GAUSSIAN PROCESS REGRESSION FOR EFFICIENT DETECTION OF FABRICATION INACCURACIES IN MICROSENSORS

POLITECNICO
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PHD COURSE: ADVANCED STATISTICAL METHODS FOR COMPLEX DATA

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OUTLINE

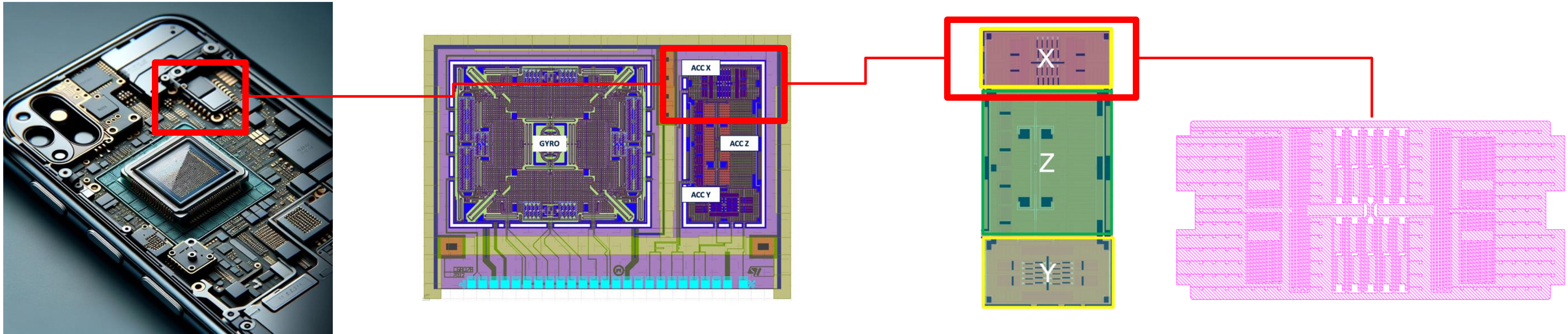
- Context and Motivation
- Gaussian Process Regression
- A Comparison with Kriging
- GPR for Online Learning
- Numerical Results

Objective

Calibration of MEMS accelerometers:

- Fabrication may lead geometrical layout to differ up to 10% w.r.t. the intended one.
- The sensitivity of the device w.r.t. external accelerations is highly impacted by fabrication inaccuracies.
- Sensitivity is generally estimated using labor intensive mechanical tests.

Calibration of MEMS accelerometer <u>using cheap electronic tests</u>



GENERAL FRAMEWORK - METROPOLIS HASTINGS

- Measurements are stored in $\mathrm{y}^{\mathrm{exp}} \in R^d$.
- Uncertain parameters are stored in $\mathrm{x} \in R^p$
- The two are connected by a **forward model** f_{HF}:

$$\mathrm{y}^{\mathrm{exp}} = f_{HF}(x) + \varepsilon, \qquad \varepsilon \sim N(0, \Sigma)$$

- Goal: infer the **posterior distribution** of x:

$$\pi(\, x \mid \mathrm{y}^{\mathrm{exp}}\,) = \frac{\pi(\, \mathrm{y}^{\mathrm{exp}} \mid x\,)\pi(x)}{\pi(\mathrm{y}^{\mathrm{exp}})}$$

- Standard approach: Metropolis-Hastings

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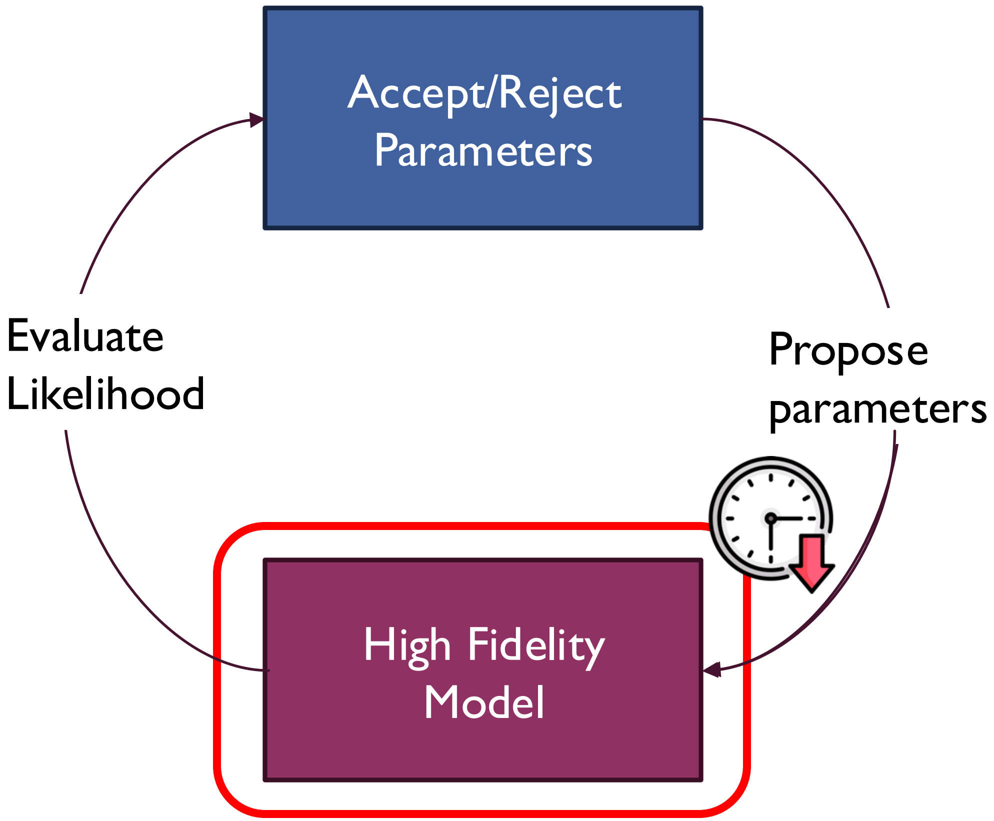


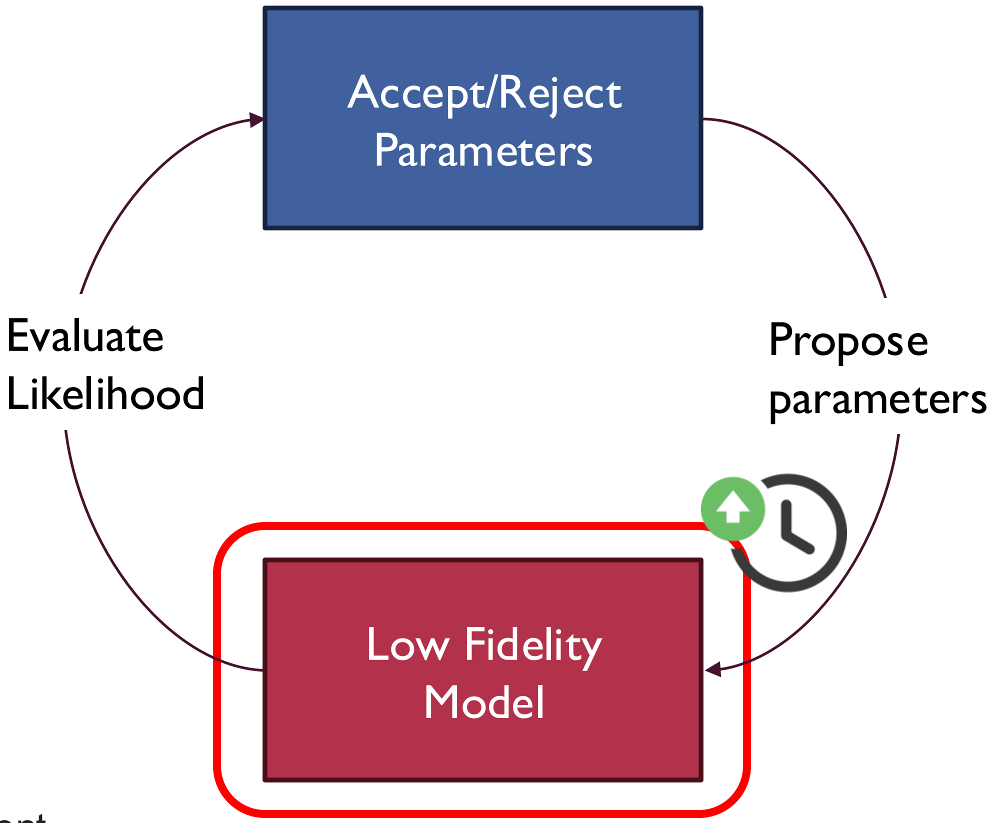
Benjamin Peherstorfer, Karen Willcox, and Max Gunzburger. Survey of multifidelity methods in uncertainty propagation, inference, and optimization. Siam Review,60(3):550–591, 2018.

