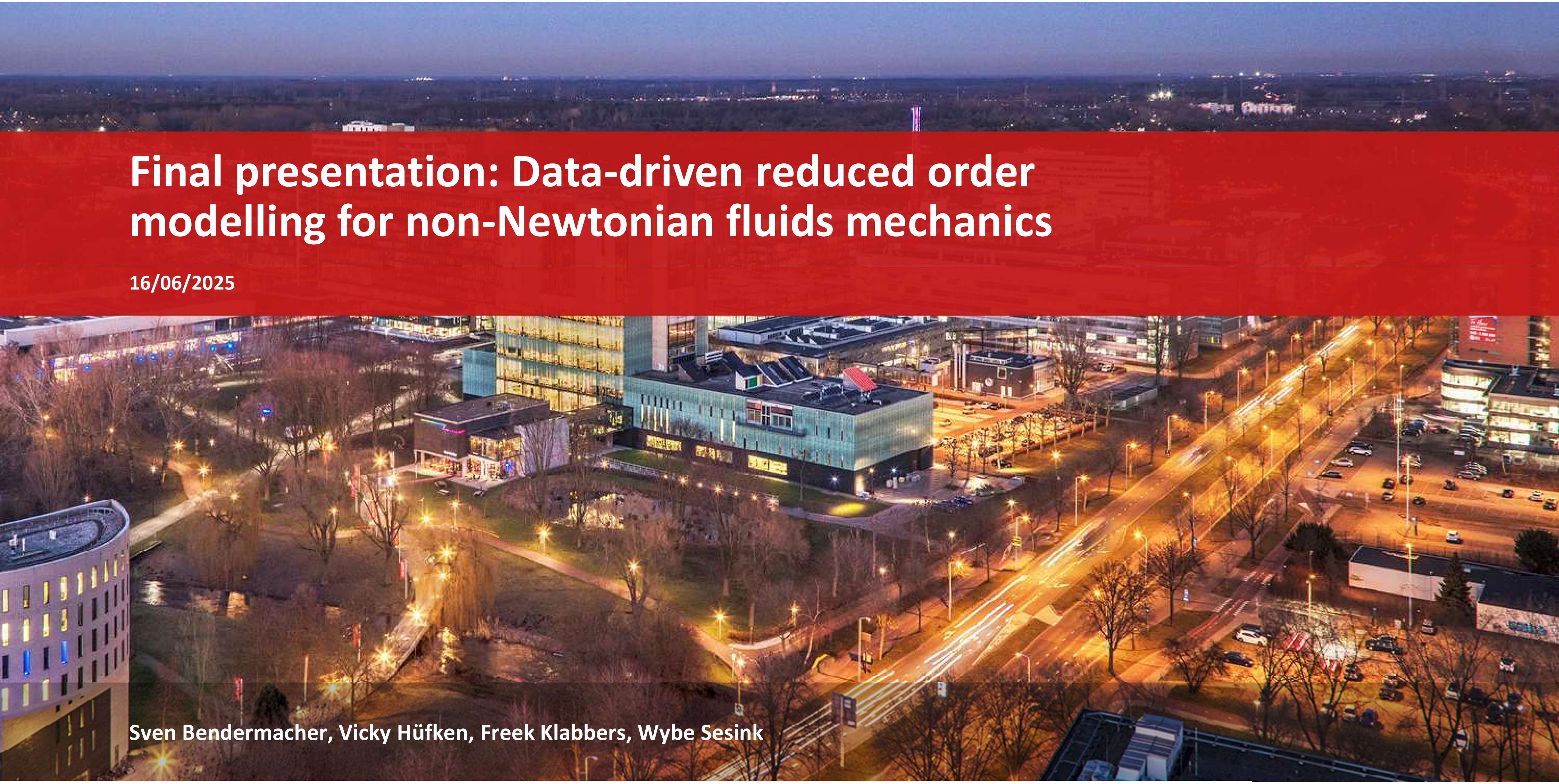


Final presentation: Data-driven reduced order modelling for non-Newtonian fluids mechanics

16/06/2025

Sven Bendermacher, Vicky Hüfken, Freek Klabbers, Wybe Sesink

AIES, Group internship Team 5

EINDHOVEN UNIVERSITY OF TECHNOLOGY

Incentive: Measuring Fluid Parameters

[1]

