering design
 - Bottleneck → Data cost
 - Advantage → Prior information

Incorporate prior information into surrogate models

Contents

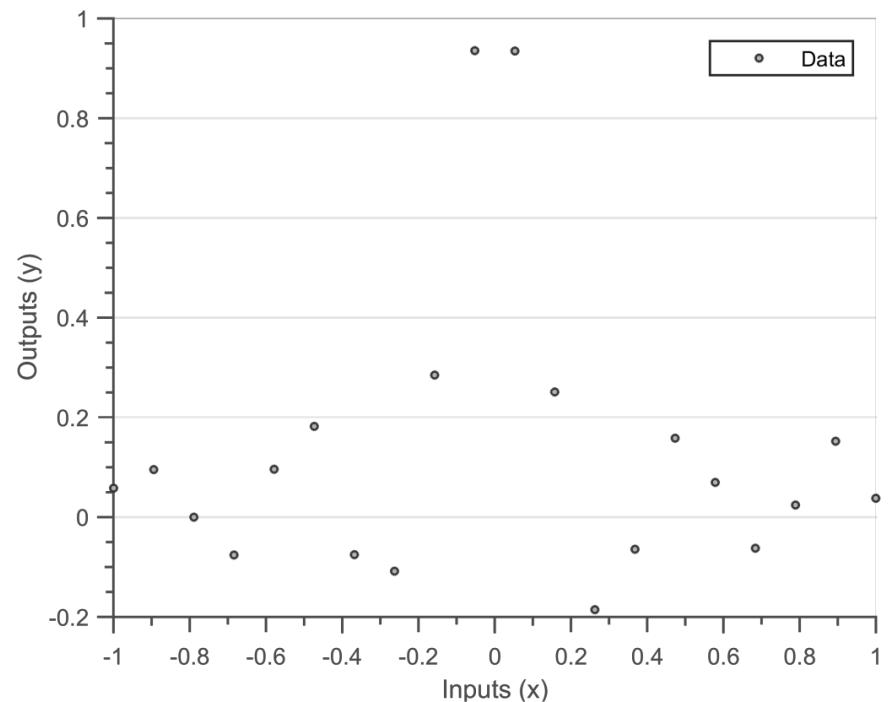
1. Gaussian Process Regression
2. Adding information of multiple outputs
 - Multi-task Gaussian Process
 - Incorporating relationships
 - Scaling Solutions
3. Adding information of patterns
 - Detecting onset of non-linearity
 - Shock Interpolation
4. Conclusions

Gaussian Process Regression

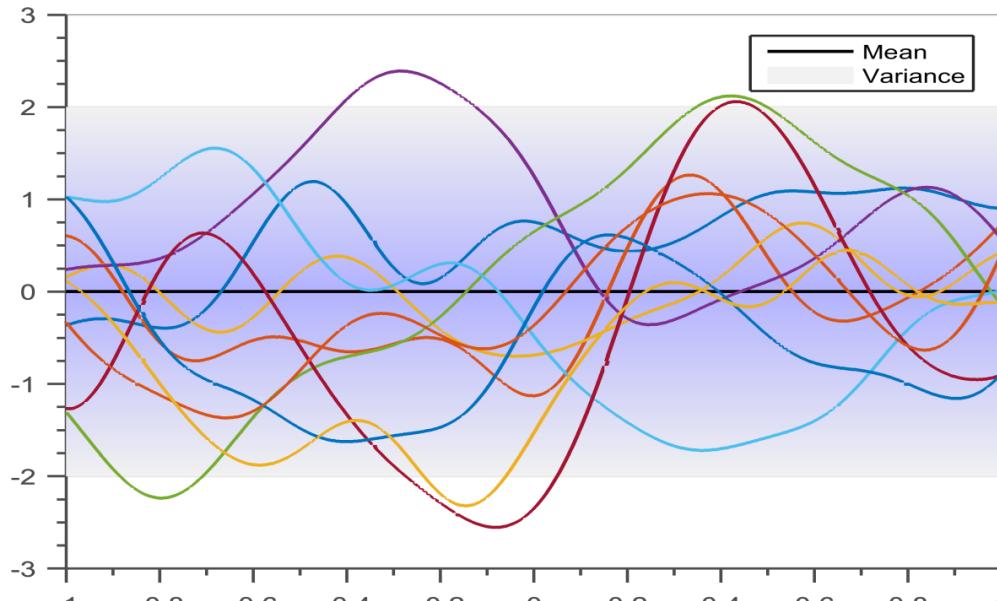
Regression

- Objective:

Find → $f: R^{D_{inputs}} \rightarrow R^{D_{outputs}}$



Gaussian Process



Prior

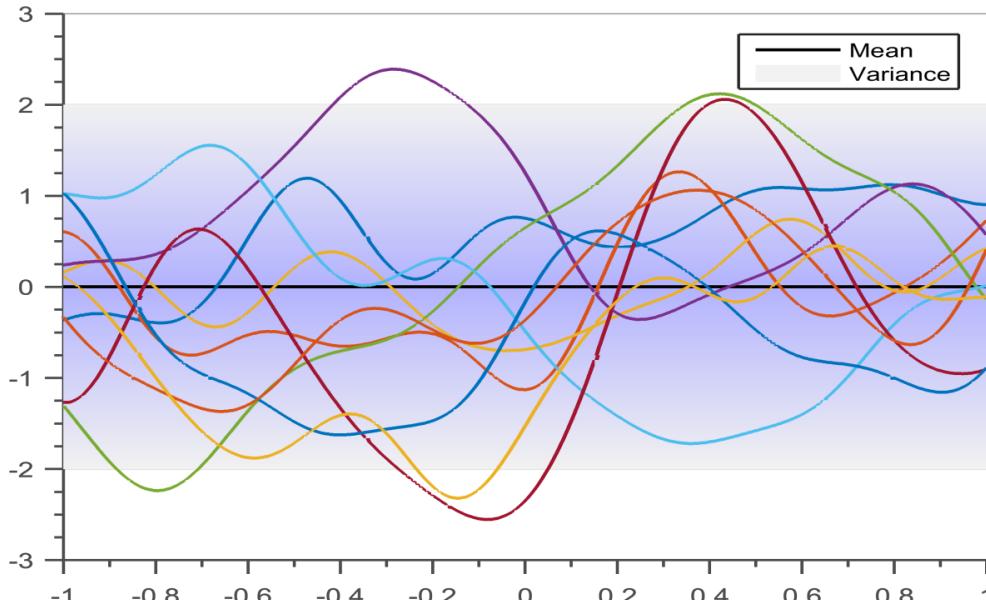
$$p(f|M) = GP(0, K(\theta))$$

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

References:

- [G. Matheron. 1962] → Kriging
- [C. Rasmussen et. al. 2005] → Gaussian Process

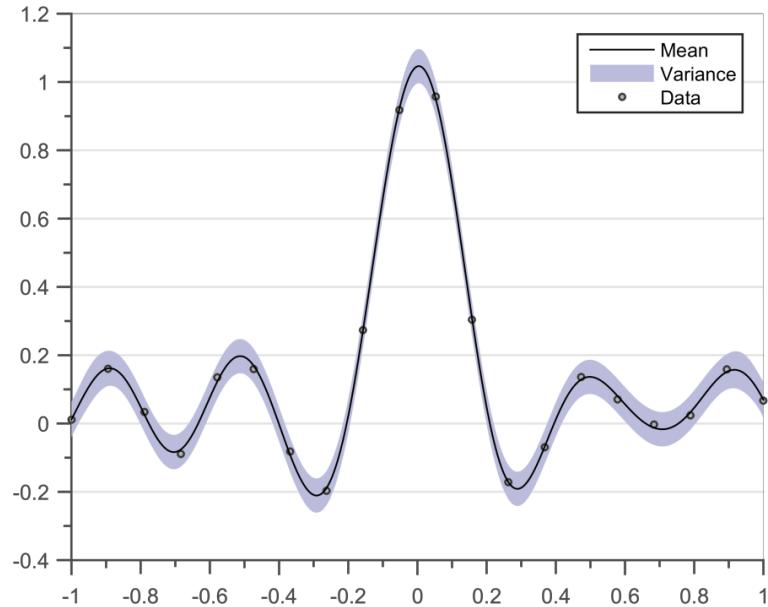
Gaussian Process Regression (GPR)



Prior

$$p(f|M) = GP(0, K(\theta))$$

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



Posterior

$$m(x_*) = K_* [K + \sigma_n^2 I]^{-1} y$$

$$\text{var}(x_*, x'_*) = K_{**} + \sigma_n^2 I - K_*^T [K + \sigma_n^2 I]^{-1} K_*$$

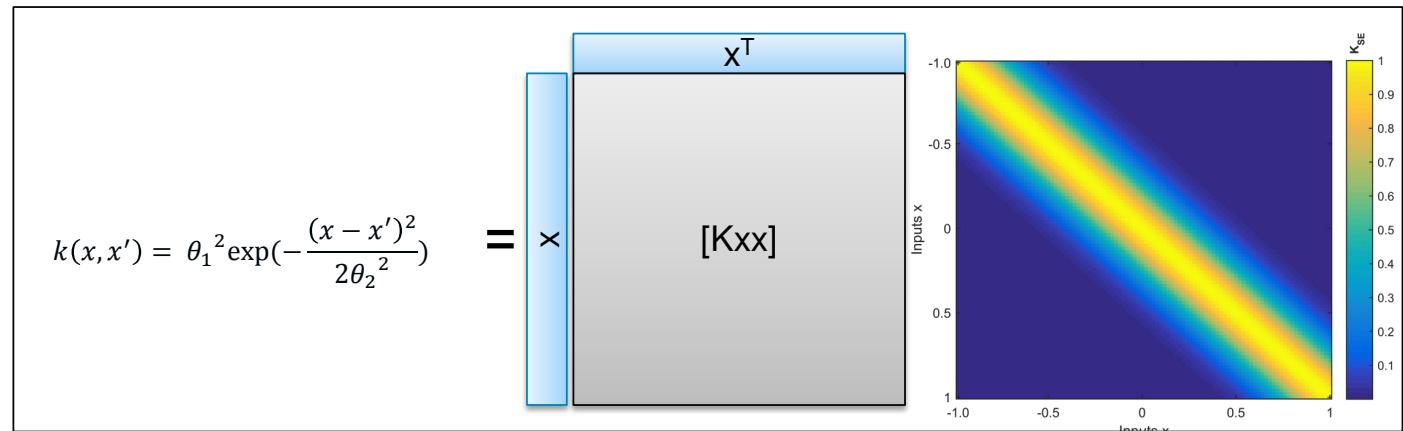
References:

- [G. Matheron. 1962] → Kriging
- [C. Rasmussen et. al. 2005] → Gaussian Process

Matrix view of Gaussian Process

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

$$x^*$$



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

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

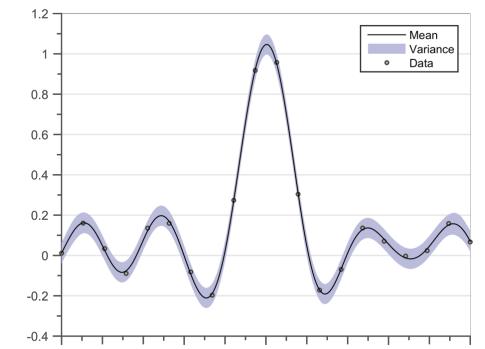
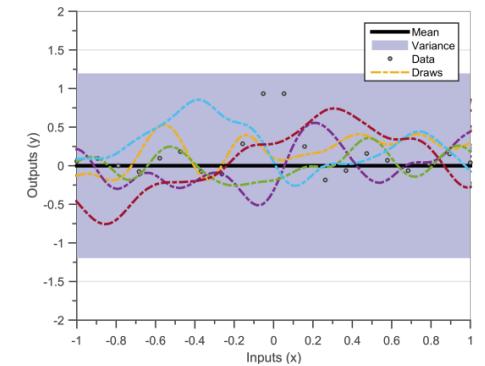
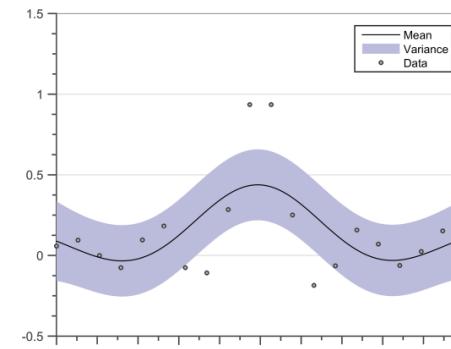
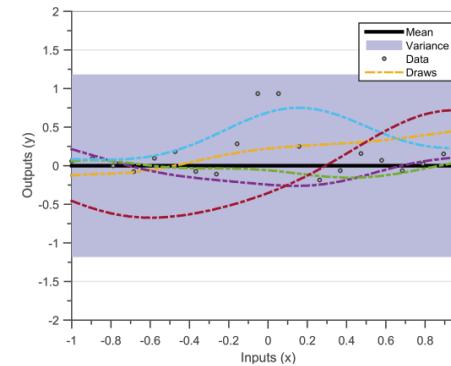
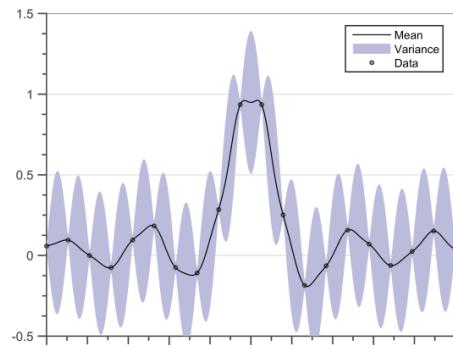
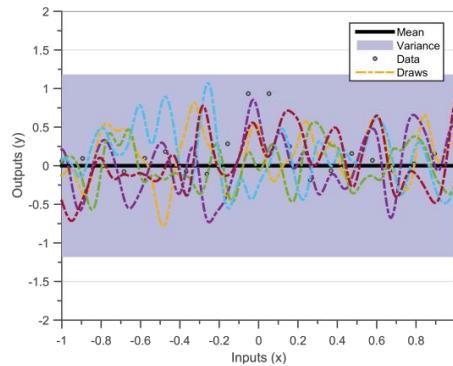
$$\text{cov}(y^*) = [K_{x^*x^*}] - \begin{matrix} [K_{x^*x}] \\ \vdots \\ [K_{xx}]^{-1} \end{matrix} [K_{x^*x}]^T$$

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

Optimizing marginal likelihood

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

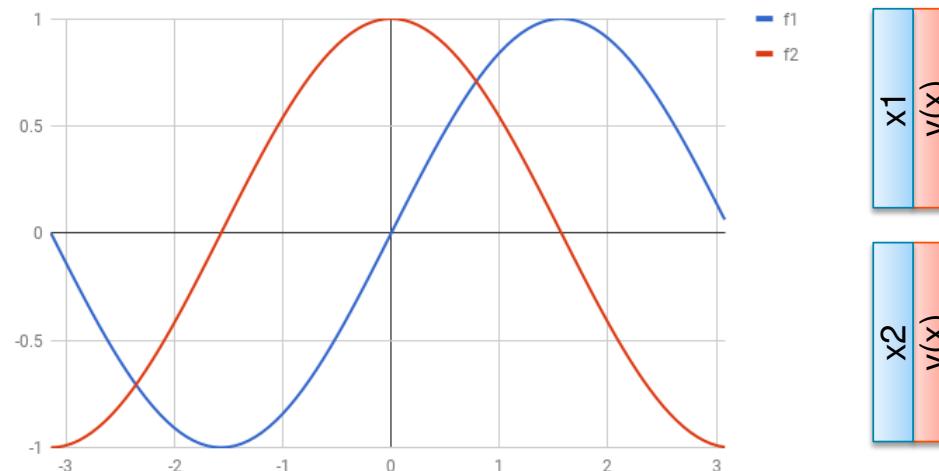
- It is a combination of **data-fit term**, a **complexity penalty term** and a **normalization term**



Adding information of multiple outputs

Multi-task Gaussian Process

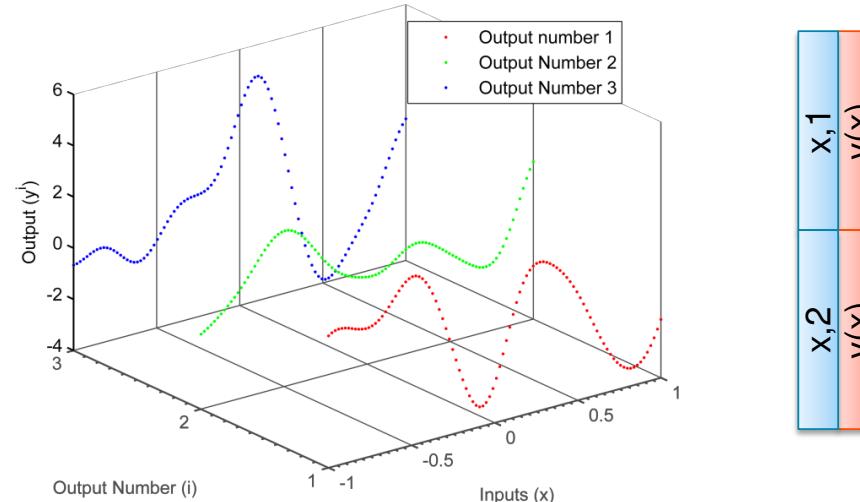
- Case 1: When the outputs are non-correlated



- Define prior independently $\rightarrow p(f_1) = GP(0, K_1)$ and $p(f_2) = GP(0, K_2)$
- Maximize ML
- Calculate mean and variance

Multi-Task Gaussian Process

Case 2: When the outputs are related but the relation is unknown



- Joint prior:

$$PR(f_1 | f_2) = GP \begin{pmatrix} 0 \\ 0 \end{pmatrix} \left| \begin{matrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{matrix} \right.$$

- Maximize marginal likelihood
- Calculate mean and variance

References:

- [Michael Osborne. Thesis, 2010]

Matrix view of Multi task Gaussian Process

$$\begin{bmatrix} X,1 \\ X,2 \end{bmatrix} \quad \begin{bmatrix} y(x) \\ y(x) \end{bmatrix}$$

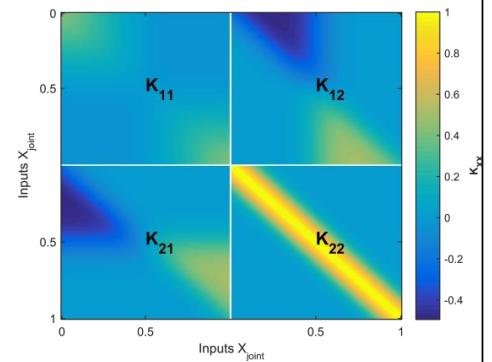
$$x^*$$

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

$$K = k_{output} k_{input}$$

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

$$= \begin{bmatrix} X,1 \\ X,2 \end{bmatrix} \begin{bmatrix} [K_{11}] & [K_{12}] \\ [K_{21}] & [K_{22}] \end{bmatrix} \begin{bmatrix} X,1 \\ X,2 \end{bmatrix}$$