GENERAL FRAMEWORK - LOW FIDELITY

- Replace the forward model with a low fidelity approximation f_{LF}:

$$y^{\exp} \approx f_{LF}(x) + \varepsilon, \qquad \varepsilon \sim N(0, \Sigma)$$

- Huge gains in sampling efficiency
- The surrogate determines the accuracy of the estimate



Zacchei, Filippo, et al. "Neural networks based surrogate modeling for efficient uncertainty quantification and calibration of MEMS accelerometers." *International Journal of Non-Linear Mechanics* 167 (2024): 104902.

SURROGATE MODELING

- Surrogate models replace computationally expensive forward models, enabling efficient Bayesian inference.
- This transforms the inverse problem into a **statistical learning task**, where the surrogate approximates the high-fidelity model behavior.

Gaussian Process Regression!

Key Considerations:

✅ **Error Quantification:**

- We must estimate surrogate errors **accurately**, as they propagate into the **posterior distribution** and may bias inference.

✅ **Data Efficiency:**

- Surrogates must be trained on **fewer samples** than needed for direct MCMC, making **data efficiency** essential.

GAUSSIAN PROCESS REGRESSION

A **Gaussian Process** is a distribution over functions:

$f(x) \sim GP(m(x), k(x, x'))$

- $m(x)$: mean function (often assumed zero)
- $k(x, x')$: covariance (kernel) function

🔍 Gaussian Process Regression

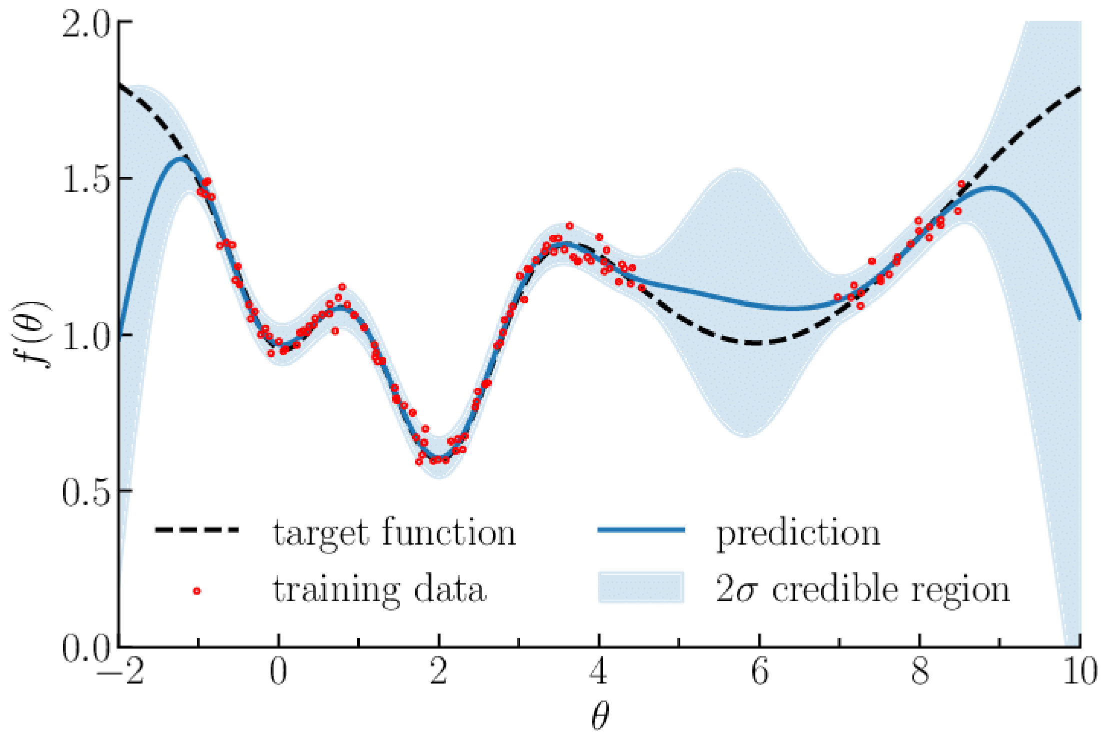
Given training data $D = \{X, y\}$ and observation noise σ_n^2, the GP posterior at a test point x^* is:

Mean prediction:

$\mu(x^*) = k^{*T} (K + \sigma_n^2 I)^{-1} y$

Predictive variance:

$*\sigma^2(x^*) = k(x^*, x^*) - k^{*T} (K + \sigma_n^2 I)^{-1} k^*$



Simple Kriging (SK): Mathematical Formulation

Consider a random field $Z(\mathbf{x})$, with known mean $m(\mathbf{x})$ and covariance function $k(\mathbf{x}, \mathbf{x}')$. We have observations:

$$Y(\mathbf{x}_i) = Z(\mathbf{x}_i) + \varepsilon_i, \quad i = 1, \ldots, n$$

The **Best Linear Unbiased Predictor (BLUP)** estimator is given by:

$$\hat{Z}(\mathbf{x}_*) = \sum_{i=1}^{n} \lambda_i Y(\mathbf{x}_i) + \lambda_0$$

Minimizing the variance of prediction error subject to unbiasedness constraint yields the SK solution:

$$\hat{\boldsymbol{\lambda}} = \Sigma^{-1}\mathbf{k}_*, \quad \hat{\lambda}_0 = m(\mathbf{x}_*) - \hat{\boldsymbol{\lambda}}^\top \mathbf{m}$$

where: - $\Sigma = [k(\mathbf{x}_i, \mathbf{x}_j)]_{i,j=1}^{n}$ - $\mathbf{k}_* = [k(\mathbf{x}_1, \mathbf{x}_*), \ldots, k(\mathbf{x}_n, \mathbf{x}_*)]^\top$
The prediction becomes explicitly:

$$\hat{Z}(\mathbf{x}_*) = m(\mathbf{x}_*) + \mathbf{k}_*^\top \Sigma^{-1}(Y - \mathbf{m})$$

with variance of prediction error:

$$\mathbb{V}[\hat{Z}(\mathbf{x}_*) - Z(\mathbf{x}_*)] = k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{k}_*^\top \Sigma^{-1}\mathbf{k}_*$$