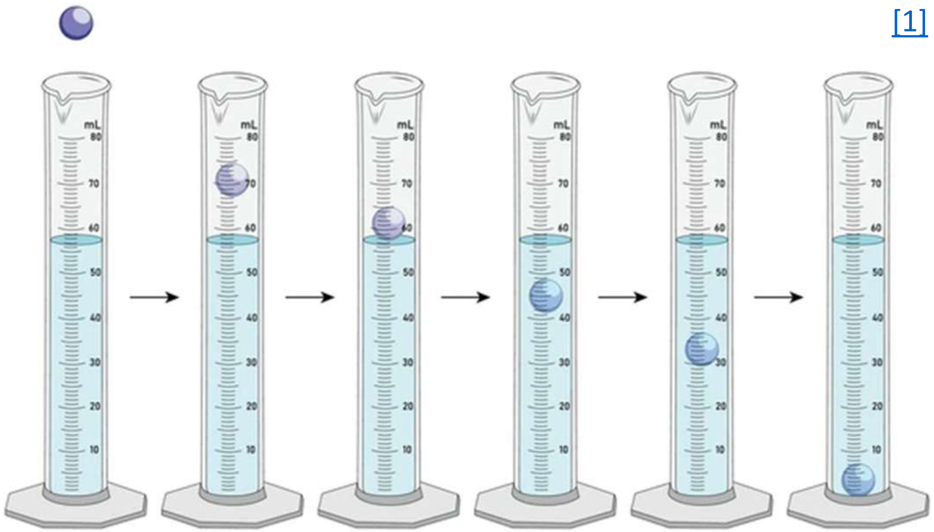
- Understanding complex fluids
- Data generation is difficult

- Non-Newtonian

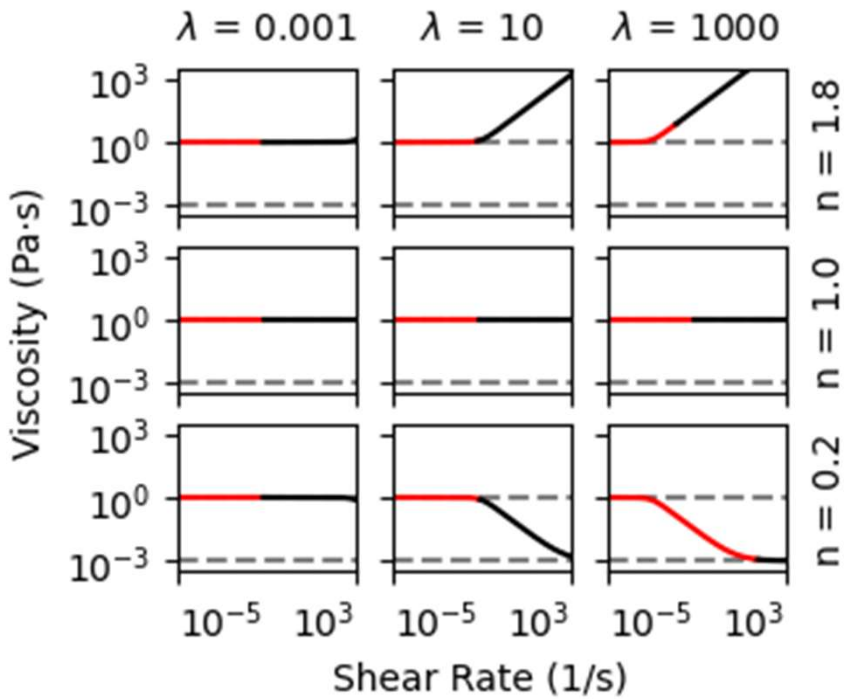
[1] https://formula82.pro/news/Pravda-o-motornom-masle-razrushaem-mifyi

Falling Sphere Rheometry

$$\eta = \eta_\infty + \frac{\eta_0 - \eta_\infty}{\left(1 + (\lambda\dot{\gamma})^2\right)^{\frac{1-n}{2}}}$$