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

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

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

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

Multi-task Gaussian Process

Case 3: When the outputs are related by a known relation/function

Given: $f_1 = g(f_2, x)$

Affine property: Iff g is a linear operator such as

$$g(a + b) = g(a) + g(b)$$

Then:

$$p\begin{pmatrix} f_1 \\ f_2 \end{pmatrix} = GP \begin{pmatrix} 0 & g(g(K_{22}, x_2), x_1) & g(K_{22}, x_2) \\ 0 & g(K_{22}, x_1) & K_{22} \end{pmatrix}$$

Example: Gradient enhanced kriging

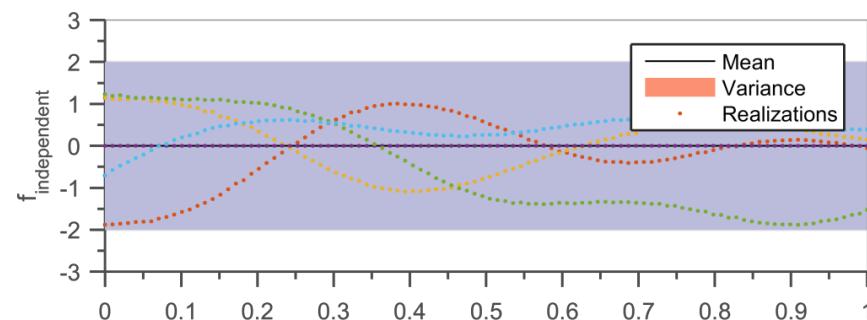
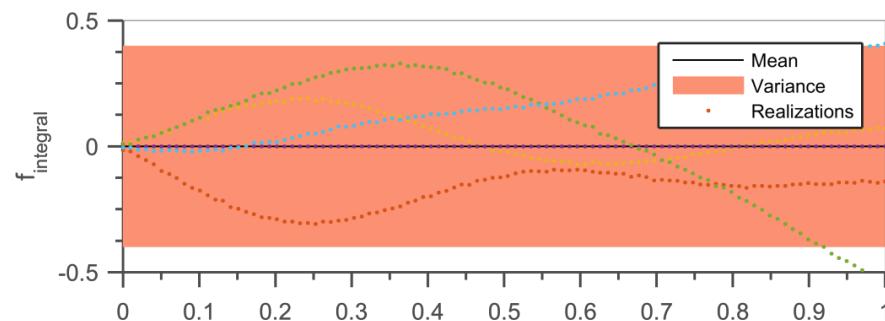
[AIAA, Chiplunkar 2016]

References:

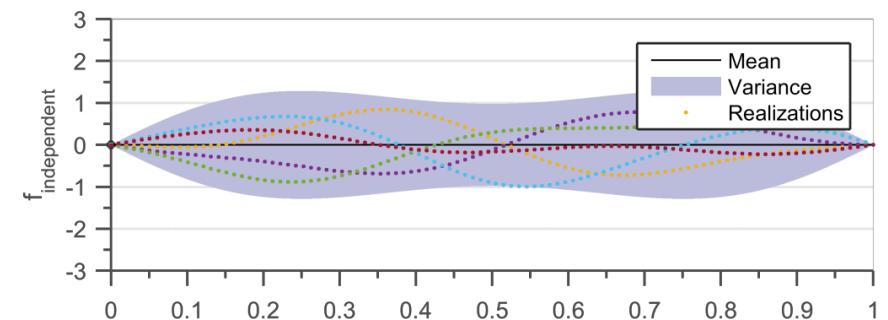
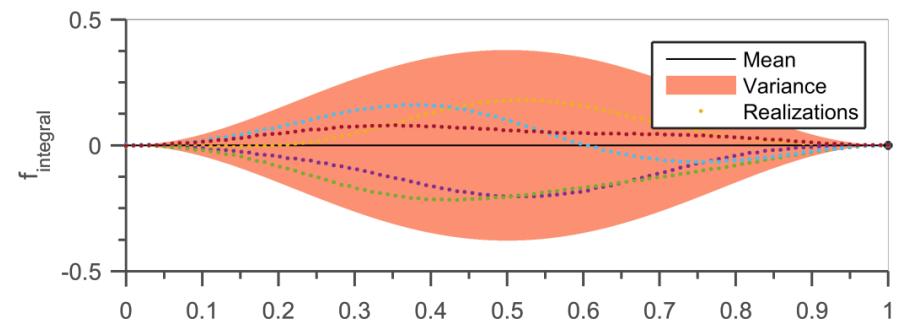
- [S. Särkkä. et. al ICANN 2011] [D. Ginsbourger, et. al arXiv, 2013] ➔ Linear processes
- [Emil M. Constantinescu et. al. SIAM 2013] ➔ Non-linear processes

Integral relation

$$f_{integral} = \int_0^x f_{independent}$$



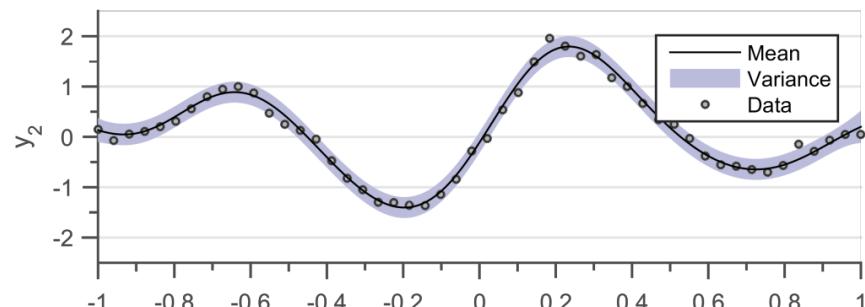
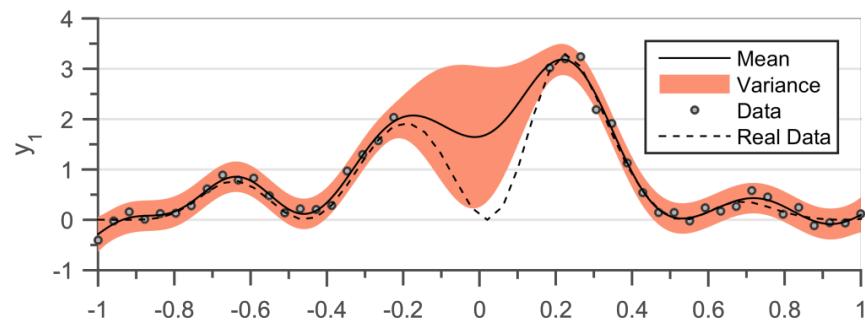
$$\begin{aligned} f_{integral} \Big|_{x=0} &= 0 \\ f_{integral} \Big|_{x=1} &= 0 \end{aligned}$$



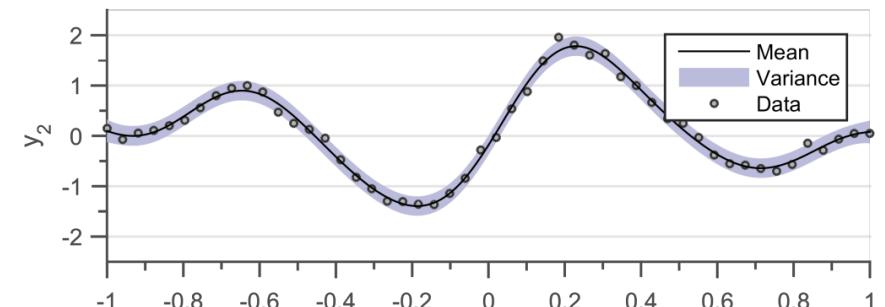
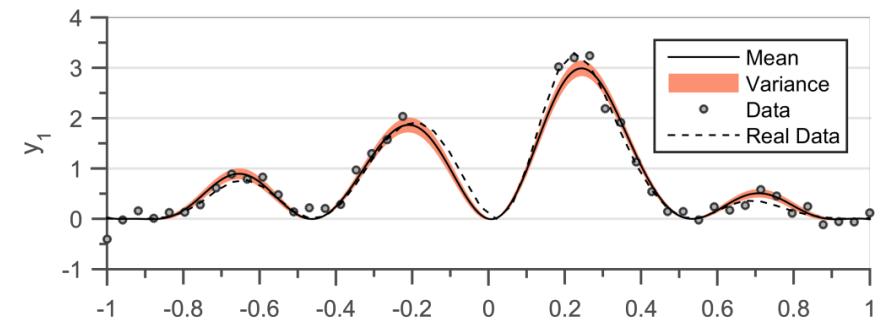
Simulated Data

Sensor malfunction

$$y_1 = (y_2)^2$$



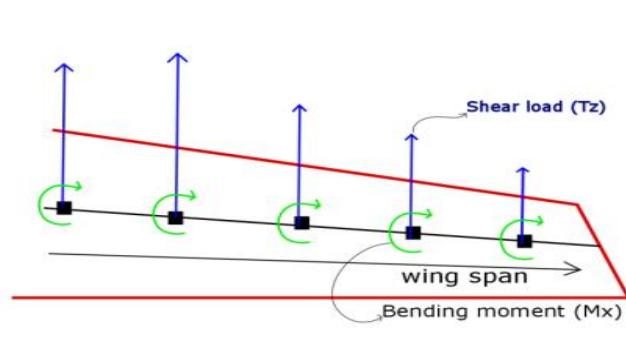
Independent GPs



Related GPs

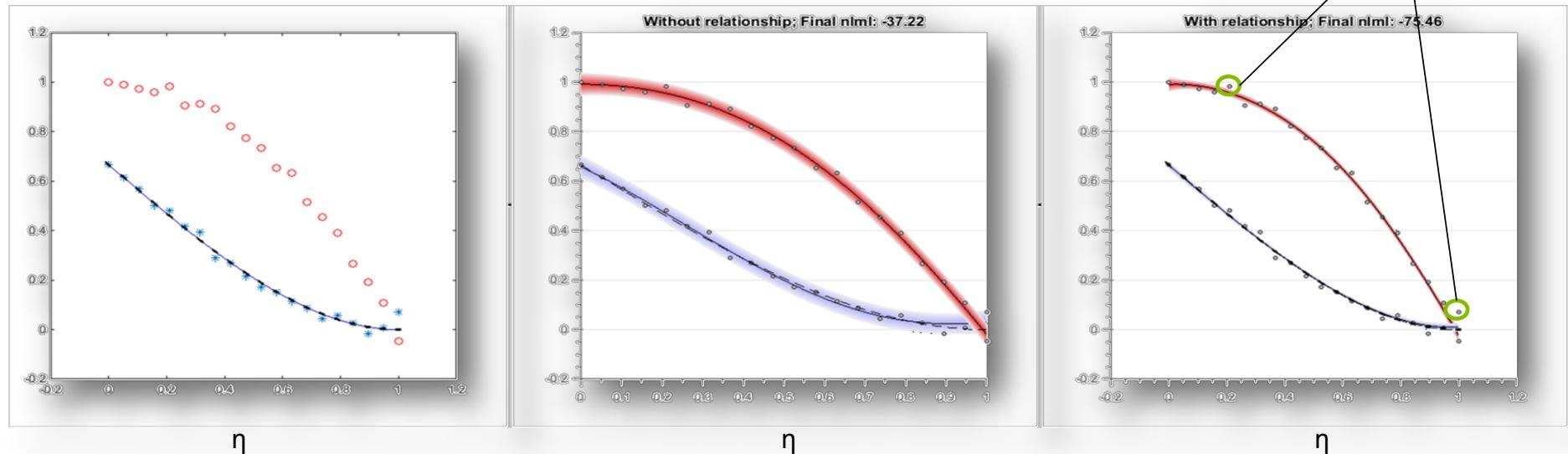
Simulated Data

Detecting faulty sensors



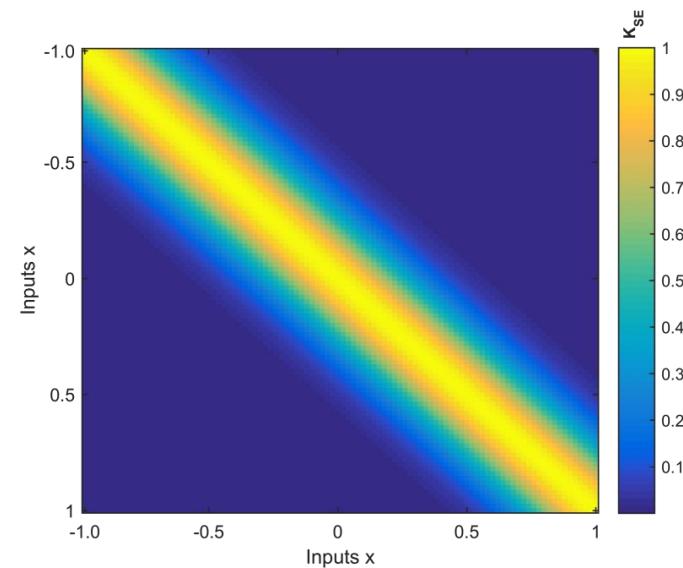
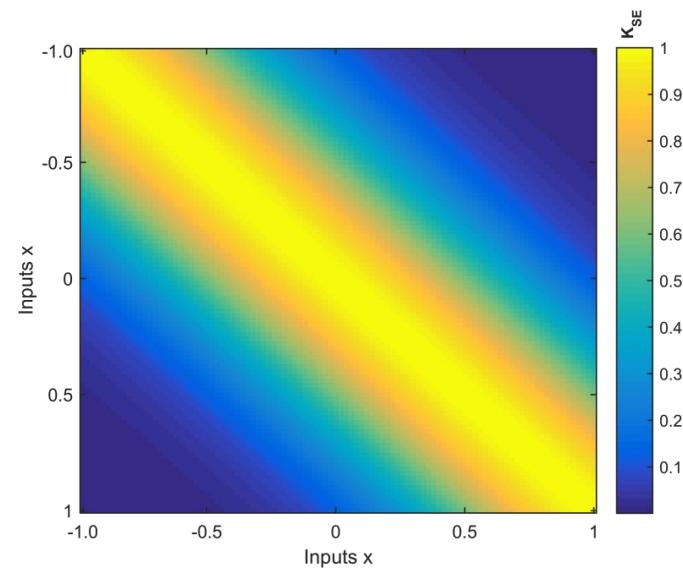
$$Mx = \int_{\eta}^{\eta_{edge}} (x - \eta) Tz \, dx$$

Wrong data point



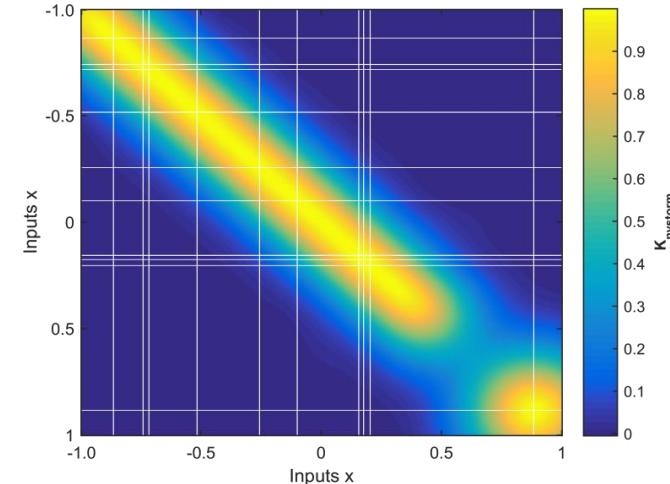
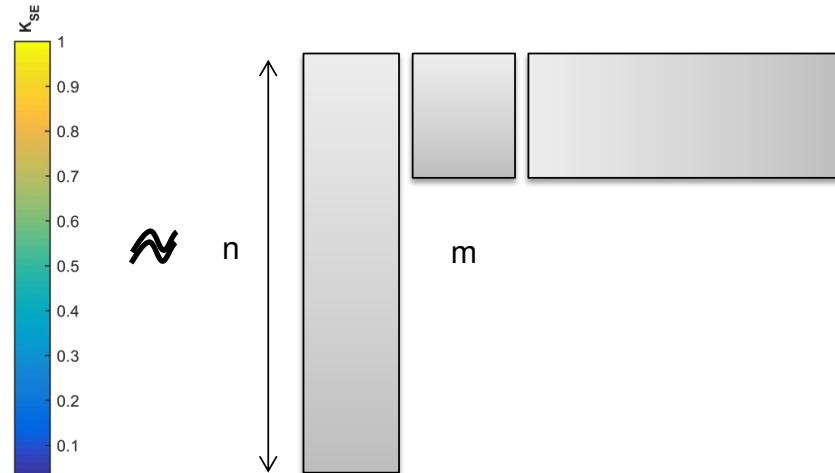
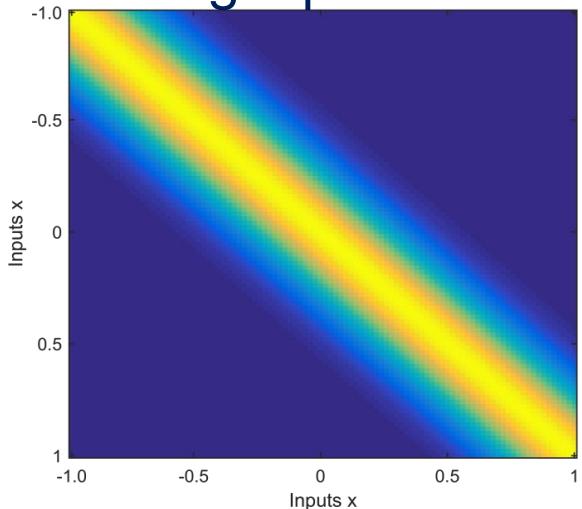
Scaling solutions