Connection: Simple Kriging and Gaussian Process Regression

Gaussian Process Regression (GPR) explicitly assumes a joint Gaussian distribution for observed values and predictions:

$$\begin{bmatrix} \mathbf{Z} \\ Z(\mathbf{x}_*) \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} m(\mathbf{X}) \\ m(\mathbf{x}_*) \end{bmatrix}, \begin{bmatrix} \Sigma & \mathbf{k}_* \\ \mathbf{k}_*^\top & k(\mathbf{x}_*, \mathbf{x}_*) \end{bmatrix}\right)$$

The GPR posterior predictive distribution at a new location $\mathbf{x}_*$ is:

$$Z(\mathbf{x}_*)|\mathbf{Z}, \mathbf{X}, \mathbf{x}_* \sim \mathcal{N}(\mu_*, \sigma_*^2)$$

with posterior mean and variance:

$$\mu_* = m(\mathbf{x}_*) + \mathbf{k}_*^\top \Sigma^{-1}(\mathbf{Z} - \mathbf{m})$$

$$\sigma_*^2 = k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{k}_*^\top \Sigma^{-1} \mathbf{k}_*$$

Key Observations: - The SK estimator coincides exactly with the posterior mean of GPR. - The SK prediction error variance matches exactly the posterior variance in GPR. - Thus, GPR generalizes SK by providing not only a point estimator (BLUP), but a full posterior predictive distribution.

Marinescu, Marius. "Explaining and Connecting Kriging with Gaussian Process Regression." *arXiv preprint arXiv:2408.02331*(2024).

Accuracy Results

Corollary 1 *Suppose $U \subseteq \mathbb{R}^{d_u}$, $\Phi \in H_k(U)$, and the random surrogate model is constructed by applying Gaussian process regression to Φ, resulting in $\Phi_N \sim GP(m_N^\Phi(u), k_N(u,u'))$. Then there exist constants $C_{\mathrm{Co}}, C'_{\mathrm{Co}} > 0$, independent of N, such that*

$$d_{\mathrm{Hell}}(\mu^y, \mu^{y,N}_{\mathrm{mean}}) \le C_{\mathrm{Co}} \left\|\Phi - m_N^\Phi\right\|_{L^2_{\mu^y}(U)},$$

Remark: accuracy is optimal when our sampling points are close to the posterior!

Theorem 3 *Suppose U is a bounded Lipschitz domain, $H_k(U)$ is isomorphic to the Sobolev space $H^\tau(U)$, and $f \in H^\tau(U)$. Further suppose that for all $N \in \mathbb{N}$,*

(i) $U_N \subseteq \mathbb{R}^{d_u}$ is compact and $U_N \subseteq \left\{u \in \mathbb{R}^{d_u} : \pi^y(u) \le C_1^2 N^{-\frac{2\tau}{d_u}}\right\}$,

(ii) the training points D_N are sampled i.i.d. from a measure ν_N with density ρ_N satisfying $\rho_N(u) \ge \rho_{\min} > 0$ for all $u \in U \setminus U_N$, and $\rho_N(u) = 0$ otherwise,

(iii) $U \setminus U_N$ is a Lipschitz domain that satisfies an interior cone condition with angle θ, and $U \setminus U_N$ is contained in the cube $B(u_c, R_c^N) = \{u \in \mathbb{R}^{d_u} : \|u - u_c\|_\infty \le R_c^N\}$, for some $u_c \in \mathbb{R}^{d_u}$ and $0 < R_c^N < C_2 \log N$.

Then there exists a constant $C_{\mathrm{Thm}} > 0$, independent of f and N, such that for all $0 \le \beta \le \tau$ and $\varepsilon > 0$ we have

$$\mathbb{E}_{\nu_N}\left[\|f - m_N^f\|_{H^\beta_{\mu^y}(U)}\right] \le C_{\mathrm{Thm}} N^{-\frac{\tau-\beta}{d_u}+\varepsilon} \|f\|_{H^\tau(U)}.$$

Furthermore, for any partitioning $U \setminus U_N \subseteq \cup_{i=1}^r B_i$, where each B_i is a bounded Lipschitz domain that satisfies an interior cone condition with angle θ', there exists a constant C'_{Thm} such that for all $0 \le \beta \le \tau$ we have

$$\mathbb{E}_{\nu_N}\left[\|f - m_N^f\|_{H^\beta_{\mu^y}(U)} \mathrm{I}_{\{h_{D_N,B_i} \le h_0(B_i), 1 \le i \le n\}}\right]$$
$$\le C'_{\mathrm{Thm}} \left(\left(\sup_{u \in U_N} \pi^y(u)\right)^{\frac{1}{2}} + \sum_{i=1}^r \left(\sup_{u \in B_i} \pi^y(u)\right)^{\frac{1}{2}} \mathbb{E}_{\nu_N}\left[h_{D_N,B_i}^{\tau-\beta}\right]\right).$$

Helin, Tapio, et al. "Introduction To Gaussian Process Regression In Bayesian Inverse Problems, With New ResultsOn Experimental Design For Weighted Error Measures." *arXiv preprint arXiv:2302.04518* (2023).

Online Gaussian Process Regression

Our goal is to train the GP model during the MCMC!

Incremental Update (Woodbury Identity):

Given previous covariance matrix inverse K_{XX}^{-1}, adding new points X':

$$K_{X,X}^{-1} \to \begin{bmatrix} K_{XX} & K_{XX'} \\ K_{X'X} & K_{X'X'} \end{bmatrix}^{-1}$$

is updated efficiently by:

$$\text{Set } B = K_{XX'}, \quad C = K_{X'X}, \quad D = K_{X'X'}$$

$$\Rightarrow \quad \begin{bmatrix} K_{XX}^{-1} + K_{XX}^{-1} B \Lambda C K_{XX}^{-1} & -K_{XX}^{-1} B \Lambda \\ -\Lambda C K_{XX}^{-1} & \Lambda \end{bmatrix}$$

where $\Lambda = (D - C K_{XX}^{-1} B)^{-1}$.