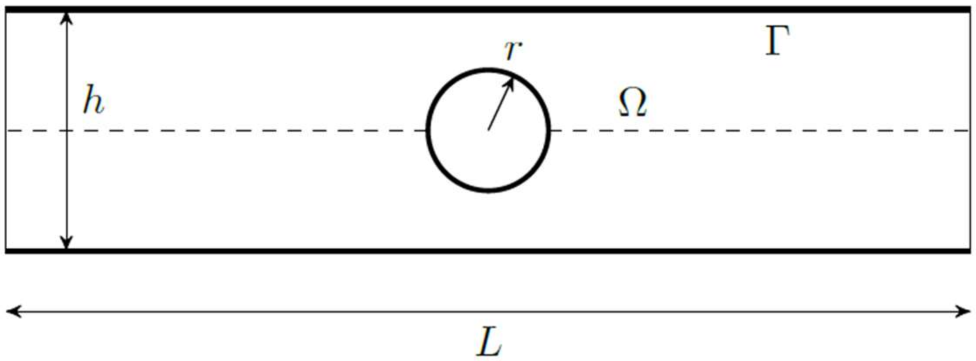
[1]



[1] https://www.shutterstock.com/image-vector/falling-sphere-viscosity-test-apparatus-laboratory-2415852693

CFD Tools for the Inverse Problem

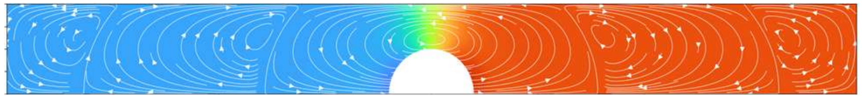
- Analysis is difficult
- CFD tools to simulate field