Learning	Storage	Mean	Variance
$O(n^3)$	$O(n^2)$	$O(n)$	$O(n^2)$



- Bottleneck → Inversion and Storage of matrix
- Infrastructure → HPC cluster

Inducing inputs



$$m(x_*) = K_{*\text{approximate}} [K_{xx\text{approximate}}]^{-1} y$$

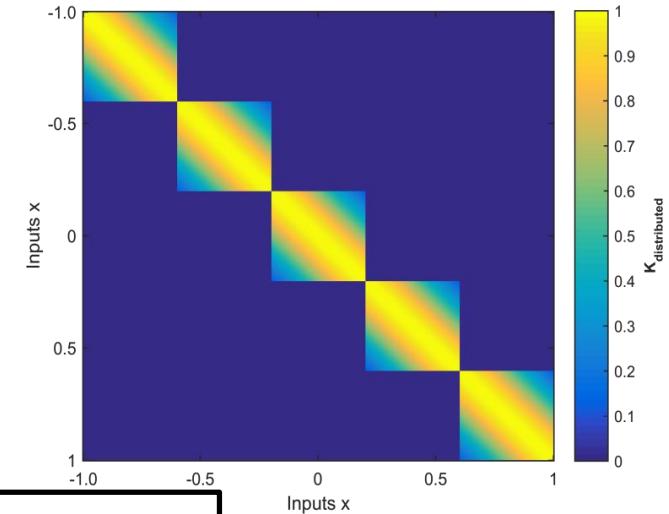
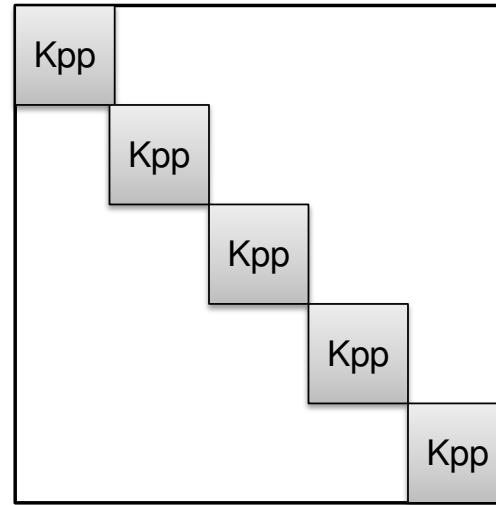
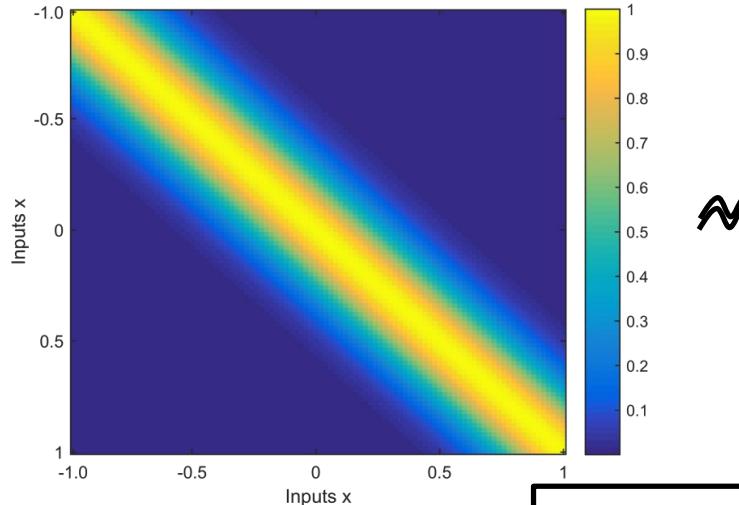
$$\text{var}(x_*, x'_*) = K_{**\text{approximate}} - K_{*\text{approximate}}^T [K_{xx\text{approximate}}]^{-1} K_{*\text{approximate}}$$

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

References:

- [C Williams et al. NIPS 2001] → Inducing inputs
- [Michalis K. Titsias. AISTATS 2009] → Variational inference

Distributed Gaussian Process



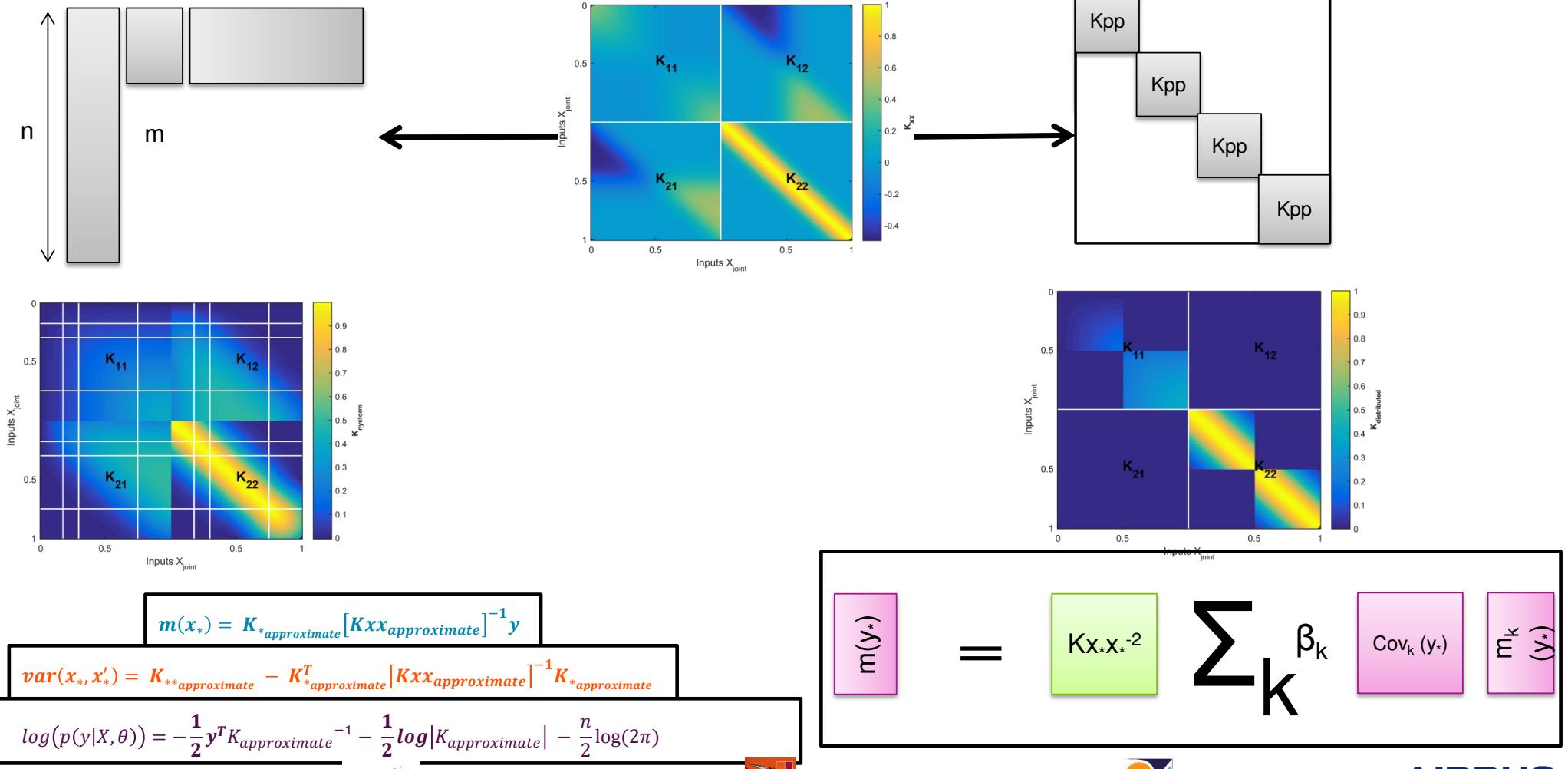
$$m(y^*) = Kx_*x_*^{-2} \sum_k \beta_k \begin{pmatrix} \text{Cov}_k(y^*) \\ m_k(y^*) \end{pmatrix}^{-2}$$

$$\beta_k = \log(K_{x^*x^*}^{-2}) - \log(\text{Cov}_k(y)^{-2})$$

References:

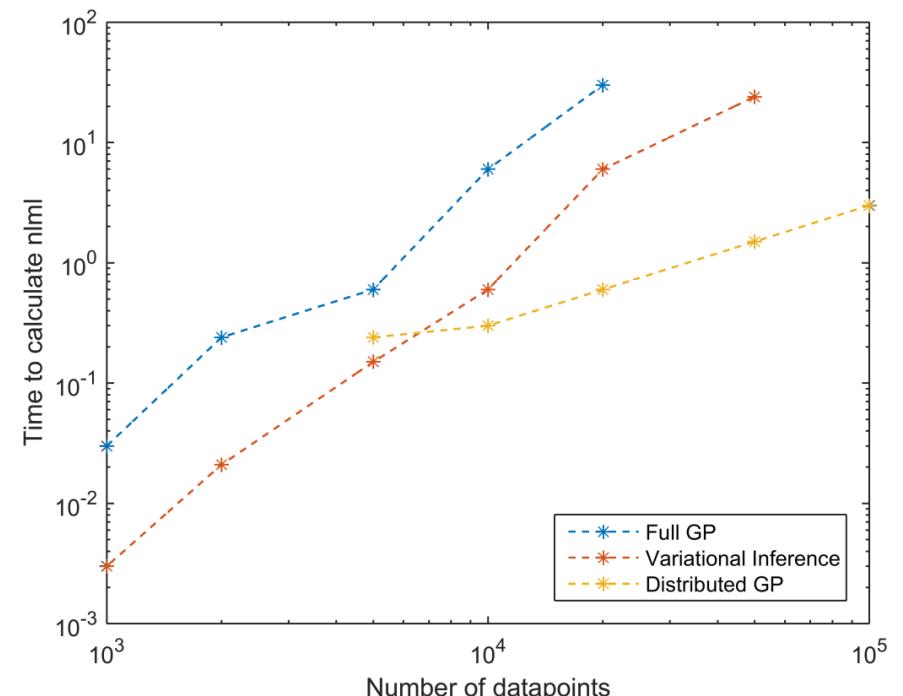
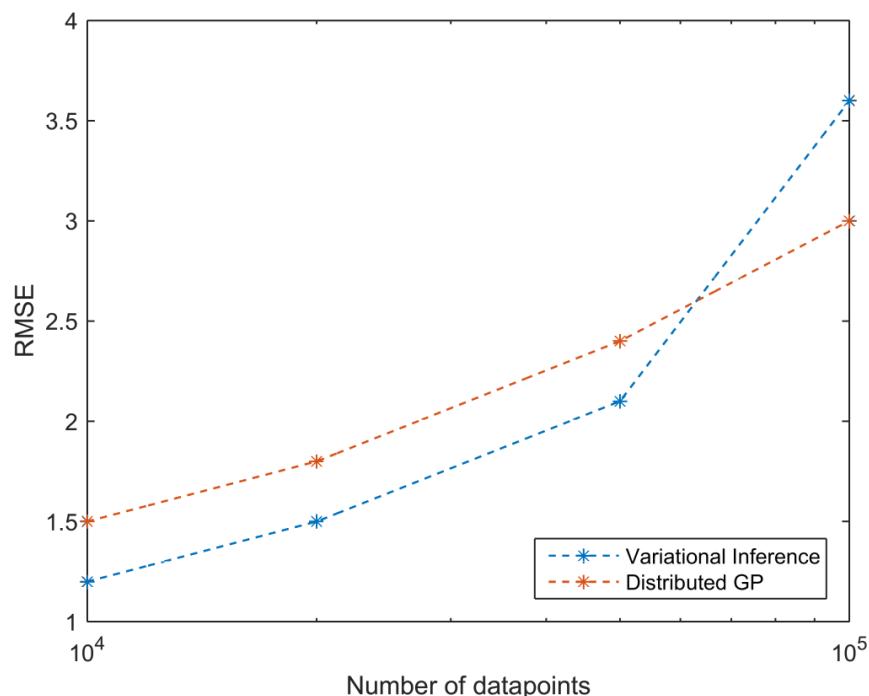
- [M Deisenroth et al. 2015]

Scaling solutions to Multi-task GP



Comparison between two approximation methods

$$f_1 = \frac{df_2}{dx}$$



Error

Simulated Data

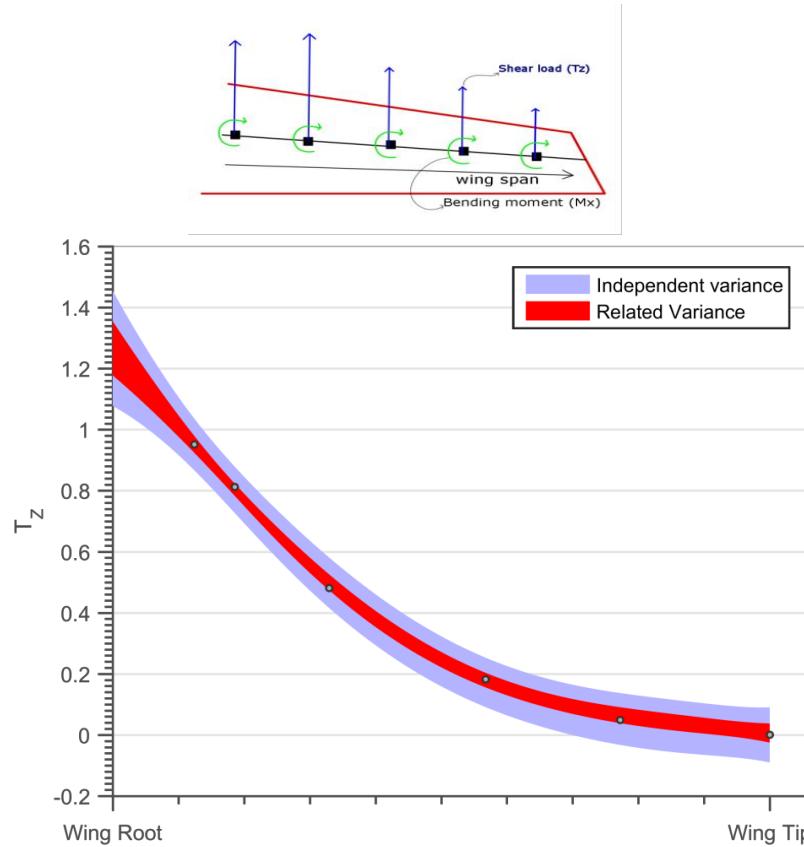


Time

[Chiplunkar et al. ICPRAM, 2016]
[Chiplunkar et al., LNCS, 2017]

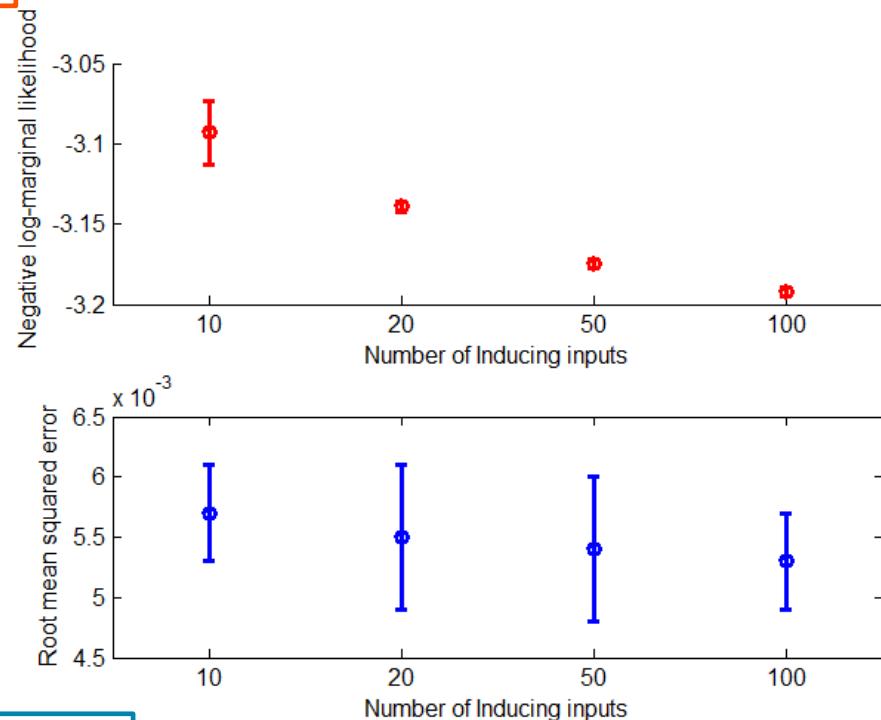


Scaling solutions to Multi-task GP



Experimental Data (flight loads)

$$Mx = \int_{\eta}^{\eta_{edge}} (x - \eta) Tz \, dx$$

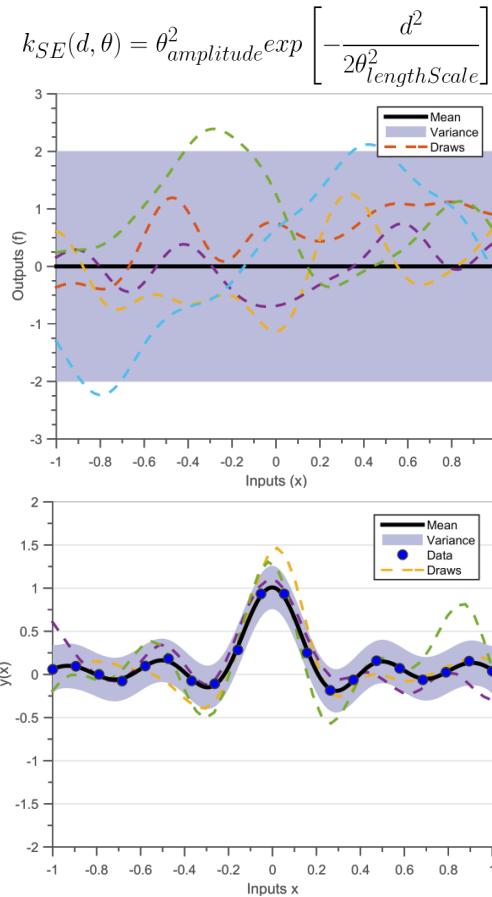


Adding information of shape

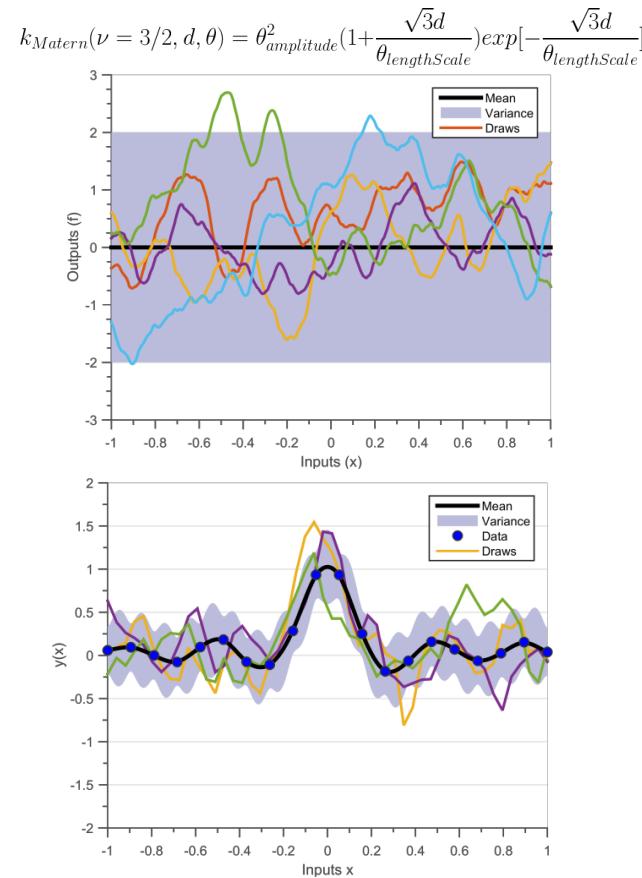
- Effect of kernels
- Detecting onset of non-linearity
- Interpolation of shock