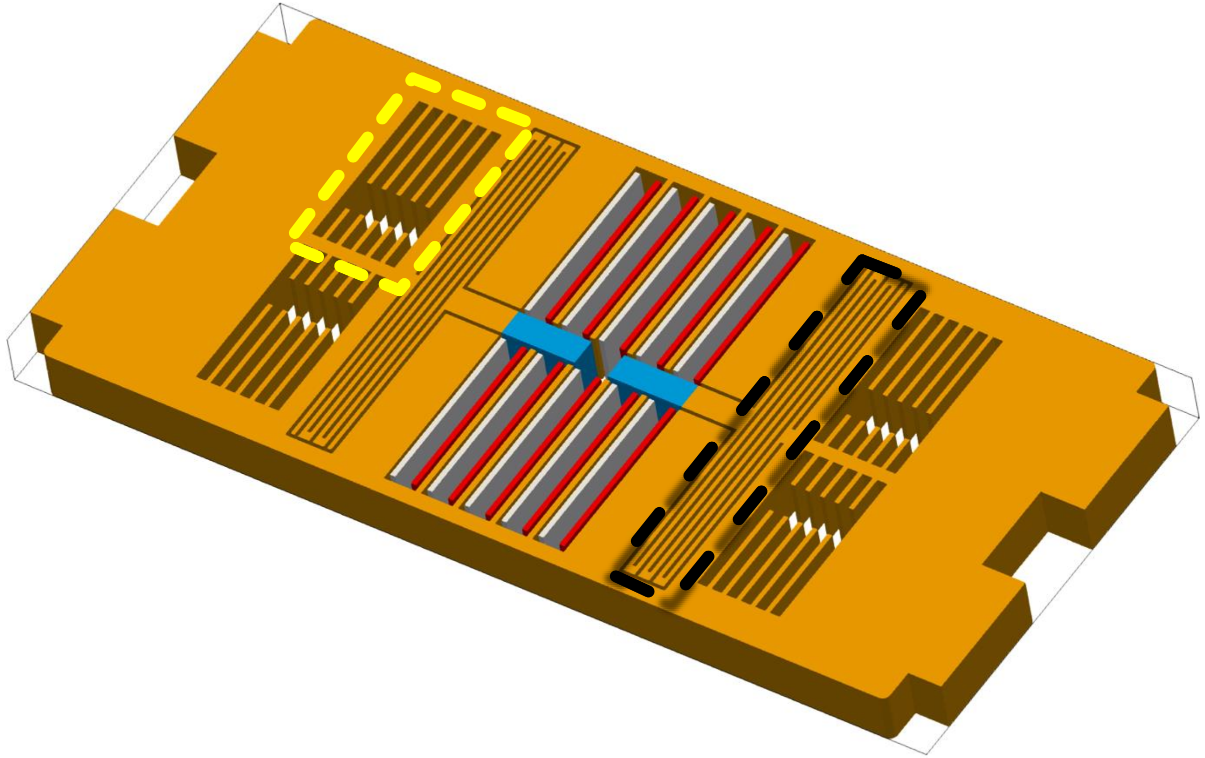
Computational Complexity:

- Naive GP inversion: $\mathcal{O}(N^3)$
- Online (incremental) update complexity: $\mathcal{O}(N^2)$ per new point

NUMERICAL RESULTS

3D Model

Components	
(purple swatch)	Shuttle mass I
(red swatch)	Left Electrodes
(grey swatch)	Right Electrodes
(blue swatch)	Anchors
(black swatch)	Folded Beams = Springs
(yellow swatch)	Air damper



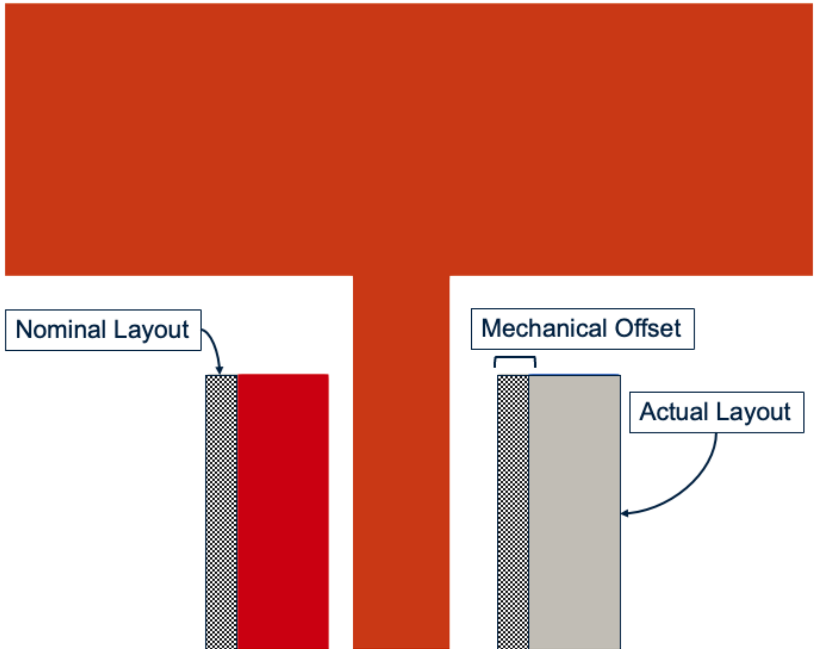
Mathematical Model

- Euler-Bernoulli elements.
- Conformal mapping for electrostatic force
- Geometric non-linearity is included.
- Small-strain assumption.
- μ embeds geometrical uncertainties

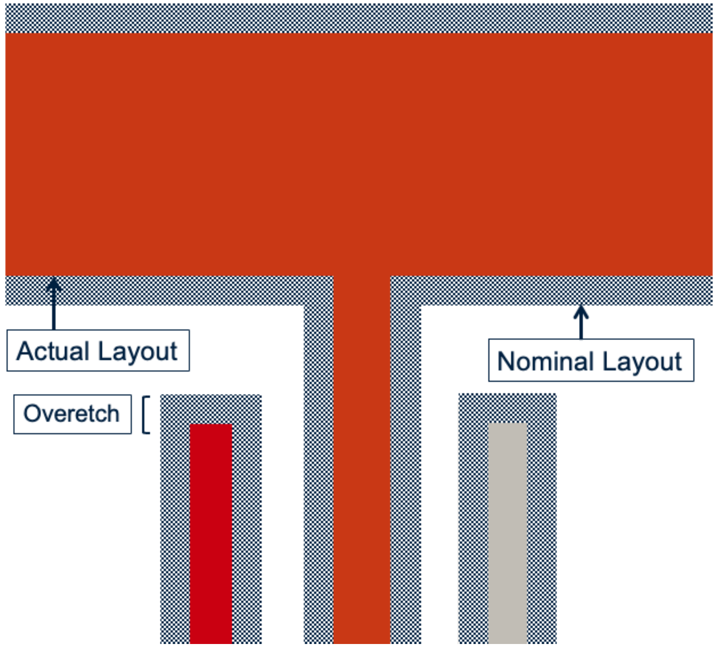
$$
\begin{aligned}
\rho_0\ddot{\mathbf{u}}(\mathbf{X},t;\boldsymbol{\mu}) + \mathbf{C}\dot{\mathbf{u}}(\mathbf{X},t;\boldsymbol{\mu}) - \nabla_{\mathbf{X}}\cdot\mathbf{P}(\mathbf{u}(\mathbf{X},t;\boldsymbol{\mu});\boldsymbol{\mu}) &= -\rho_0\mathbf{a}_0 && \text{in } \Omega_0\times\mathcal{T},\\
\mathbf{P}(\mathbf{u}(\mathbf{X},t;\boldsymbol{\mu});\boldsymbol{\mu})\cdot\mathbf{N}(\mathbf{X}) &= \mathbf{f}_{elec}(\mathbf{X}) && \text{on } \partial\Omega_{0N}\times\mathcal{T},\\
\mathbf{u}(\mathbf{X},t) &= \mathbf{0} && \text{on } \partial\Omega_{0D}\times\mathcal{T},\\
\mathbf{u}(\mathbf{X},0) &= \mathbf{0} && \text{in } \Omega_0,\\
\dot{\mathbf{u}}(\mathbf{X},0) &= \mathbf{0} && \text{in } \Omega_0,\\
\operatorname{div}(\operatorname{grad}\phi(\mathbf{x})) &= 0 && \text{in } \Omega_\infty\setminus\Omega\times\mathcal{T},\\
\phi(\mathbf{x}) &= V_k(t) && \text{on } \partial\Omega_k,\\
\operatorname{grad}\phi(\mathbf{x})\cdot\mathbf{n} &= 0 && \text{on } S_\infty.
\end{aligned}
$$