Parameters

Forward problem: CFD

Inverse problem



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Bayesian Inference

Likelihood

Prior

$$P(\theta|\,D) = \frac{P(D|\theta)P(\theta)}{P(D)}$$

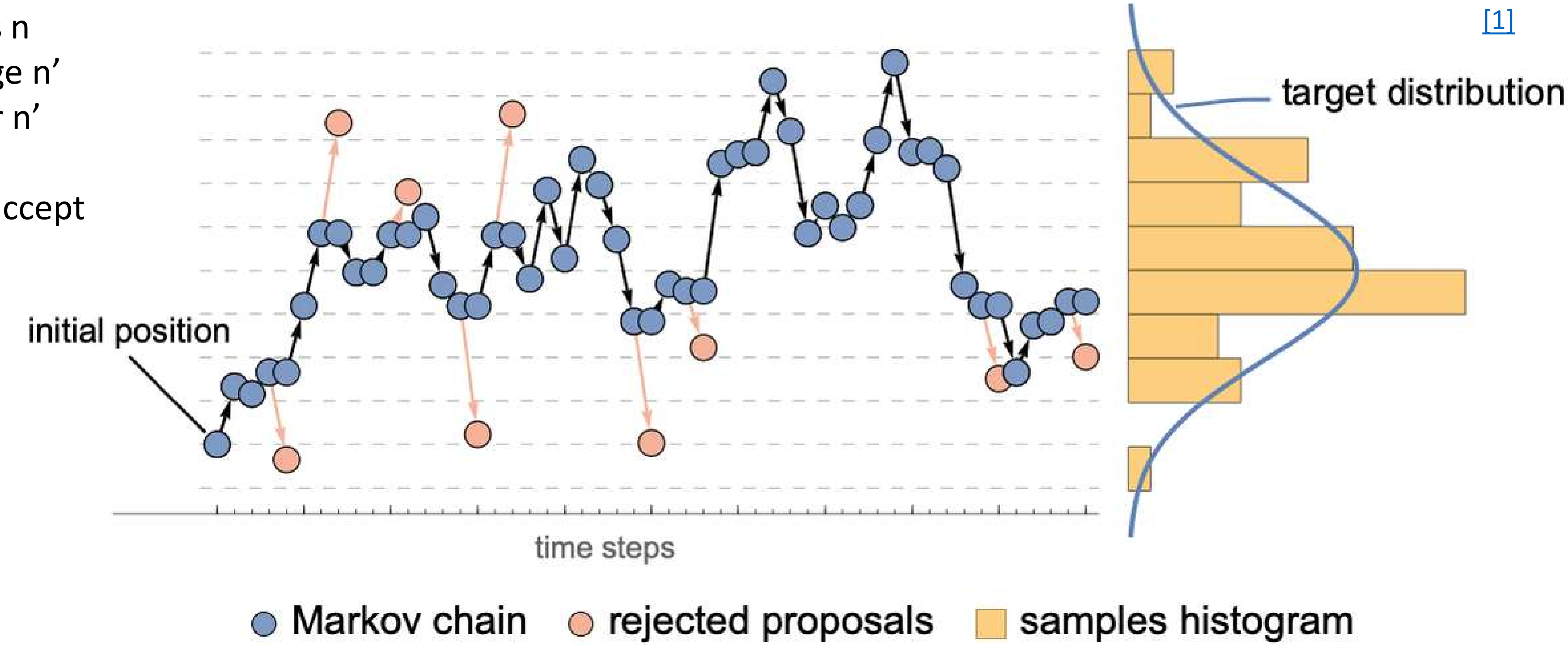
Posterior

Evidence

Markov Chain Monte Carlo

1. Initial guess n
2. Small change n’
3. Run CFD for n’
4. Likelihood
5. Choose to accept it as a next sample

[1]



[1] https://www.wolfram.com/language/introduction-machine-learning/bayesian-inference/

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Reduced Order Model

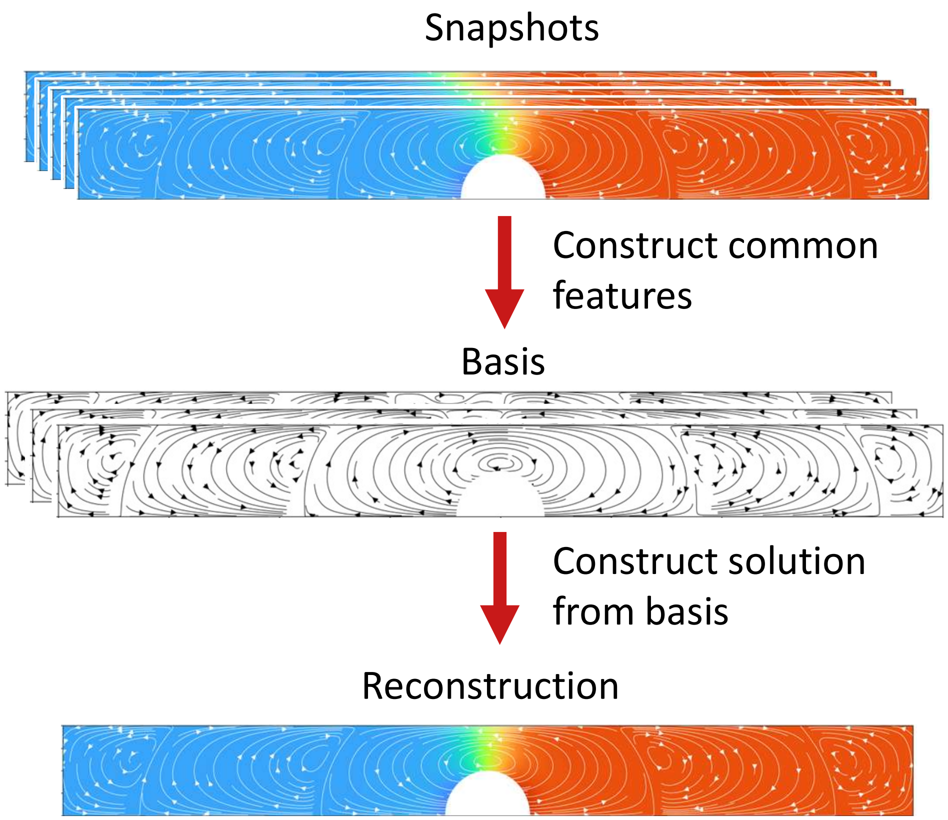
$$\mathbf{u} = \alpha_1\phi_1 + \alpha_2\phi_2 + \alpha_3\phi_3 + \alpha_4\phi_4 + \alpha_5\phi_5 + \cdots$$

Truncation:

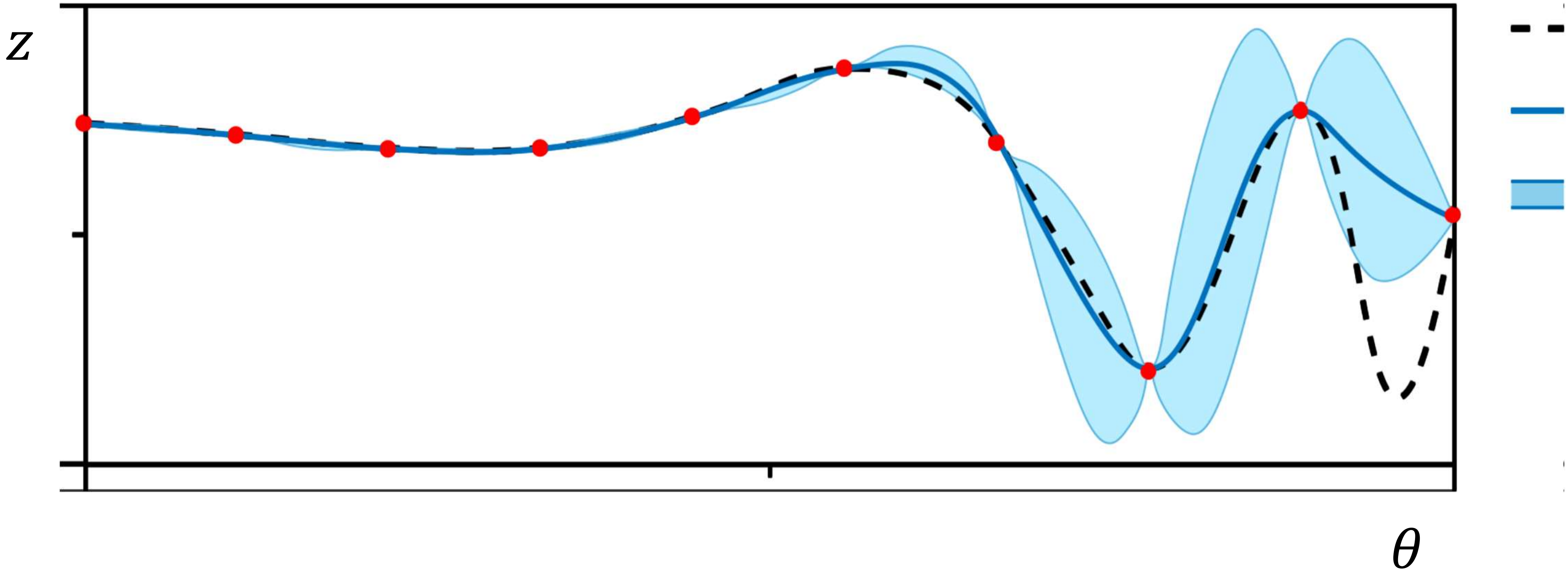
$$\mathbf{u} = \alpha_1\phi_1 + \alpha_2\phi_2 + \cdots + \alpha_n\phi_n$$

ϕ we have, α we need!

Optimal Basis ϕ: Singular Value Decomposition



Gaussian processes



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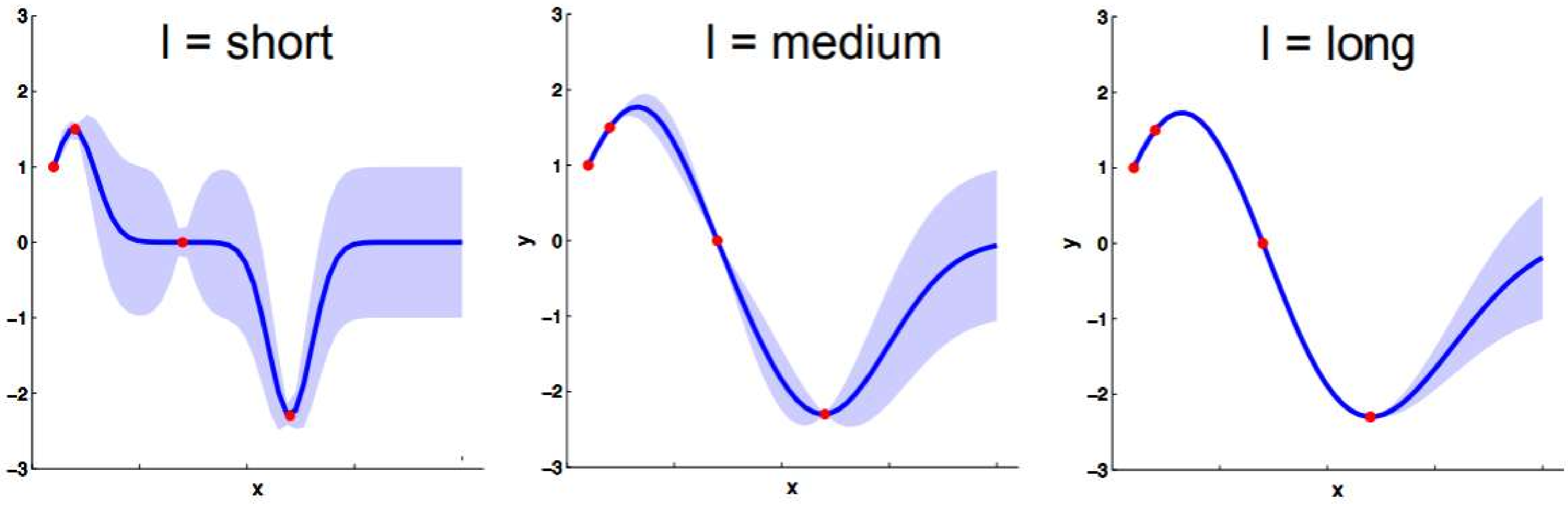
Hyperparameters