Effect of different kernels

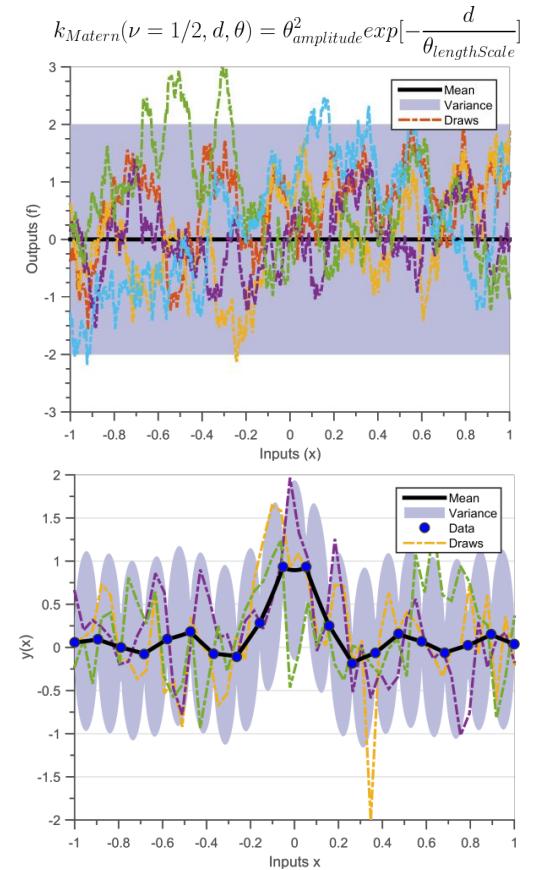
SE kernel (infinitely differentiable)



Once differentiable kernel



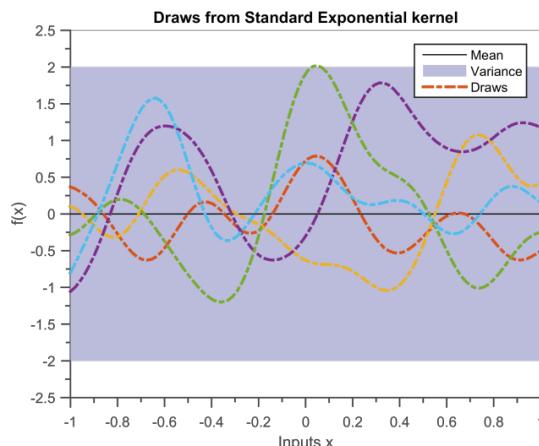
Brownian kernel



Basic Kernel Functions

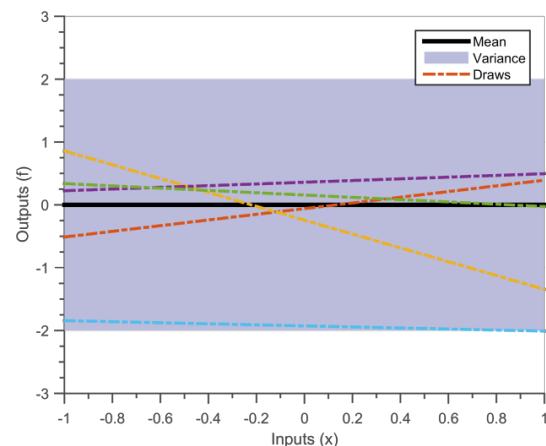
SE kernel (infinitely differentiable)

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



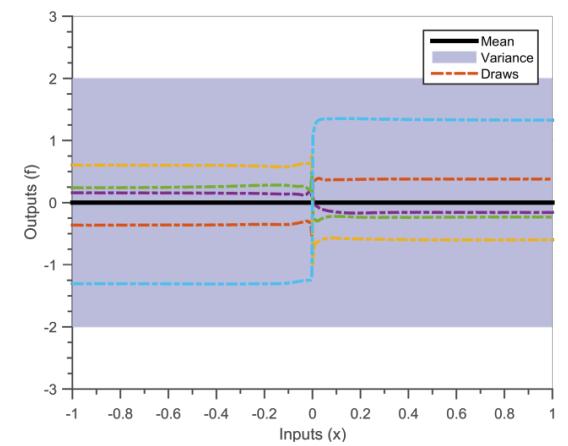
Linear kernel (Linear functions)

$$k(x, x') = \sigma_b^2 + \sigma_v^2 (x - c)(x' - c)$$



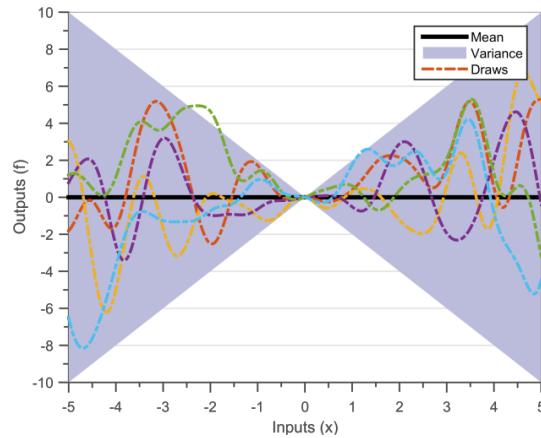
Neural Network kernel (discontinuous function)

$$k(x, x') = \sigma_1^2 \frac{2}{\pi} \sin^{-1} \left(\frac{2x\theta_2 x'}{\sqrt{(1+2x\theta_2 x)(1+2x'\theta_2 x')}} \right)$$

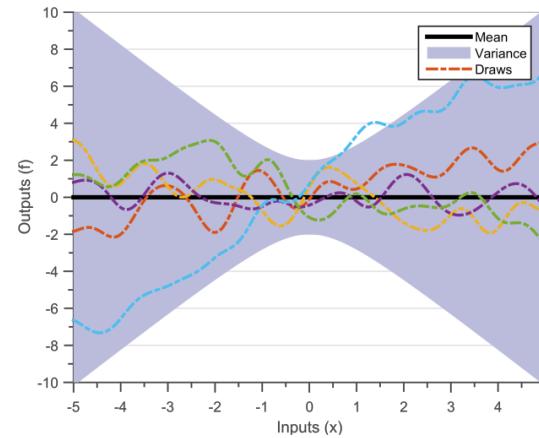


Combining different kernels

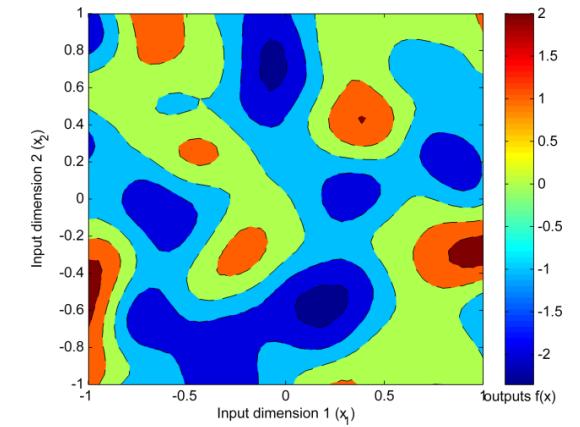
Linear (times) SE kernel



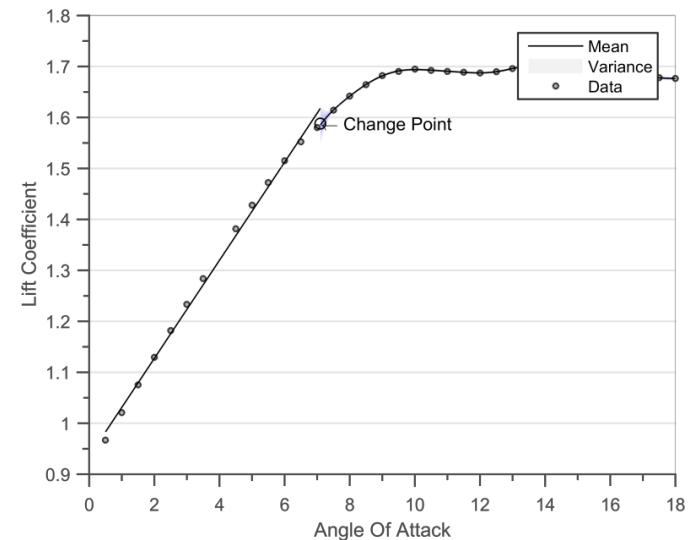
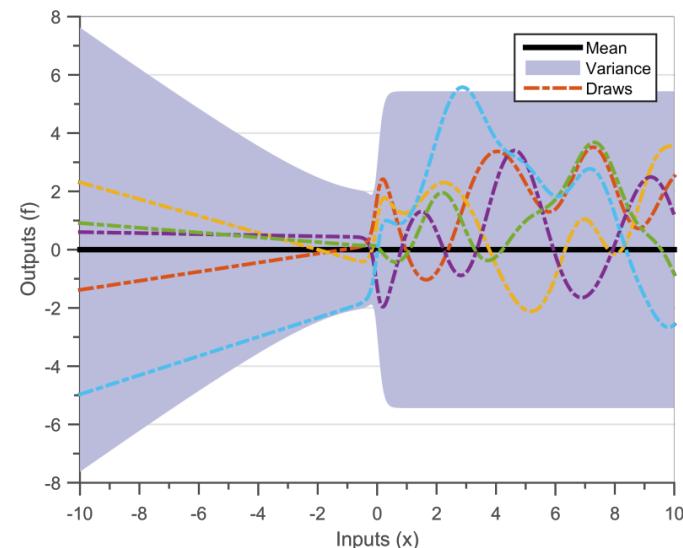
Linear (plus) SE kernel



**SE kernel (times) SE kernel
Across dimensions**



Identifying onset of non-linearity



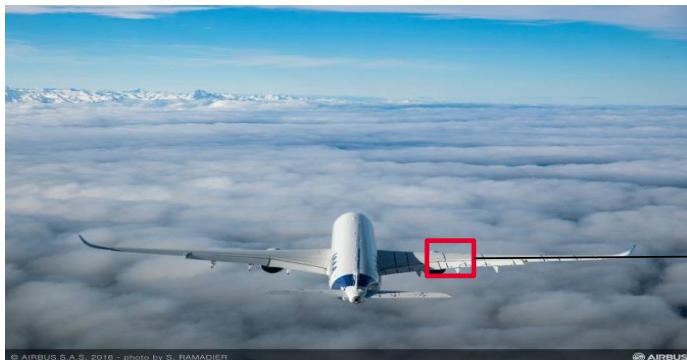
$$k_{CP}(k_1, k_2, x_1, x_2) = \text{sigm}(x_1)k_1\text{sigm}(x_2) + (1 - \text{sigm}(x_1))k_2(1 - \text{sigm}(x_2))$$

- Linear domain → Non-linear domain
- Maximize $\text{ML}(\theta)$ to estimate change-point

Experimental Data

A350-1000 : Interpolation of shock

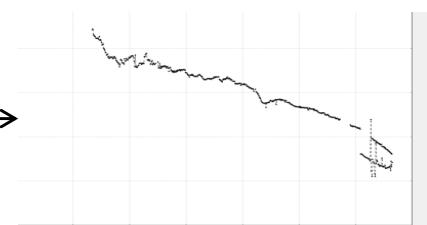
- Flight Test Instrumentation



MEMS pads

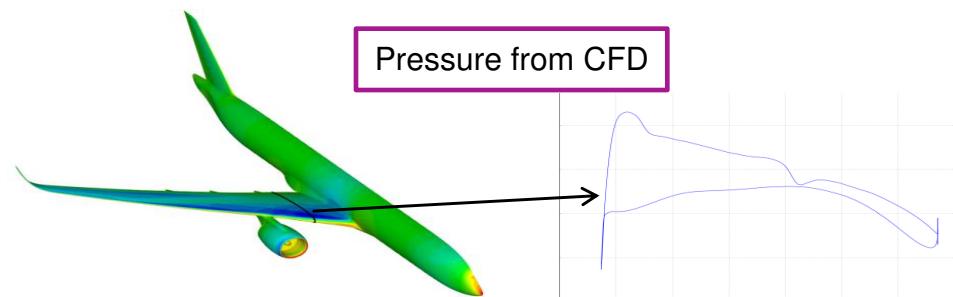


Pressure

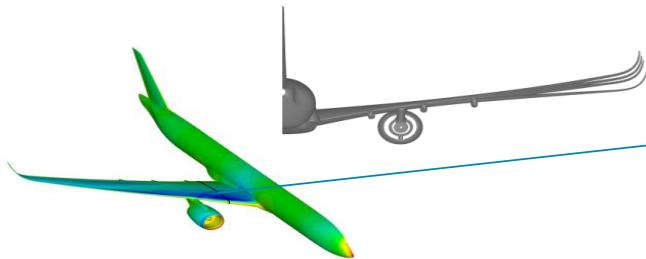


- Engineering simulations

Deformation from CSM



A350-1000 Flight test analysis



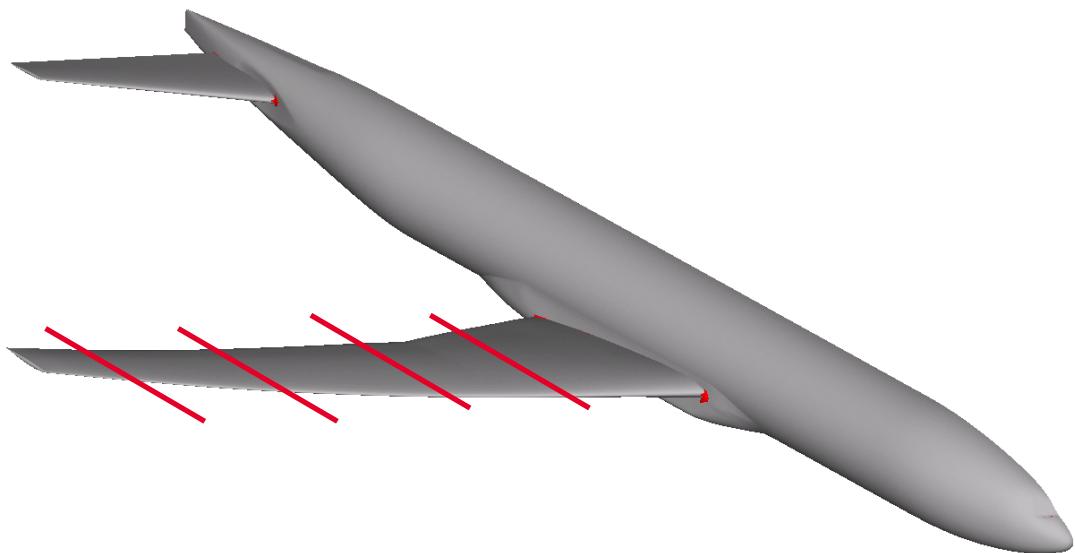
Engineering simulations



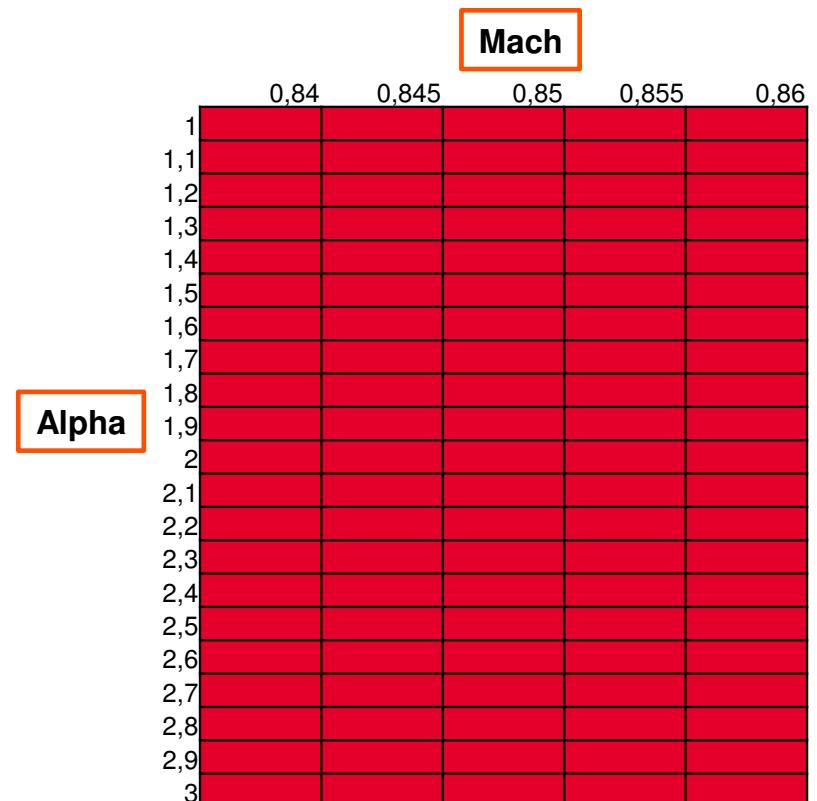
Flight Test Instrumentation

- Verify assumptions
- Extensions
- Computational bottleneck

Experimental dataset – CRM wing



<https://commonresearchmodel.larc.nasa.gov/>

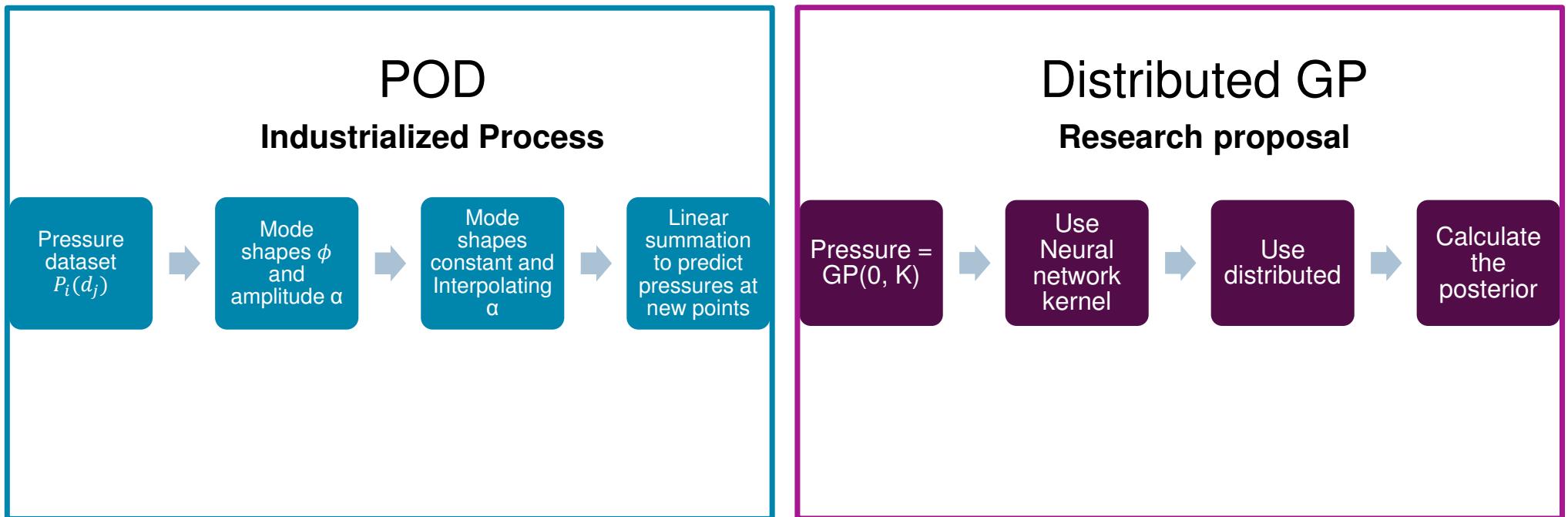


>50k data-points

References

- [L Cambier et al. AIAA 2008] → Elsa
- [John C Vassberg, et al. Journal of Aircraft, 2014] → CRM