Fabrication Inaccuracies

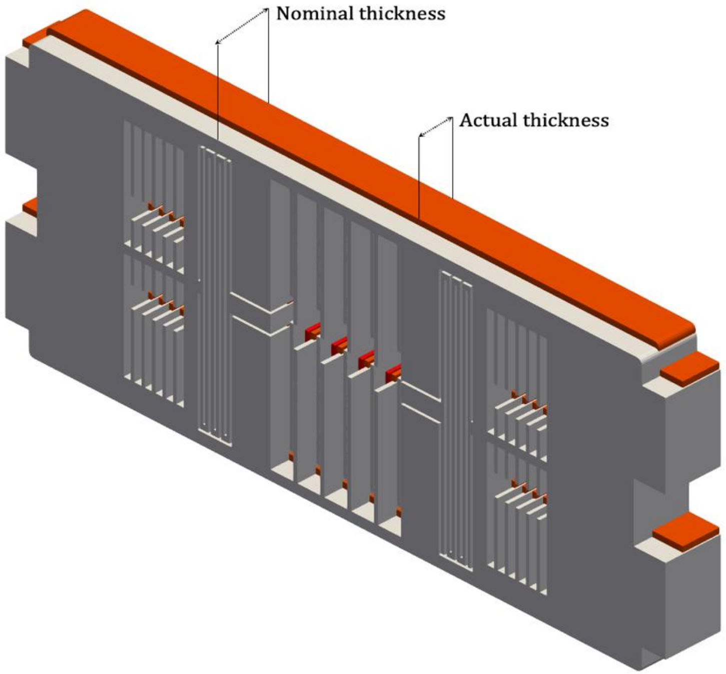
1: Mechanical Offset



2: Unilateral Overetch



3: Epipoly Thickness



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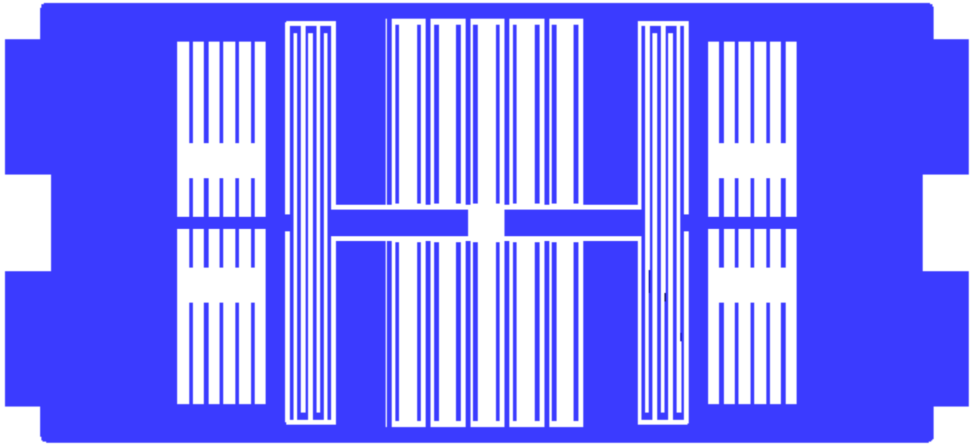
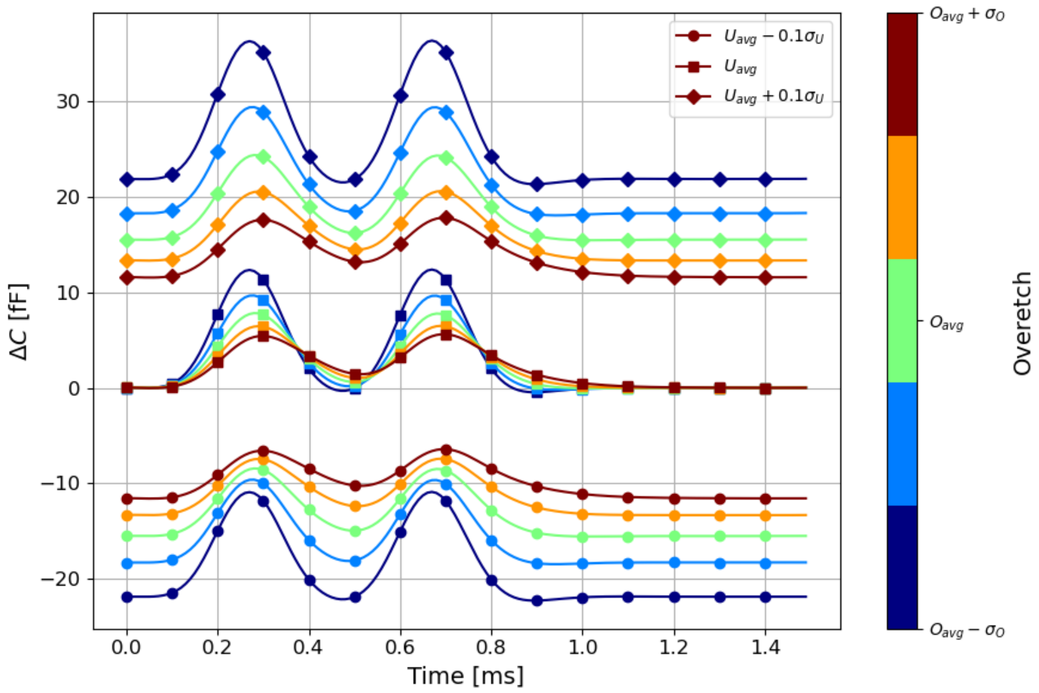
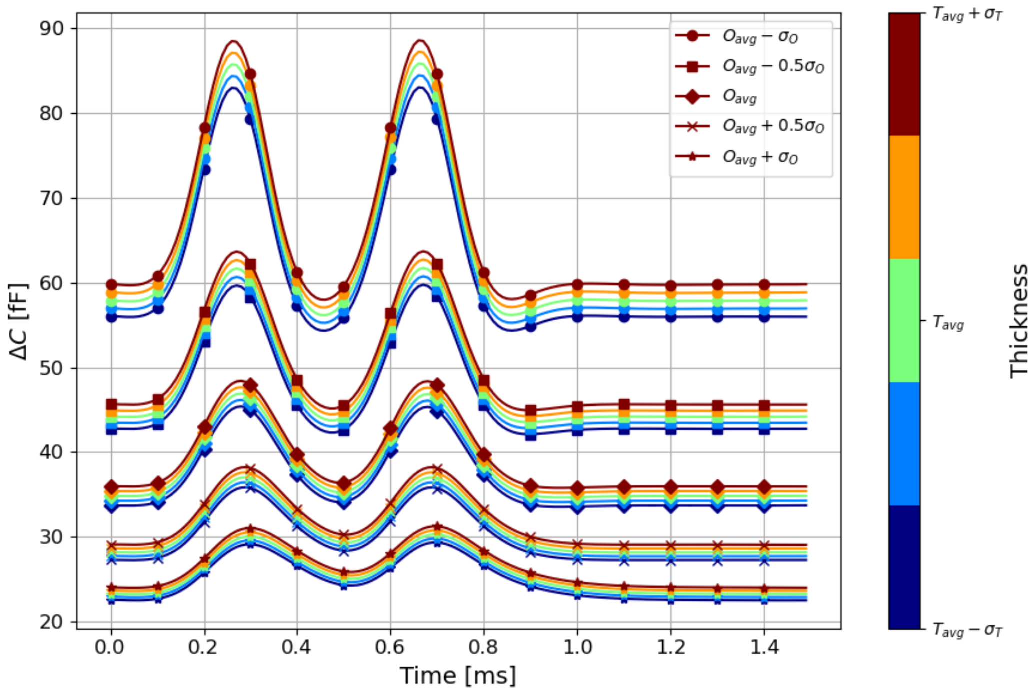
Simulation Setup

Electronic Test:

$$V_{right} = 0.9\,(1 + cos(2\pi ft))\ [V] \quad \text{for } 0 \le t \le 2T\ [s],$$
$$V_{left} = 0\ [V] \quad \text{for } t \ge 0\ [s],$$
$$V_{right} = 0\ [V] \quad \text{for } t > 2T\ [s]$$

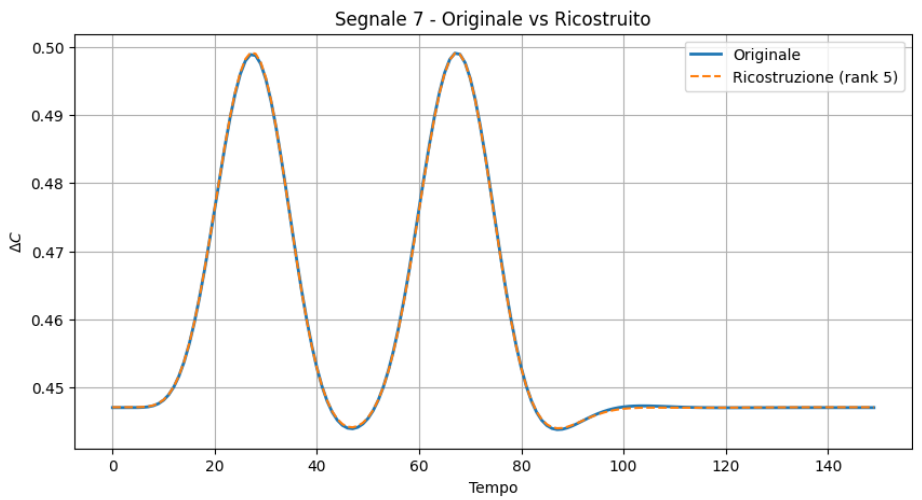


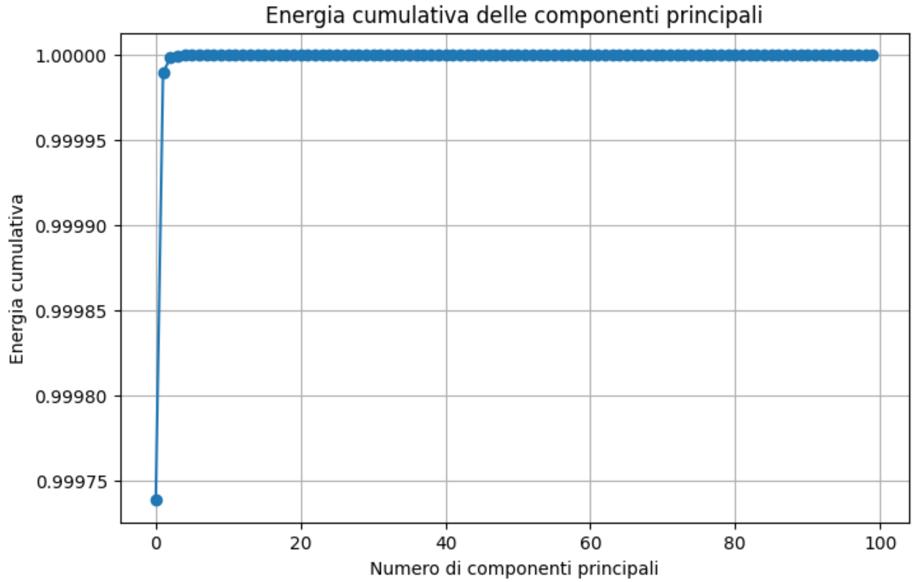




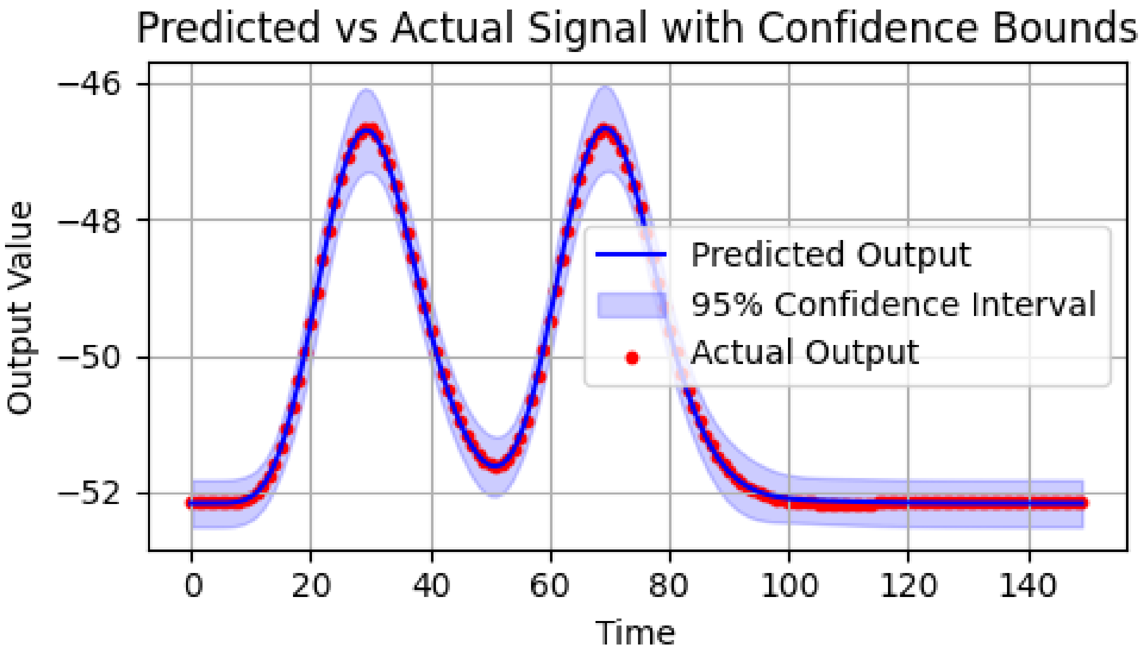
DIMENSIONALITY REDUCTION: POD-GP

- In order to have a surrogate for the time series, we decompose the signal using SVD.
- We then train an independent GP to approximate each POD mode coefficient.
- The POD guarantees that the coefficients of distinct POD modes are independent, thereby avoiding the need of a multi-output GP.





ACCURACY

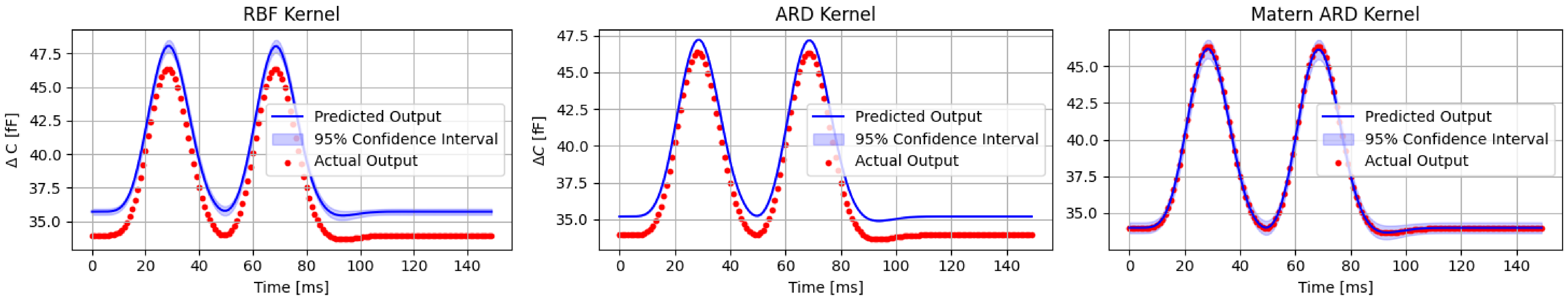


- High accuracy is obtained when increasing the number of samples.
- Our goal is to minimize the number of training data online: therefore we will stop at 100.