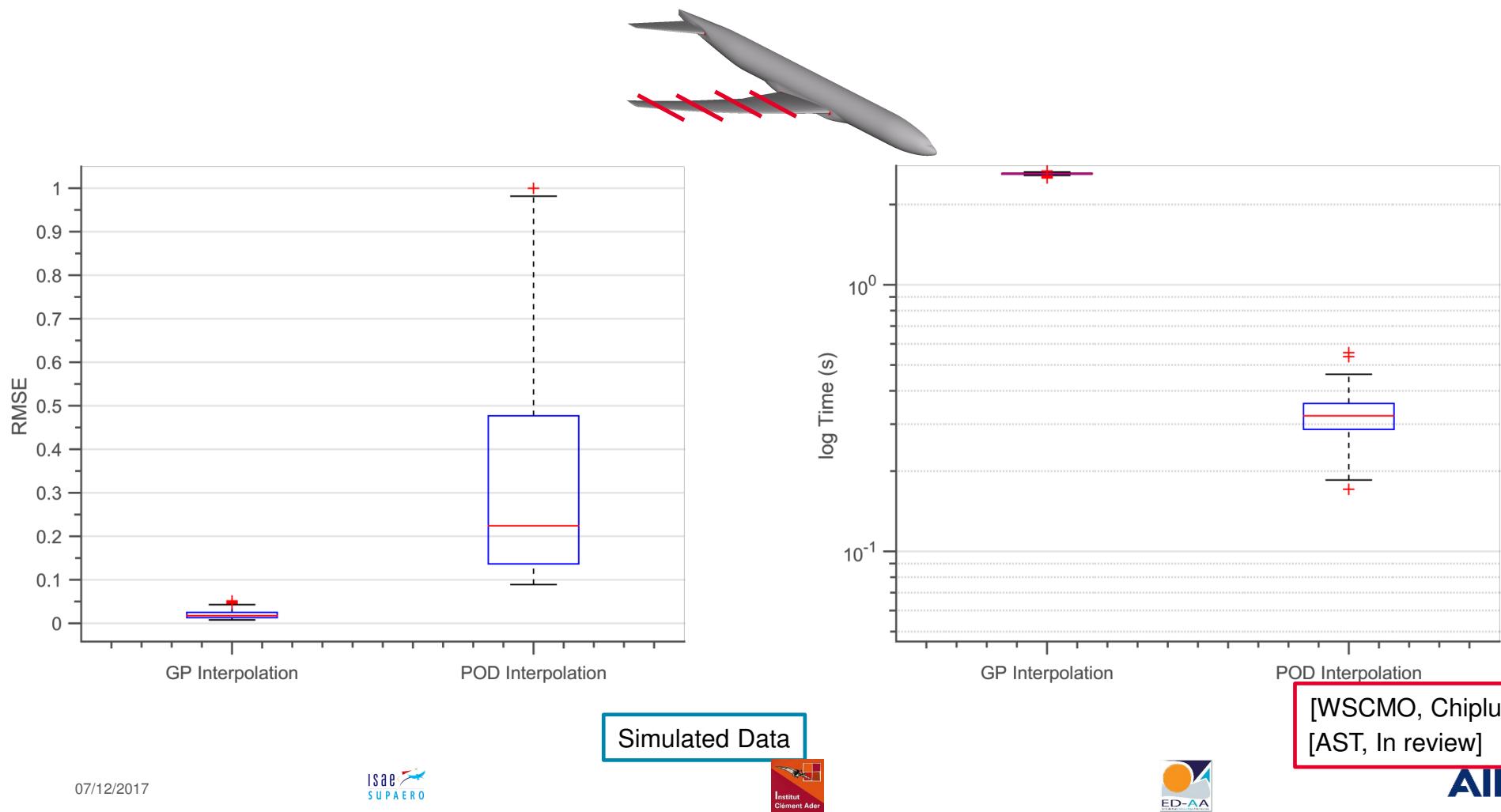
Different models



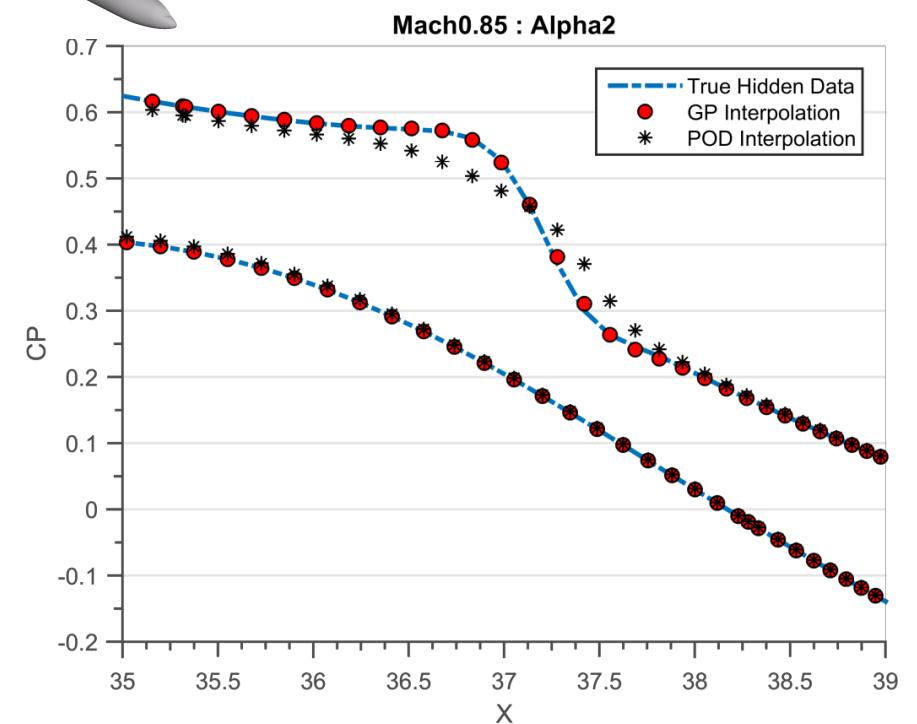
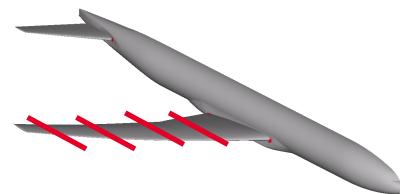
References:

- [Benjamin Rosenbaum et al SIAM 2013] → POD
- [Radford M Neal. Thesis, 2012] → Neural network kernel

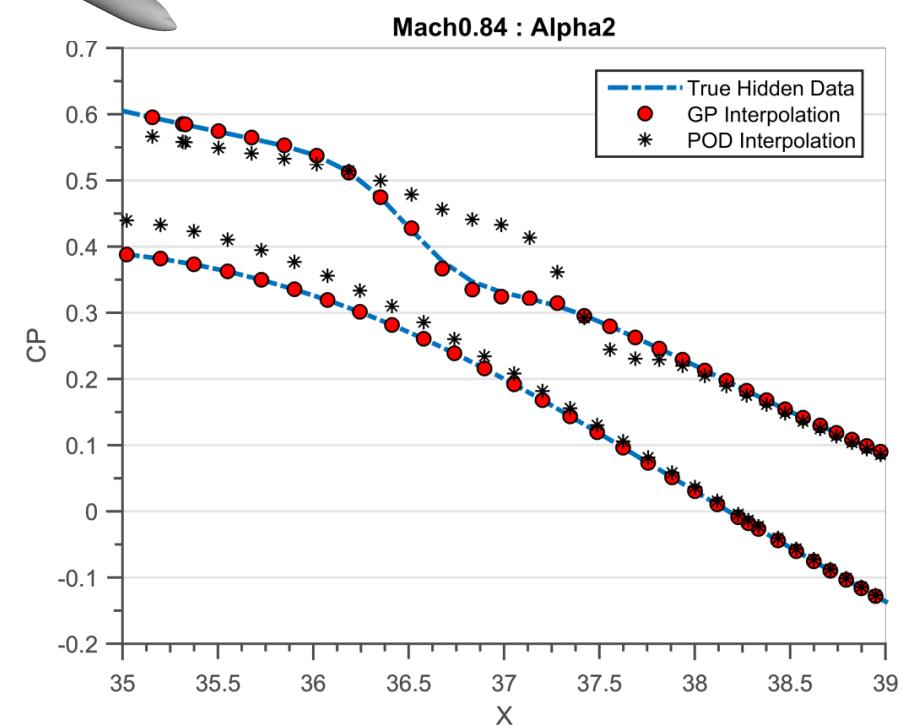
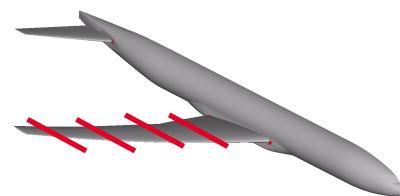
Comparison of results: Cut1 ($y/B = 0,105$)



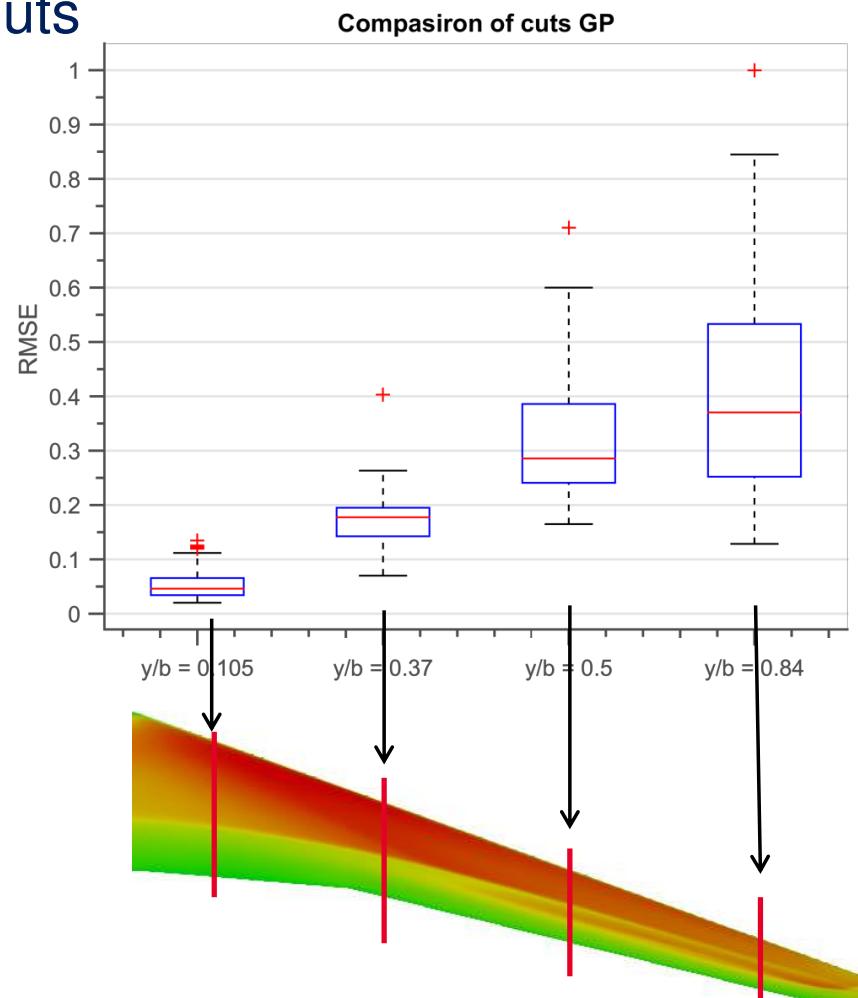
Comparison of results: Cut1 ($y/B = 0,105$)



Comparison of results: Cut1 ($y/B = 0,105$)

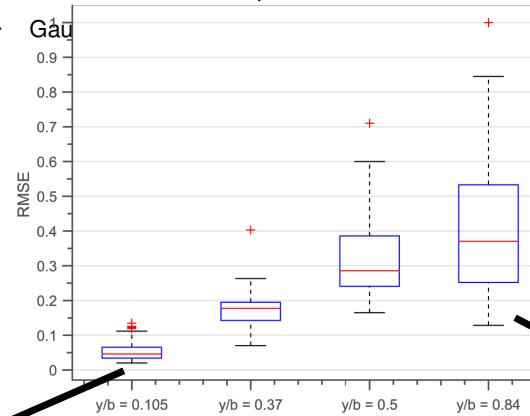


Comparison across Cuts



Motivation and Objectives →

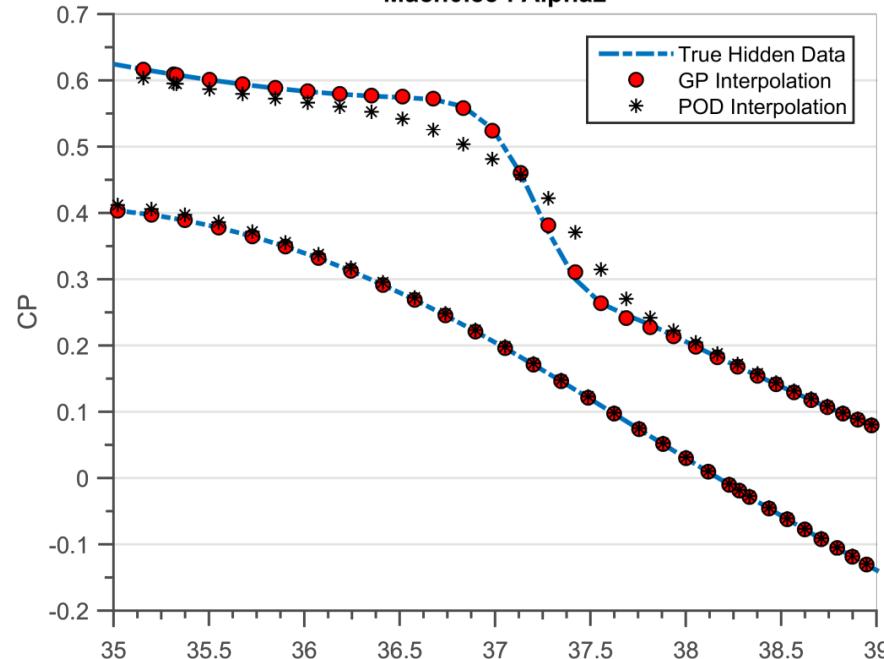
Comparison of cuts GP



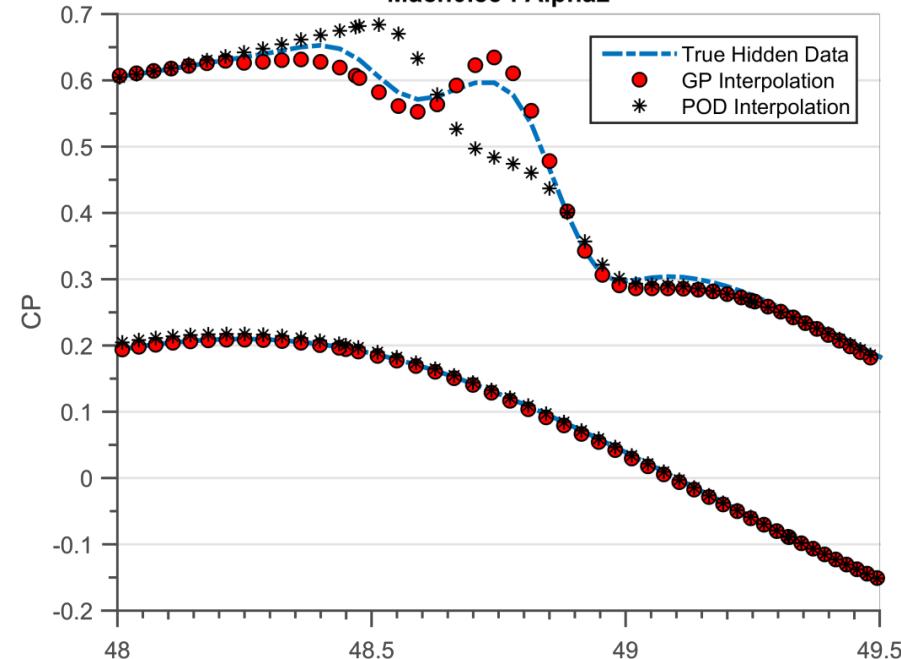
ation of multiple outputs → Adding information of shape → Conclusion

Comparison across Cuts

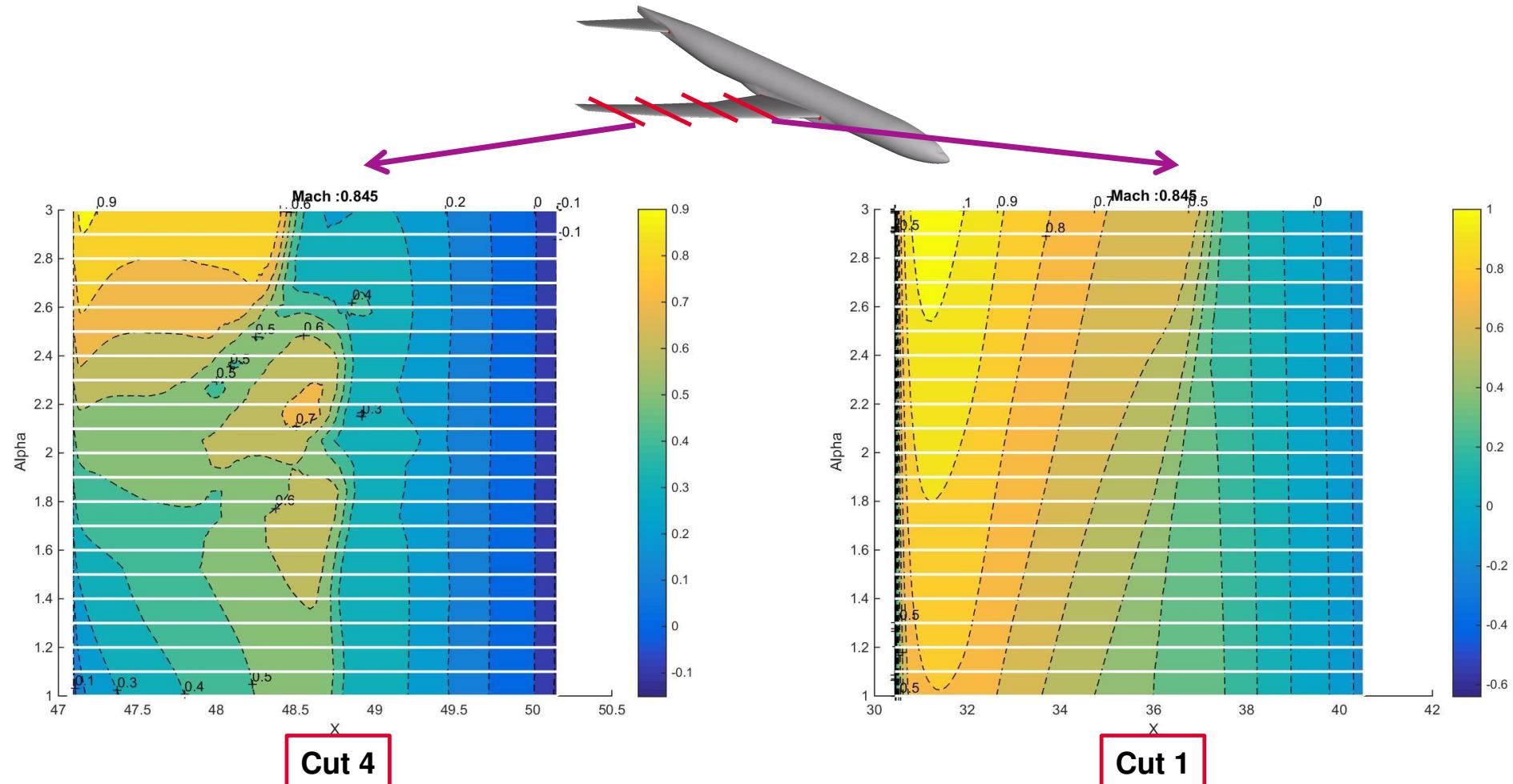
Mach0.85 : Alpha2



Mach0.85 : Alpha2



Comparison across Cuts



Conclusions and Future work

Contributions

	Additions to GP regression
Scaling multi-task GP	ICPRAM 2016 Sparse Physics-Based Gaussian Process for Multiple outputs LNCS 2017 Approximate inference in related multi-output Gaussian Process Regression
	GP + aircraft design
Identifying onset of non-linearity	SIAM 2016 - Identification of Physical Parameters Using Change-Point Kernels
Interpolating Shock position	WCSMO 2017 - Gaussian Process for Aerodynamic Pressures Prediction in Fast Fluid Structure Interaction Simulations AST Journal - In review
Identifying Structural dynamic parameters	IMAC 2017 Operational Modal Analysis in Frequency Domain using Gaussian Mixture Models
Adding relationships to GP	AIAA 2016 Adding Flight Mechanics to Flight Loads Surrogate Model