COVARIANCE KERNEL ROLE

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

$$k\left(\mathbf{x},\mathbf{x}'\right)=\exp\left(-\frac{1}{2}\sum_{d=1}^{D}\frac{\left(x_d-x_d'\right)^{2}}{\ell_d^{2}}\right)$$



$$k_{5/2}\left(\mathbf{x},\mathbf{x}'\right)=\left(1+\sqrt{5r^{2}\left(\mathbf{x},\mathbf{x}'\right)}+\frac{5}{3}r^{2}\left(\mathbf{x},\mathbf{x}'\right)\right)\exp\left(-\sqrt{5r^{2}\left(\mathbf{x},\mathbf{x}'\right)}\right)$$

where

$$r^{2}\left(\mathbf{x},\mathbf{x}'\right)=\sum_{d=1}^{D}\frac{\left(x_d-x_d'\right)^{2}}{\ell_d^{2}}$$

ACTIVE SAMPLING STRATEGY

- Use a Delayed Acceptance Algorithm for solving the inverse problem.
- At coarse level we use the GP - likelihood, adjusted by the covariance.

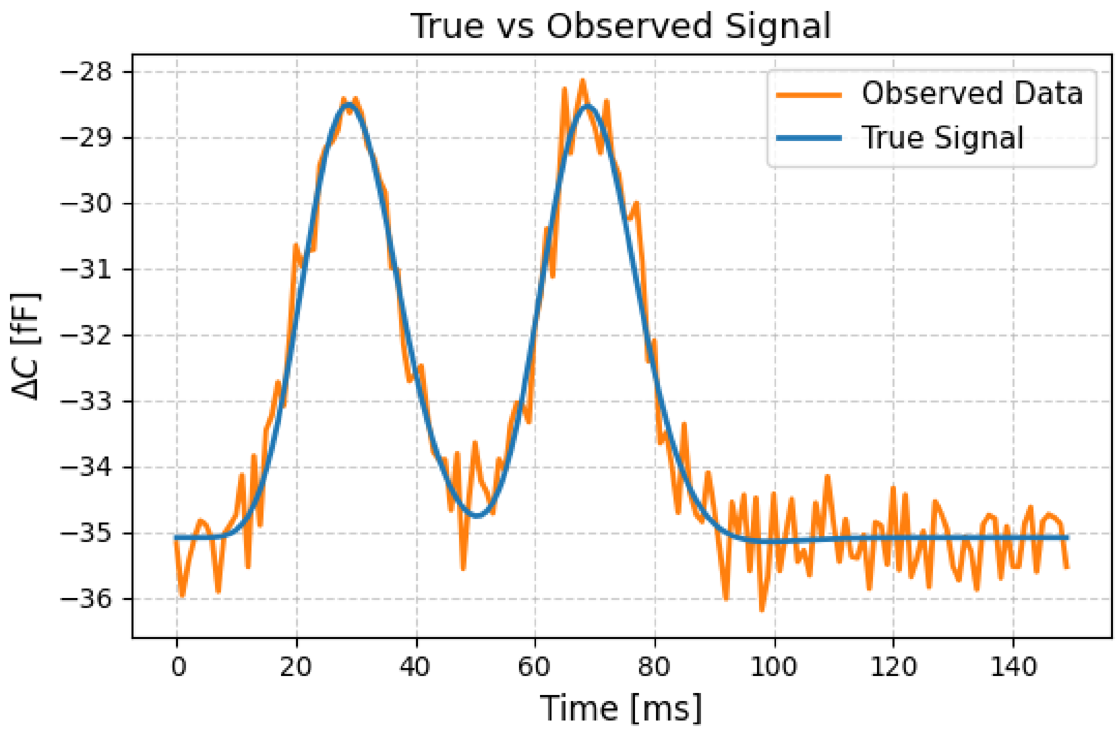
$$\mathcal{L}_{\mathrm{GP}}(y \mid \mathbf{x}) = \mathcal{N}\left(y \mid \mu_{\mathrm{GP}}(\mathbf{x}), \Sigma_{\mathrm{obs}} + \Sigma_{\mathrm{GP}}(\mathbf{x})\right)$$

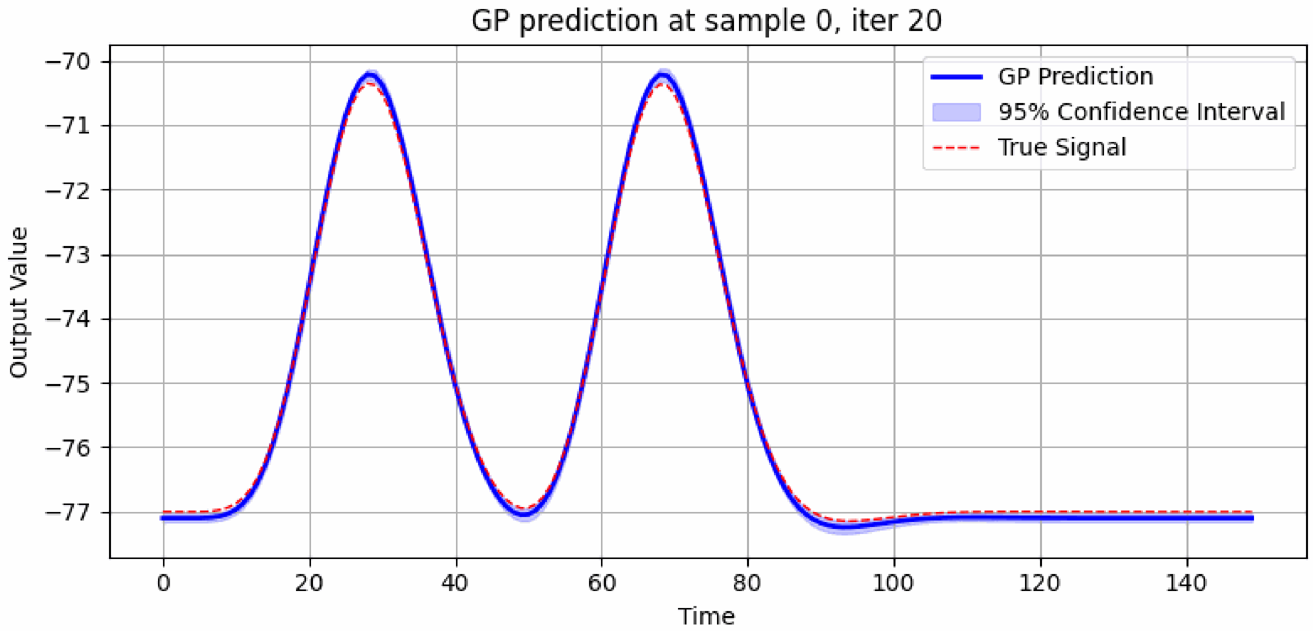
- At fine level, we use the FOM.