Conclusions

- Manipulate covariance function → Incorporate prior information
- Several applications were proposed
 1. Change point kernel
 2. Operational Modal analysis
 3. Shock detection using adapted kernels
 4. Merging experimental and simulation data
 5. Incorporate functional relationships
- Scalability solutions

Future works

- Real time comparison between simulation and experiment
- Uncertainty quantification
- Adding shape information
- Adding relationships
 - Filtering
 - Identify faulty sensors
 - MDO optimization
- Adding simulation data
 - Model updating
 - Extrapolation

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19. E Bosco, A Chiplunkar, J Morlier, Estimation of Modal Parameters Confidence Intervals: A Simple Numerical Example, 2013
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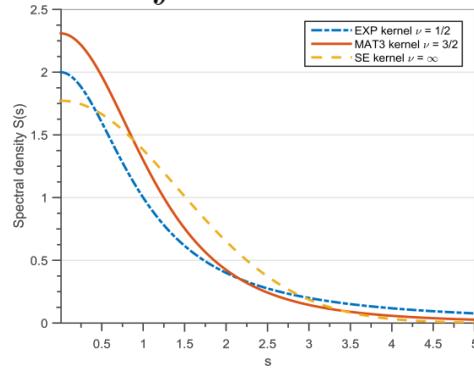
Thank you

Questions?

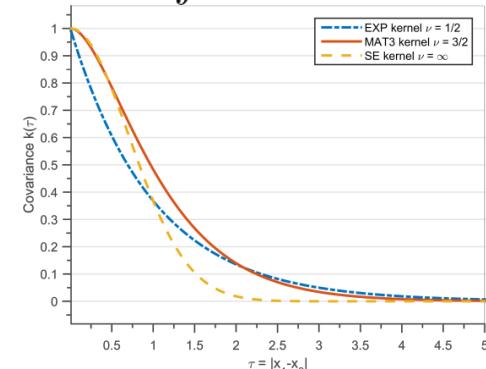
Bochners' theorem

Fourier transform of a stationary covariance function exists and is a positive finite measure

$$S(s) = \int k(\tau) e^{-2\pi i s^T \tau} d\tau$$



$$k(\tau) = \int S(s) e^{2\pi i s^T \tau} ds$$



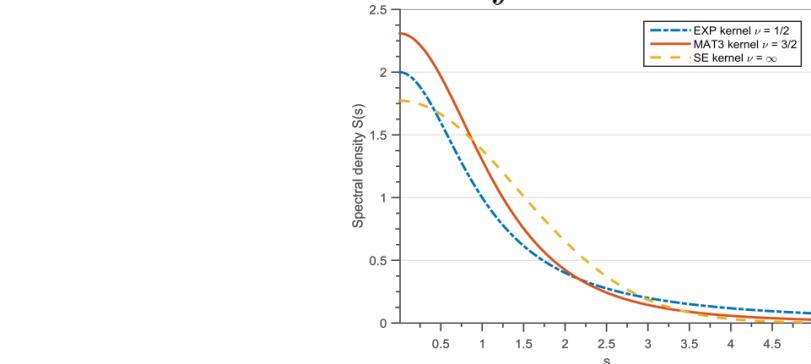
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S. Bochner, M. Tenenbaum et H. Pollard. Lectures on fourier integrals. Annals of mathematics studies. Princeton University Press, 1959

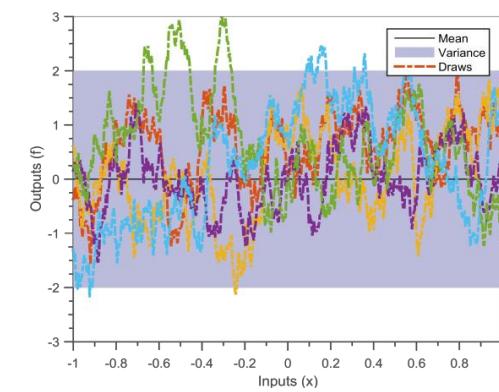
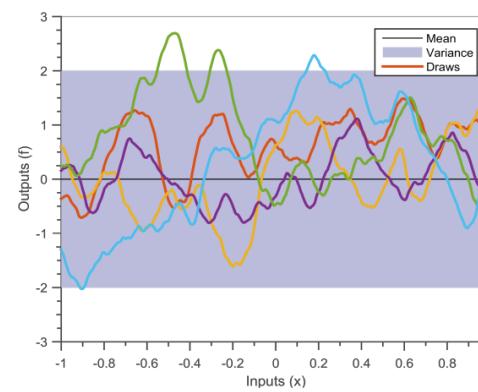
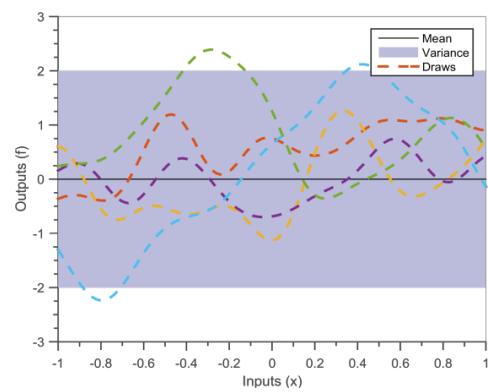
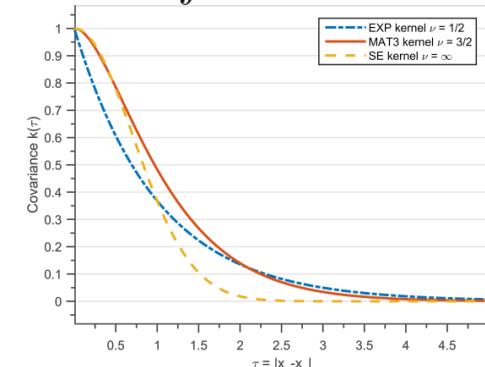
Bochners' theorem

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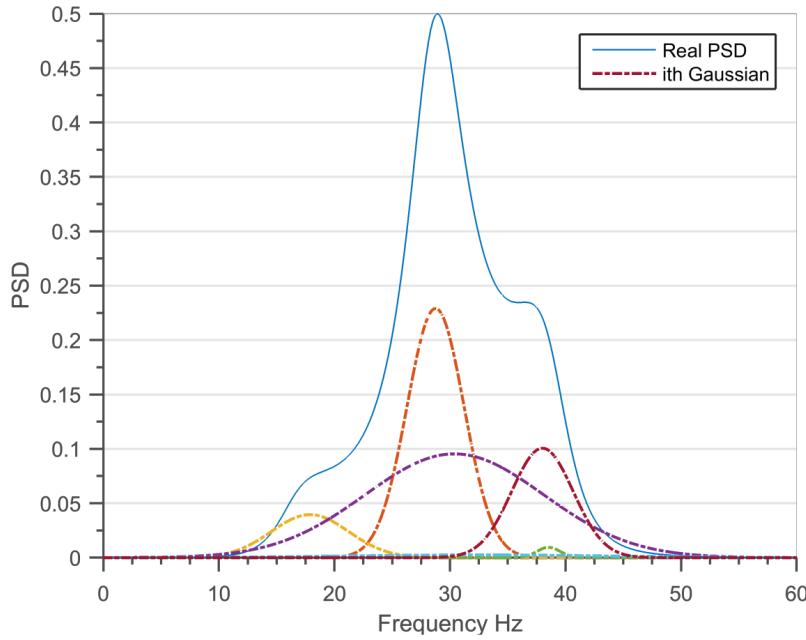
$$S(s) = \int k(\tau) e^{-2\pi i s^T \tau} d\tau$$



$$k(\tau) = \int S(s) e^{2\pi i s^T \tau} ds$$



Spectral mixture kernel



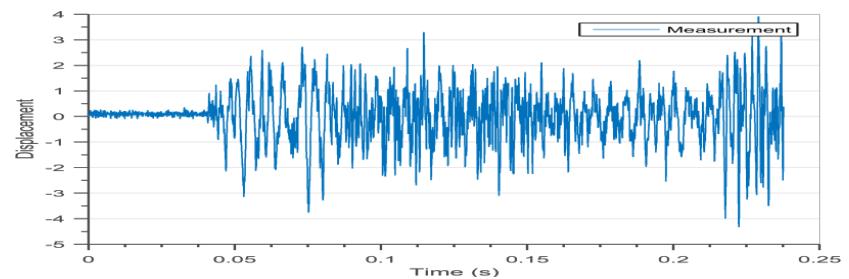
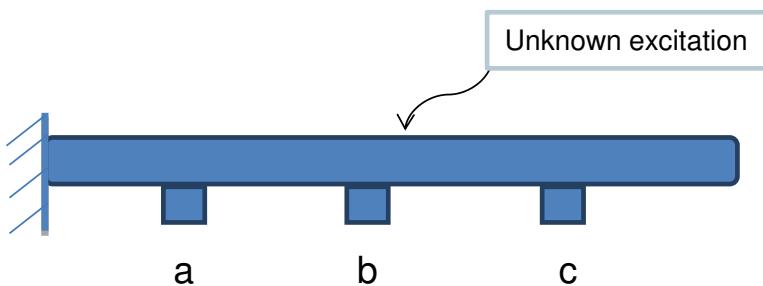
$$S_{SM}(s, \mu, \sigma, w) = \sum_{q=1}^Q \frac{w_q}{\sqrt{2\pi\sigma_q^2}} \left(\exp \left[-\frac{(s - \mu_q)^2}{2\sigma_q^2} \right] + \exp \left[-\frac{(-s - \mu_q)^2}{2\sigma_q^2} \right] \right)$$

$$k_{SM}(d, \mu, \sigma, w) = \sum_{q=1}^Q w_q \cos(2\pi\mu_q) \exp[-2\pi^2 d^2 \sigma_q^2]$$

References:

Wilson, A. G. and Adams, R. P., Gaussian Process Kernels for Pattern Discovery and Extrapolation Supplementary Material

Application - Operational Modal analysis



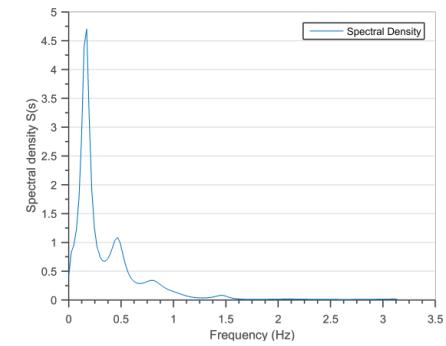
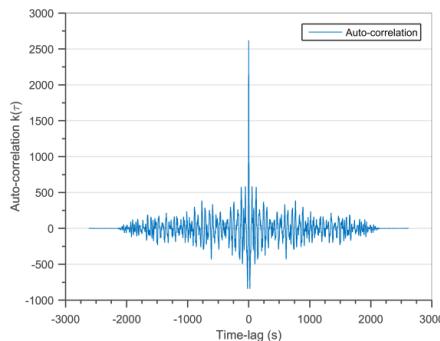
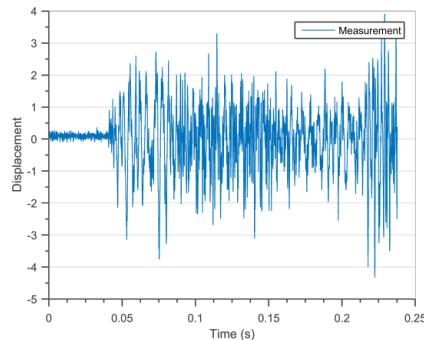
1. Sample is subjected to unknown random excitations
2. Can be used to perform damage-detection or structural health monitoring
3. Peaks in the power spectral density give us the modes of the structure

[IMAC, Chiplunkar 2017b]

References:

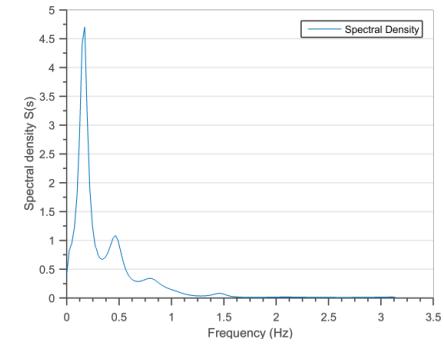
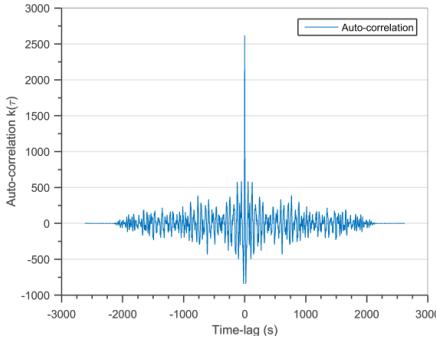
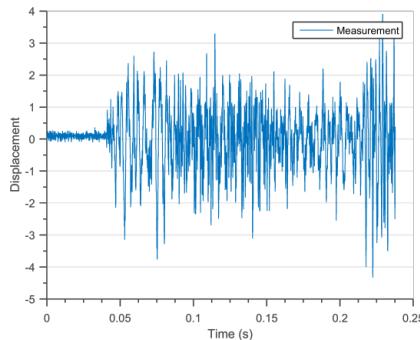
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Operational Modal analysis



Displacement	Autocorrelation	Power spectral density
$x(t)$	$k(\tau) = \int x(t)x(t - \tau)dt$	$S(s) = \text{fourier}(k(\tau))$

Operational Modal analysis

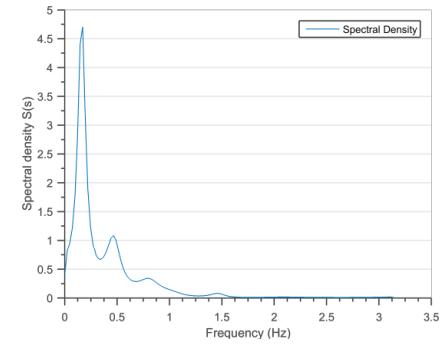
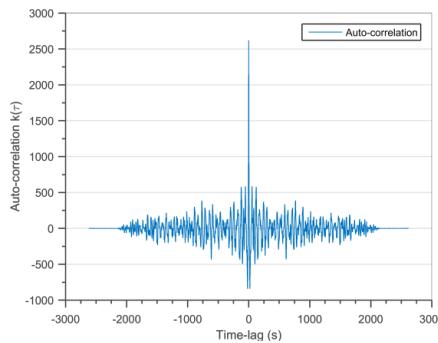
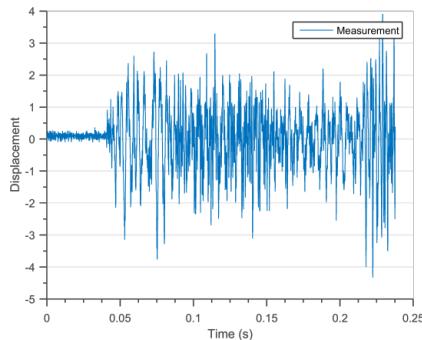


Displacement	Autocorrelation	Power spectral density
	$k(\tau) = \int x(t)x(t - \tau)dt$	$S(s) = \text{fourier}(k(\tau))$
$M\{\ddot{x}(t)\} + C\{\dot{x}(t)\} + K\{x(t)\} = \{f(t)\}$		
	$k(\tau) = \sum A_i \exp(-\lambda_i \tau) \sin(B_i \tau)$	$S(s) = \frac{\sum a_k(s)^k}{\sum b_l(s)^l}$

References:

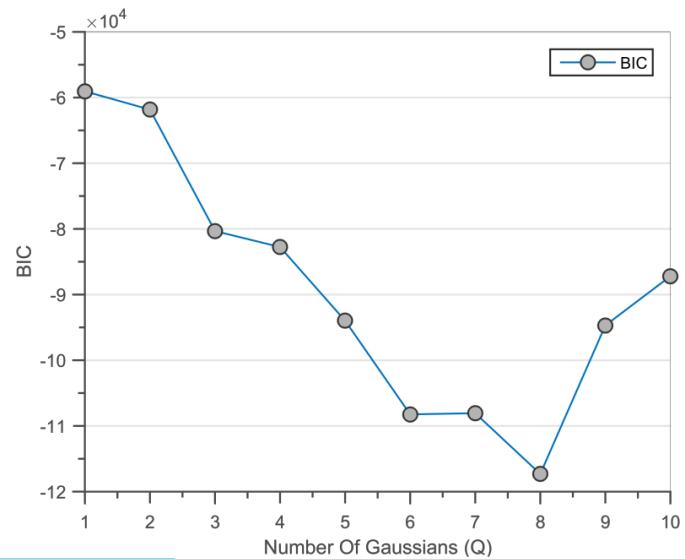
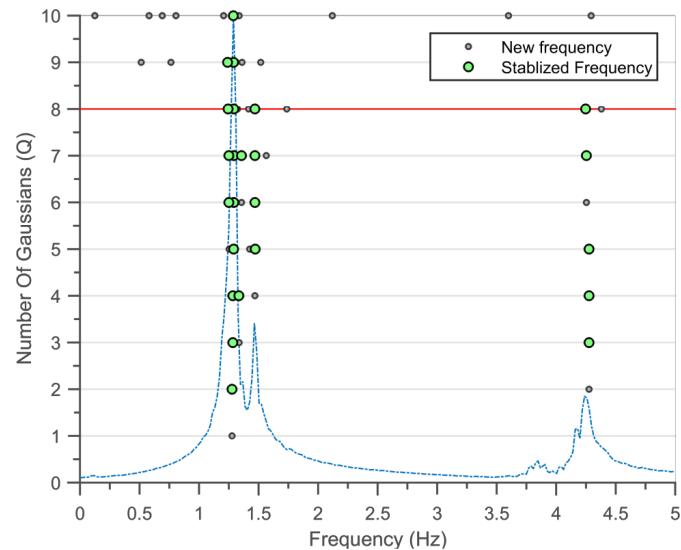
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 Randall J Allemang et DL Brown. A unified matrix polynomial approach to modal identification. Journal of Sound and Vibration, 1998

Operational Modal analysis



Displacement	Autocorrelation	Power spectral density
$x(t)$	$k(\tau) = \int x(t)x(t - \tau)dt$	$S(s) = \text{fourier}(k(\tau))$
$M\{\ddot{x}(t)\} + C\{\dot{x}(t)\} + K\{x(t)\} = \{f(t)\}$		
	$k(\tau) = \sum A_i \exp(-\lambda_i \tau) \sin(B_i \tau)$	$S(s) = \frac{\sum a_k(s)^k}{\sum b_l(s)^l}$
Spectral Mixture Covariance		
$x(t) = GP(0, cov_{SM}(t, t'))$	$k_{SM}(d, \mu, \sigma, w) = \sum_{q=1}^Q w_q \cos(2\pi\mu_q) \exp[-2\pi^2 d^2 \sigma_q^2]$	$S_{SM}(s, \mu, \sigma, w) = \sum_{q=1}^Q \frac{w_q}{\sqrt{2\pi\sigma_q^2}} \left(\exp\left[-\frac{(s - \mu_q)^2}{2\sigma_q^2}\right] + \exp\left[-\frac{(-s - \mu_q)^2}{2\sigma_q^2}\right] \right)$

Results on HCT dataset

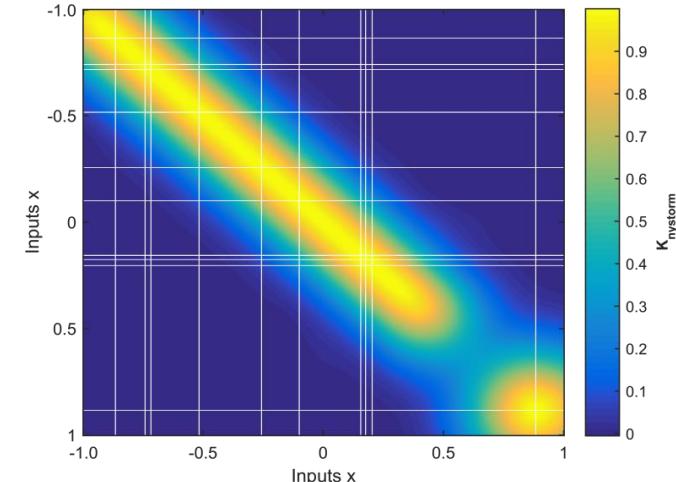
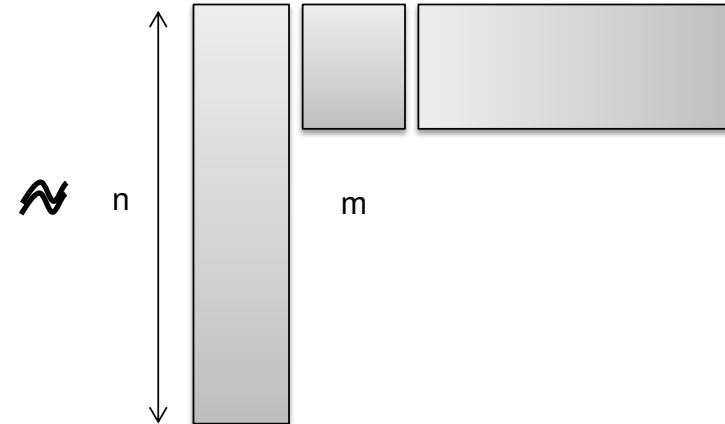
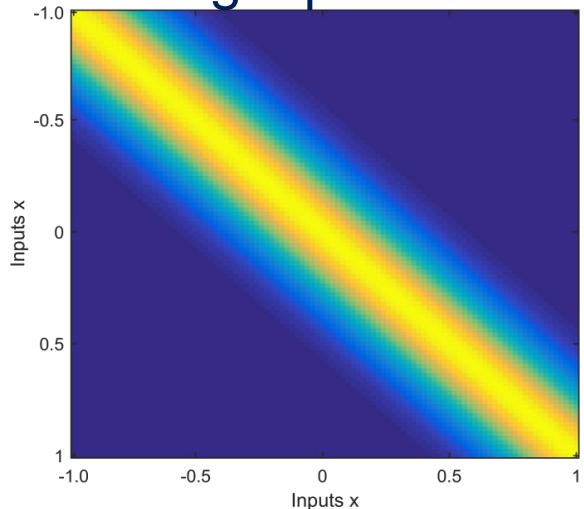


	From paper	FRF
Freq1	1,23	1,242
Freq2	1,27	1,292
Freq3	1,43	1,470
Freq4	3,86	3,866
Freq5	4,25	4,247

Experimental Data (HCT dataset)

Scaling solutions to a GP

Inducing inputs



$$\mathbf{m}(\mathbf{x}_*) = \mathbf{K}_{*\text{approximate}} [\mathbf{K}_{xx\text{approximate}}]^{-1} \mathbf{y}$$

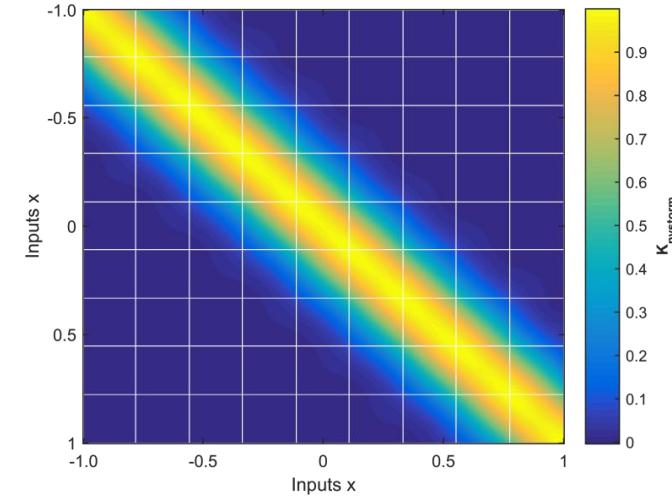
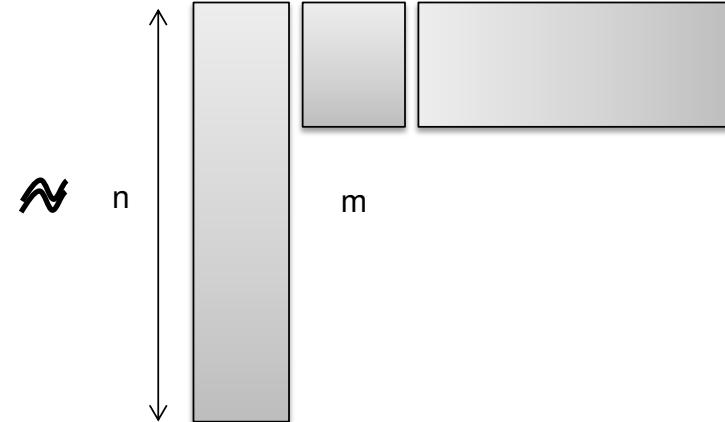
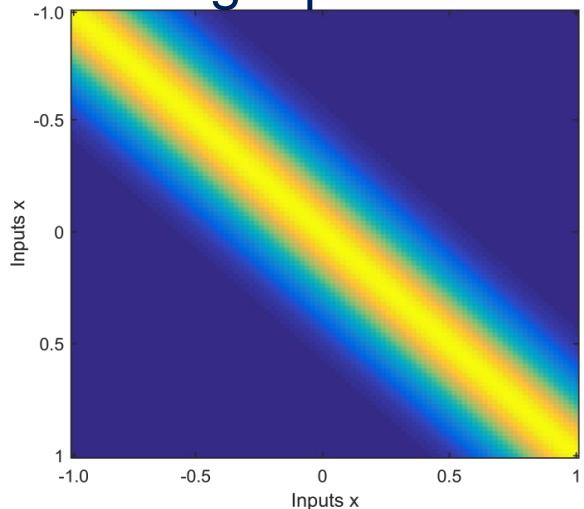
$$\text{var}(\mathbf{x}_*, \mathbf{x}'_*) = \mathbf{K}_{**\text{approximate}} - \mathbf{K}_{*\text{approximate}}^T [\mathbf{K}_{xx\text{approximate}}]^{-1} \mathbf{K}_{*\text{approximate}}$$

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

References:

- Michalis K. Titsias. Variational learning of inducing variables in sparse Gaussian processes. In In Artificial Intelligence and Statistics 2009
 Christopher KI Williams et Matthias Seeger. Using the Nyström method to speed up kernel machines. In Advances in neural information processing systems, 2001

Inducing inputs



$$\mathbf{m}(\mathbf{x}_*) = \mathbf{K}_{*\text{approximate}} [\mathbf{K}_{xx\text{approximate}}]^{-1} \mathbf{y}$$

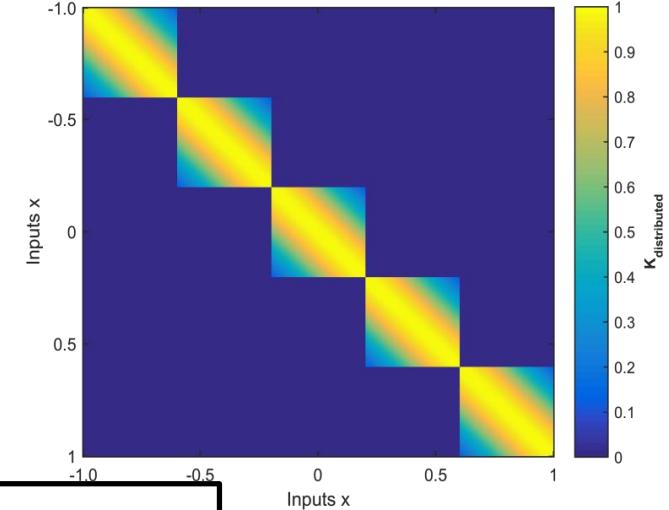
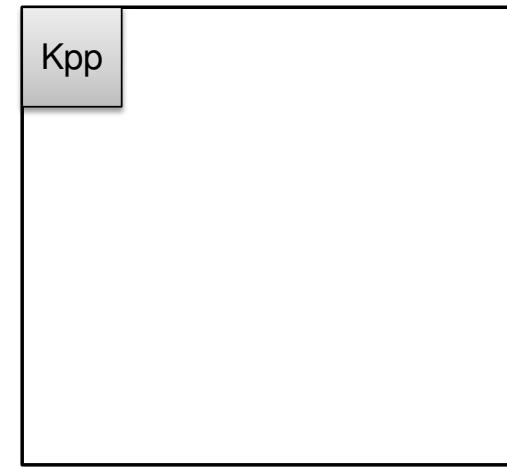
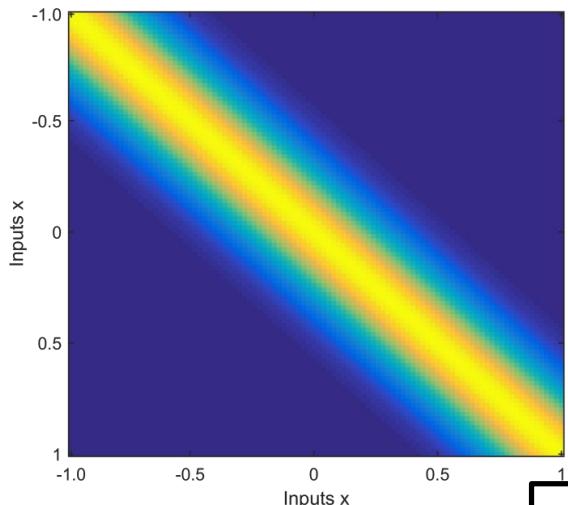
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Distributed Gaussian Process



$$m(y^*) = Kx_*x_*^{-2} \sum_k \beta_k \begin{pmatrix} Cov_k(y^*) \\ m_k(y^*) \end{pmatrix}^2$$

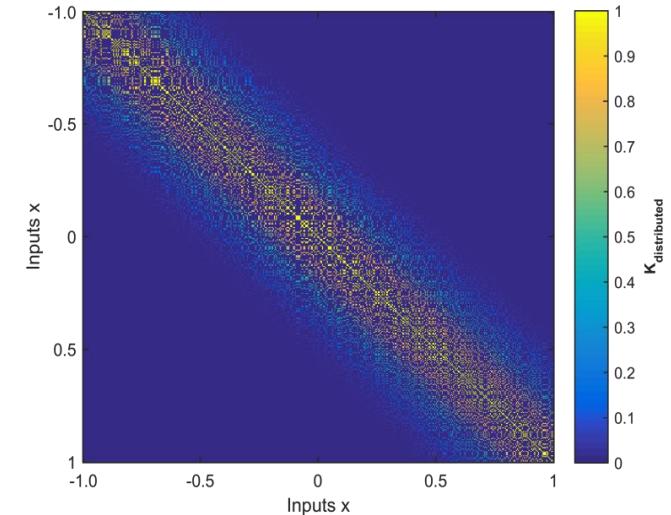
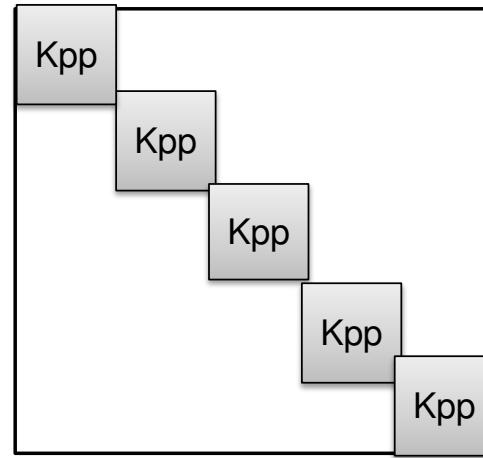
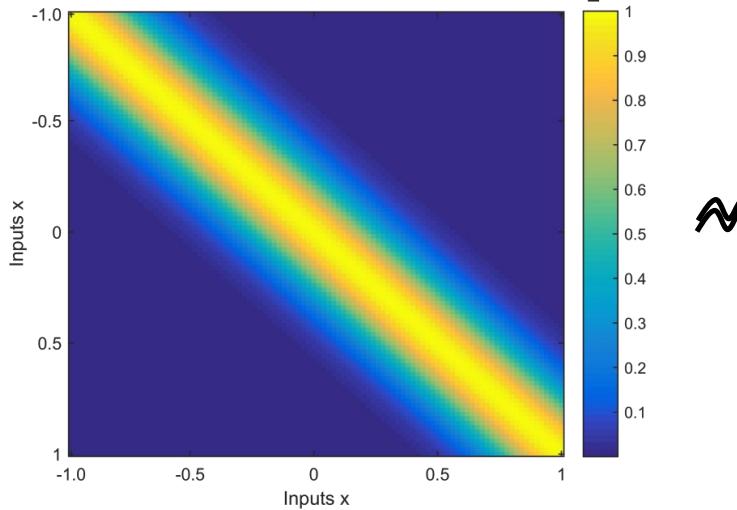
$$\beta_k = \log(K_{x_*x_*}^{-2}) - \log(Cov_k(y)^{-2})$$

References:

Tao Chen et Jianghong Ren. Bagging for Gaussian process regression. Neurocomputing, 2009.

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Distributed Gaussian Process