$$\mathcal{L}_{\mathrm{FOM}}(y \mid \mathbf{x}) = \mathcal{N}\left(y \mid \mathcal{F}(\mathbf{x}), \Sigma_{\mathrm{obs}}\right)$$

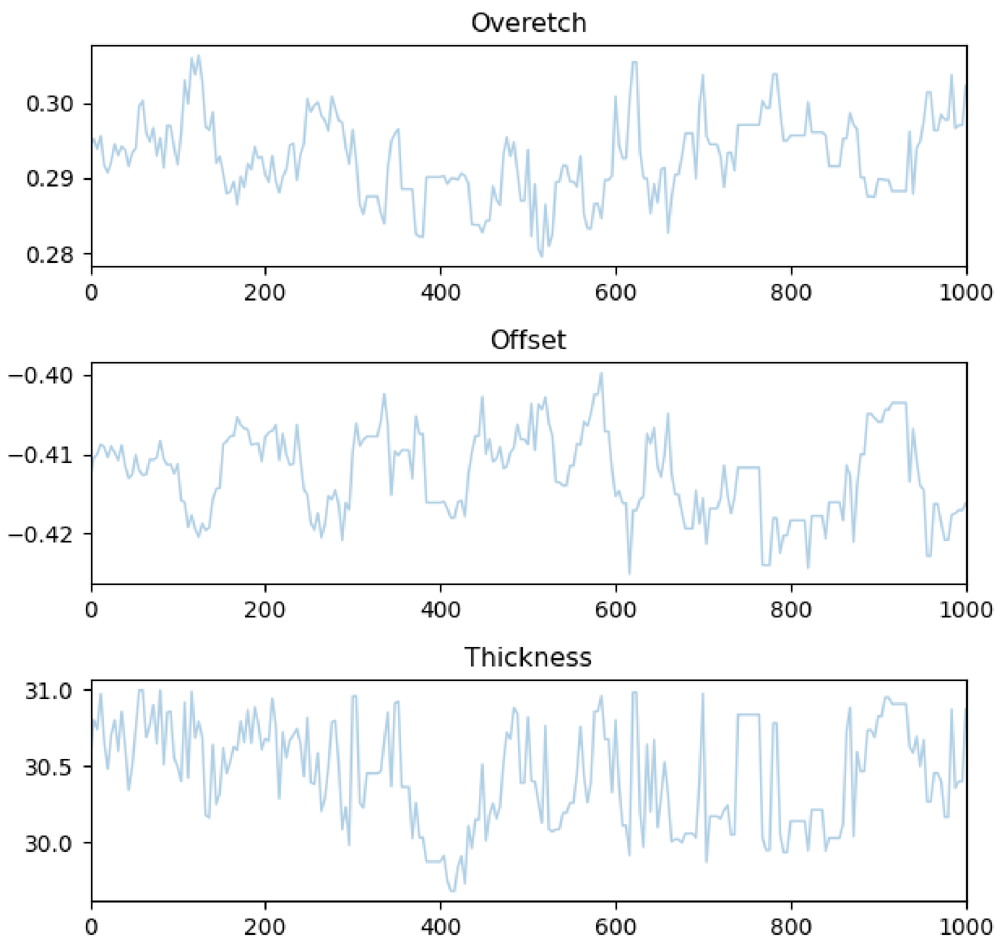
- Every 5 steps, we fit the GP introducing New Point.
- When the GP standard deviation becomes negligigble, we stop training and switch to only surrogate

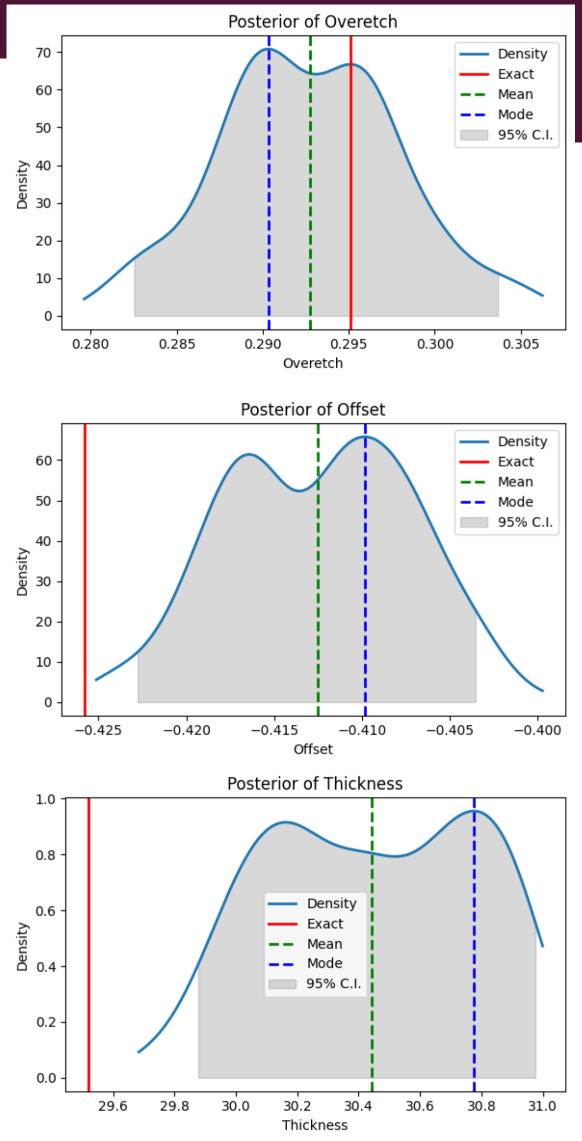
ONLINE SAMPLING





GP - MCMC


Overetch
0.30
0.29
0.28
0
200
400
600
800
1000
Offset
−0.40
−0.41
−0.42
0
200
400
600
800
1000
Thickness
31.0
30.5
30.0
0
200
400
600
800
1000


Posterior of Overetch
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Density
Overetch
0.280
0.285
0.290
0.295
0.300
0.305
Posterior of Offset
Density
Exact
Mean
Mode
95% C.I.
Density
Offset
−0.425
−0.420
−0.415
−0.410
−0.405
−0.400
Posterior of Thickness
Density
Exact
Mean
Mode
95% C.I.
Density
Thickness
29.6
29.8
30.0
30.2
30.4
30.6
30.8
31.0

CONCLUSION

- The active sampling allows to reduce by a factor of 4 the total number of samples need to train the GP.
- Numerical Issues in inverse correction reduce the effectiveness of the method, for which a regularization is introduced, limiting the accuracy of the method.
- Preconditioning techniques should be investigated.
- In general, the method allows to drastically reduce the computational times needed for MCMC with good accuracy.

BIBLIOGRAPHY

- Marinescu, Marius. "Explaining and Connecting Kriging with Gaussian Process Regression." *arXiv preprint arXiv:2408.02331*(2024).
- Helin, Tapio, et al. "Introduction To Gaussian Process Regression In Bayesian Inverse Problems, With New ResultsOn Experimental Design For Weighted Error Measures." *arXiv preprint arXiv:2302.04518* (2023).
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- [2] Benjamin Peherstorfer, Karen Willcox, and Max Gunzburger. Survey of multifidelity methods in uncertainty propagation, inference, and optimization. Siam Review,60(3):550–591, 2018.