$$m(y^*) = Kx_*x_*^{-2} \sum_k \beta_k \text{Cov}_k(y^*) \text{E}^k(y^*)$$

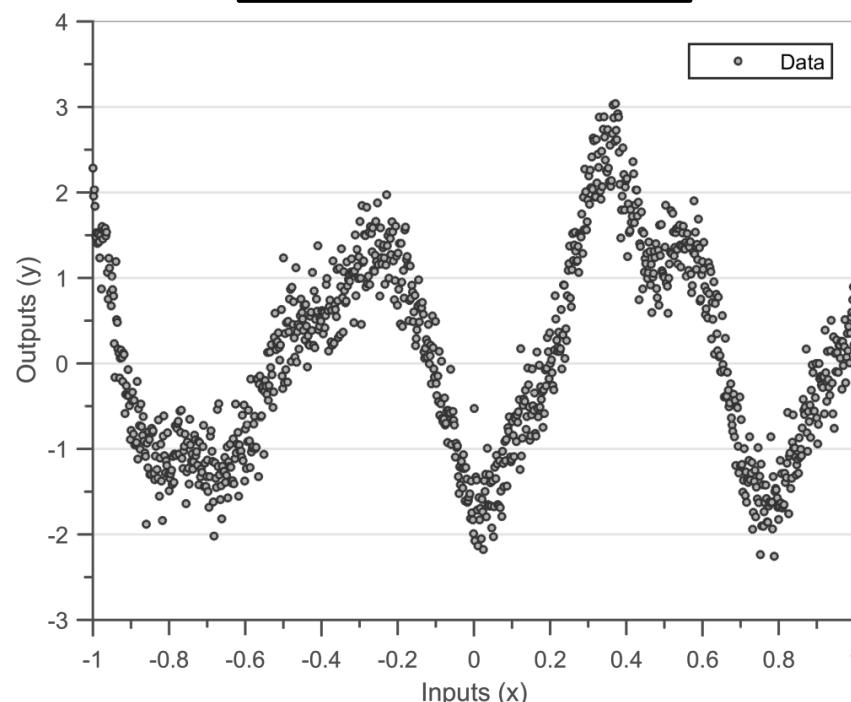
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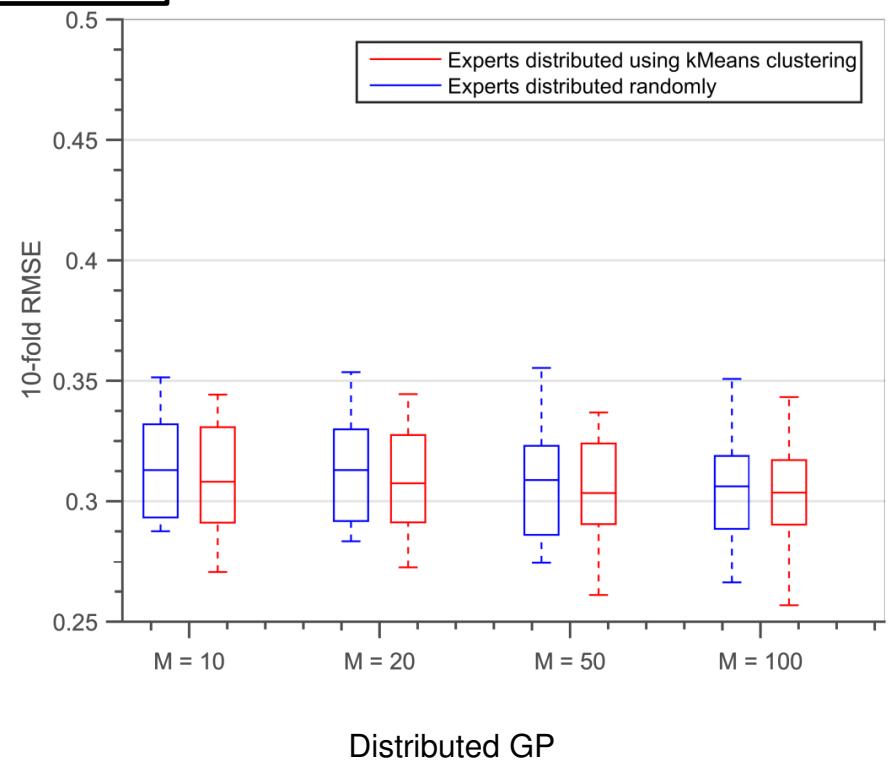
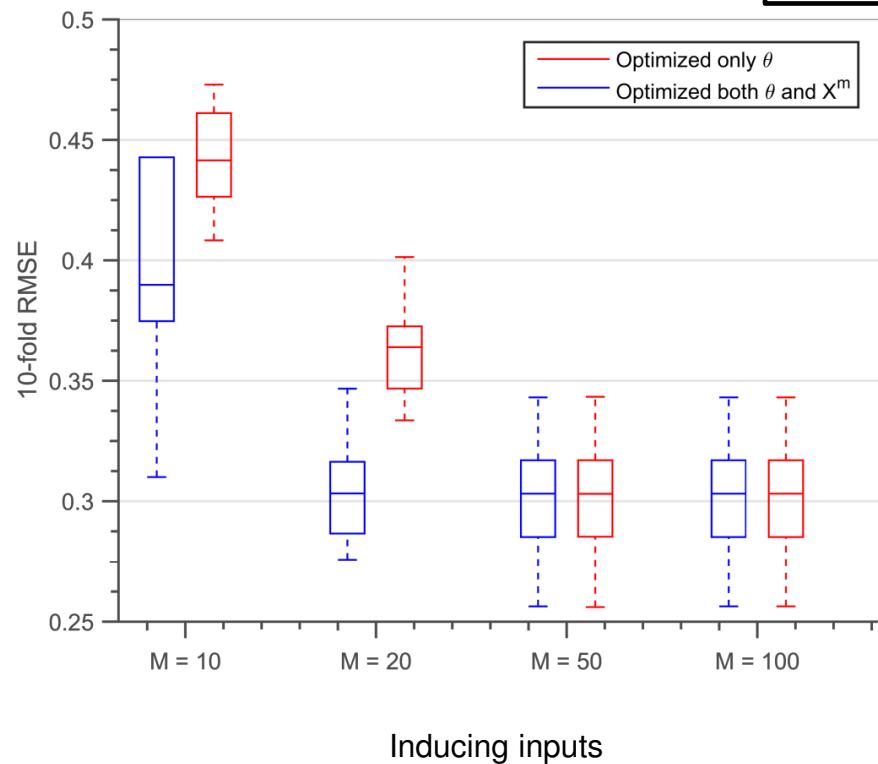
Comparison between two approximation methods

- $f(x) = \text{GP}(0, K_{\text{se}}(1, 0.1))$
- $y(x) = f(x) + (0.3)^*\text{rand}$
- $N = 1000$
- 10 fold Cross-validation



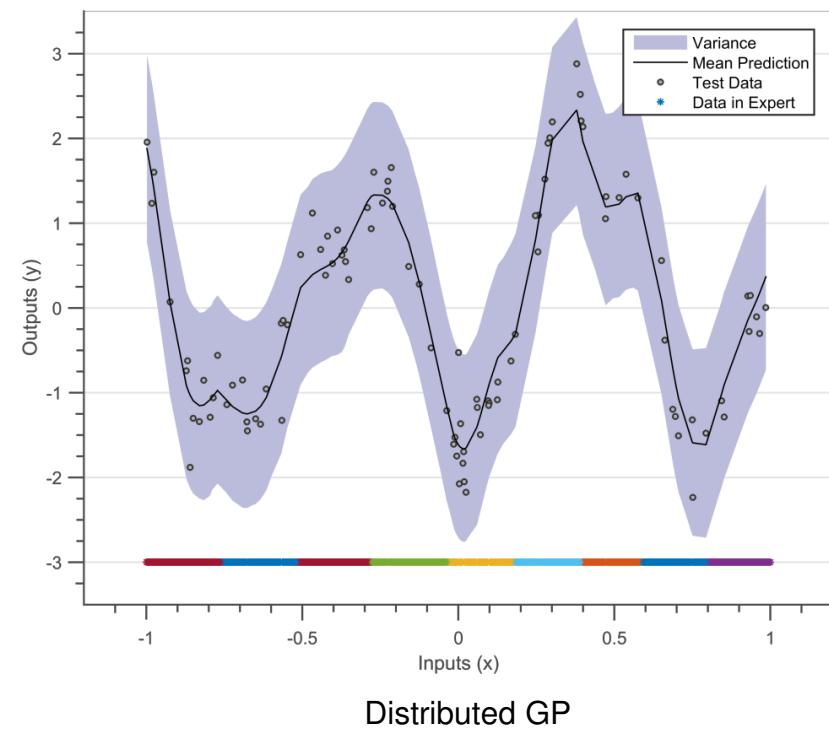
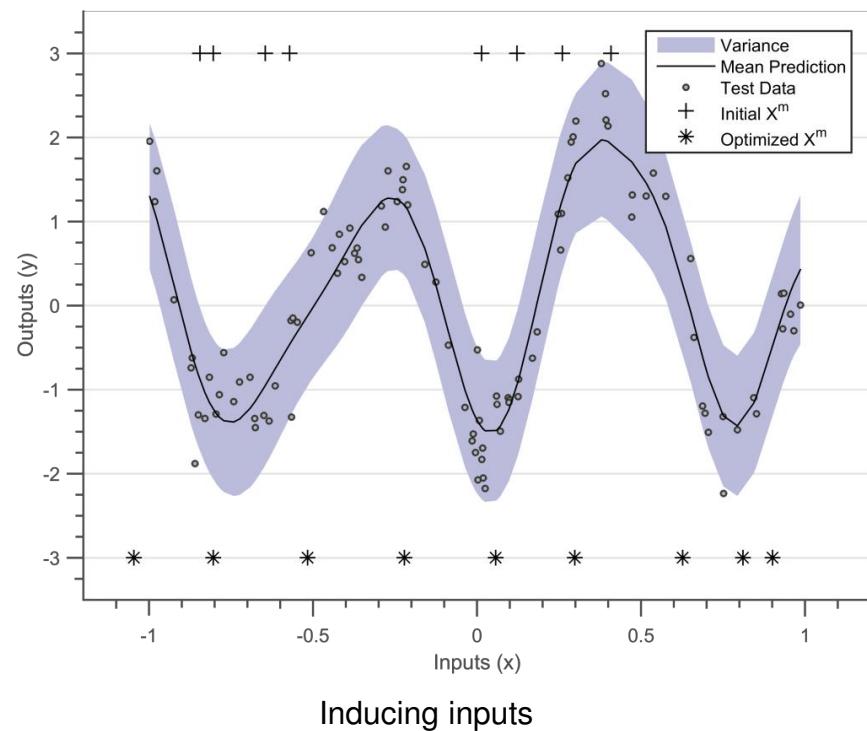
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- $y(x) = f(x) + (0.3)^*\text{rand}$
- $N = 1000$
- 10 fold Cross-validation



Multi-Output Gaussian Process /Non-Linear

Case 3: When the outputs are related by a known relation/function

Given: $f_1 = g(f_2, x)$

If g is **non-linear**

$$p\left(\begin{matrix} f_1 \\ f_2 \end{matrix} \middle| M\right) = GP\left(\begin{matrix} 0 & g(g(K_{22}, x_2), x_1) & g(K_{22}, x_2) \\ 0 & g(K_{22}, x_1) & K_{22} \end{matrix}\right)$$

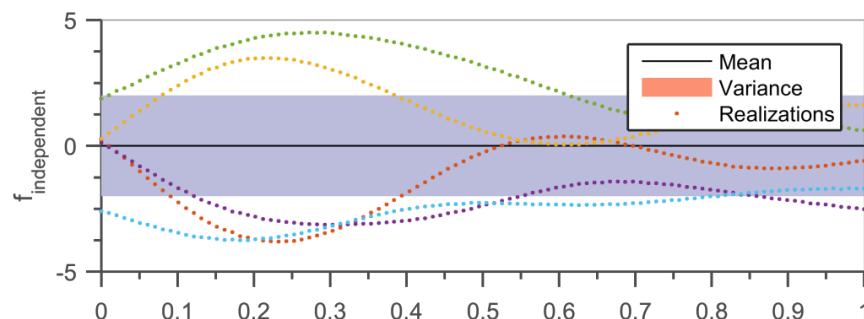
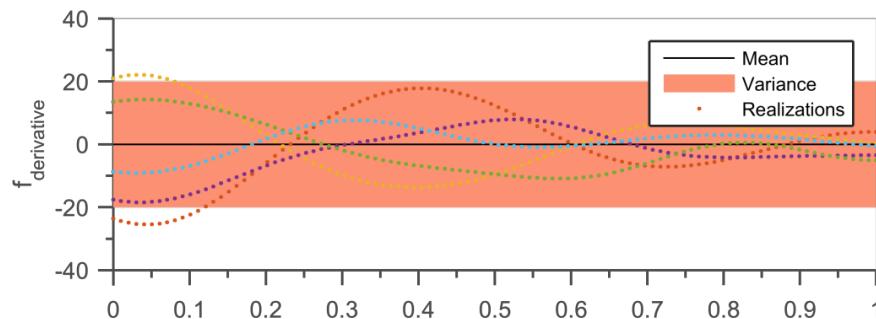
Is not a gaussian

$$p\left(\begin{matrix} f_1 \\ f_2 \end{matrix} \middle| M\right) = GP\left(\begin{matrix} 0 & LK_{22}L^T & LK_{22} \\ 0 & K_{22}L^T & K_{22} \end{matrix}\right) \{L = \frac{\partial g}{\partial y_2}\}$$

First order taylor series expansion

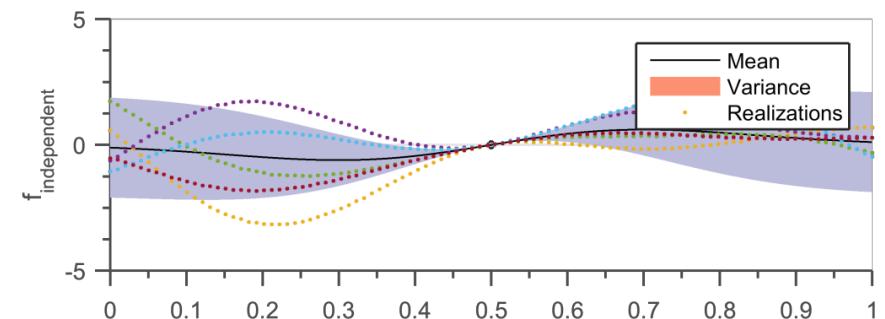
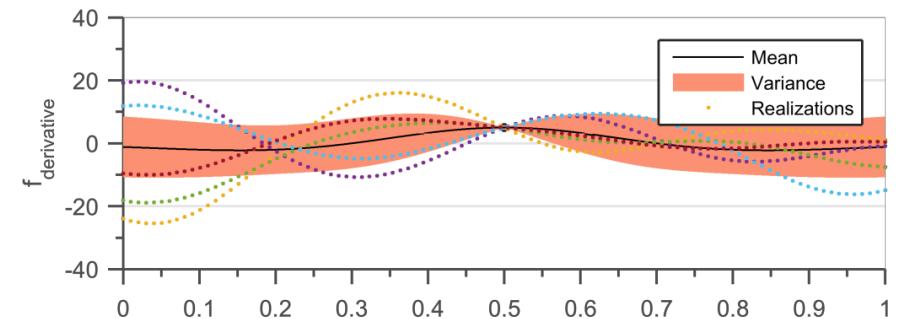
Differential relation

$$f_{derivative} = \frac{df_{independent}}{dx}$$

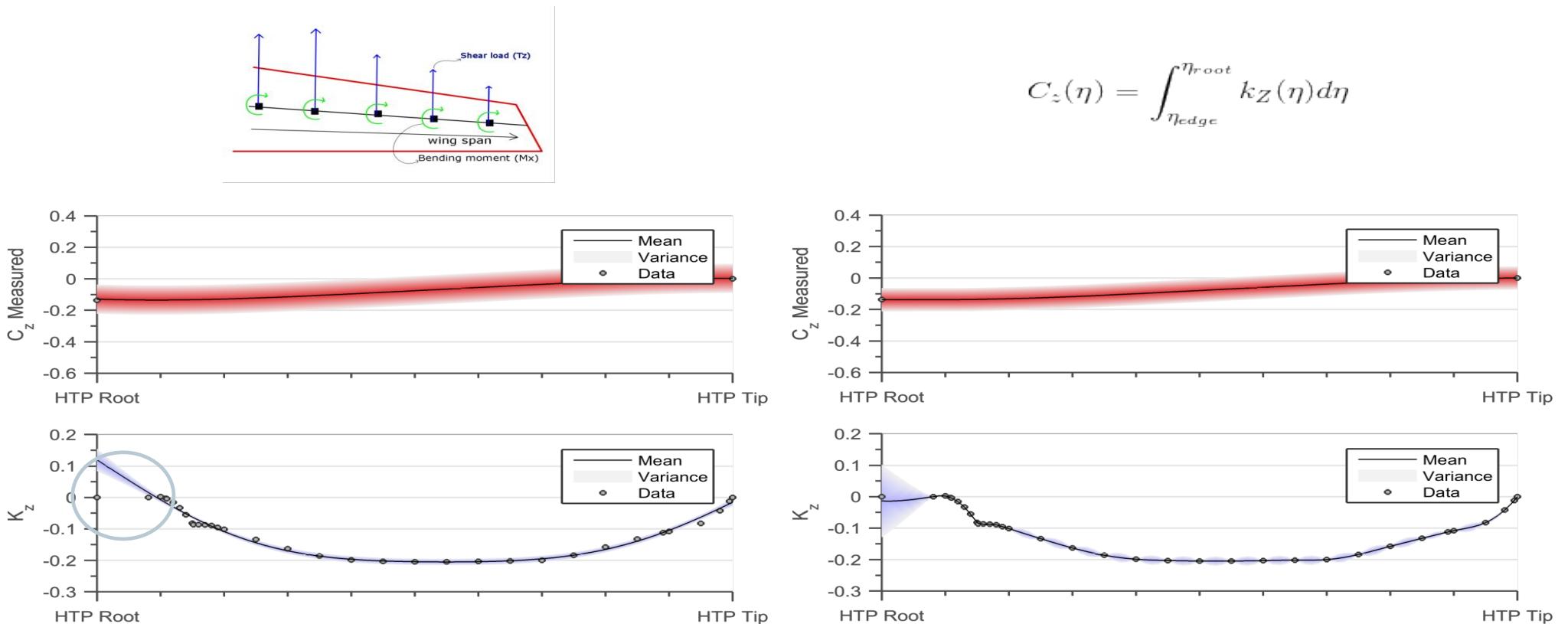


$$f_{derivative} \Big|_{x=0} = 5$$

$$f_{independent} \Big|_{x=0} = 0$$



Flight test - Relationship between C_z and K_z



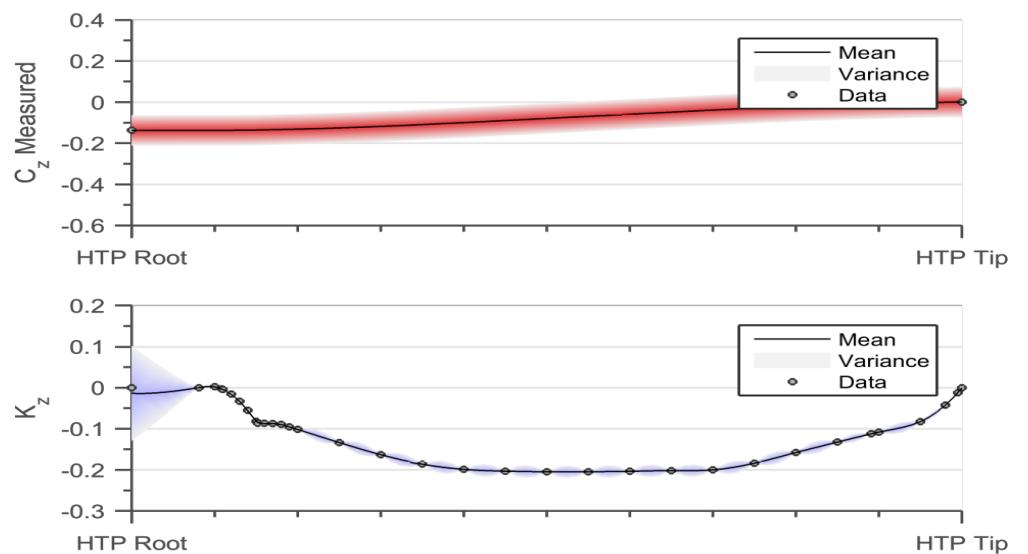
$$k_{SE}(x, x', \theta) = \theta_1^2 \exp\left[-\frac{d^2}{2\theta_2^2}\right]$$



66

07/12/2017

$$C_z(\eta) = \int_{\eta_{edge}}^{\eta_{root}} k_Z(\eta) d\eta$$



$$k_{Mat2}(x, x', \theta) = \theta_1^2 \left(1 + \frac{\sqrt{5}d}{\theta_2} + \frac{5d^2}{3\theta_2^2} \right) \exp\left[-\frac{\sqrt{5}d}{\theta_2}\right]$$



AIRBUS

Kriging vs Gaussian Process

Topics	Kriging	Gaussian Process
Original Formulation	[Matheron, G., 1967] [Petrie, Gregg M., et al. 2002]	
New formulation	[Kennedy, Marc C., et al 2001]	[Rasmussen et al 2006]
Multi-fidelity Optimization	[Kennedy, et al 2000] [Jones, Donald R. 2001]	[Mockus, Jonas. 2012] [Maatouk, Hassan, et al 2017]
Constrained Optimization	[Sasena, 2002]	
GEK	[Liu, Weiyu. 2003]	[Solak, Ercan, et al. 2003]
Dimensionality Reduction	[Bouhlel, M., et al. 2016]	[Tripathy, Rohit et al 2016]
Parallel approximations		[Deisenroth, et al 2015]. [Duvenaud 2014]; [Wilson 2011]
Automatic kernel		