[1]



[1] https://thegradient.pub/gaussian-process-not-quite-for-dummies/

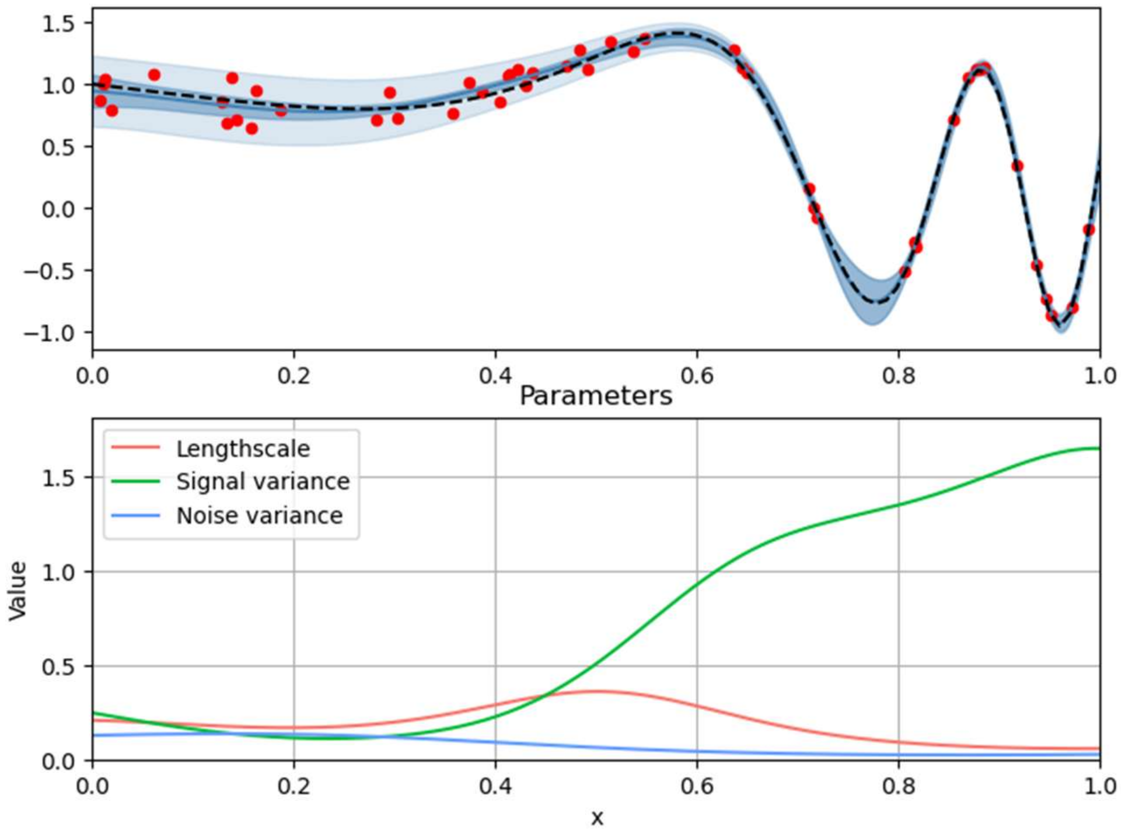
Non – Stationary Gaussian Process

Normal GP:

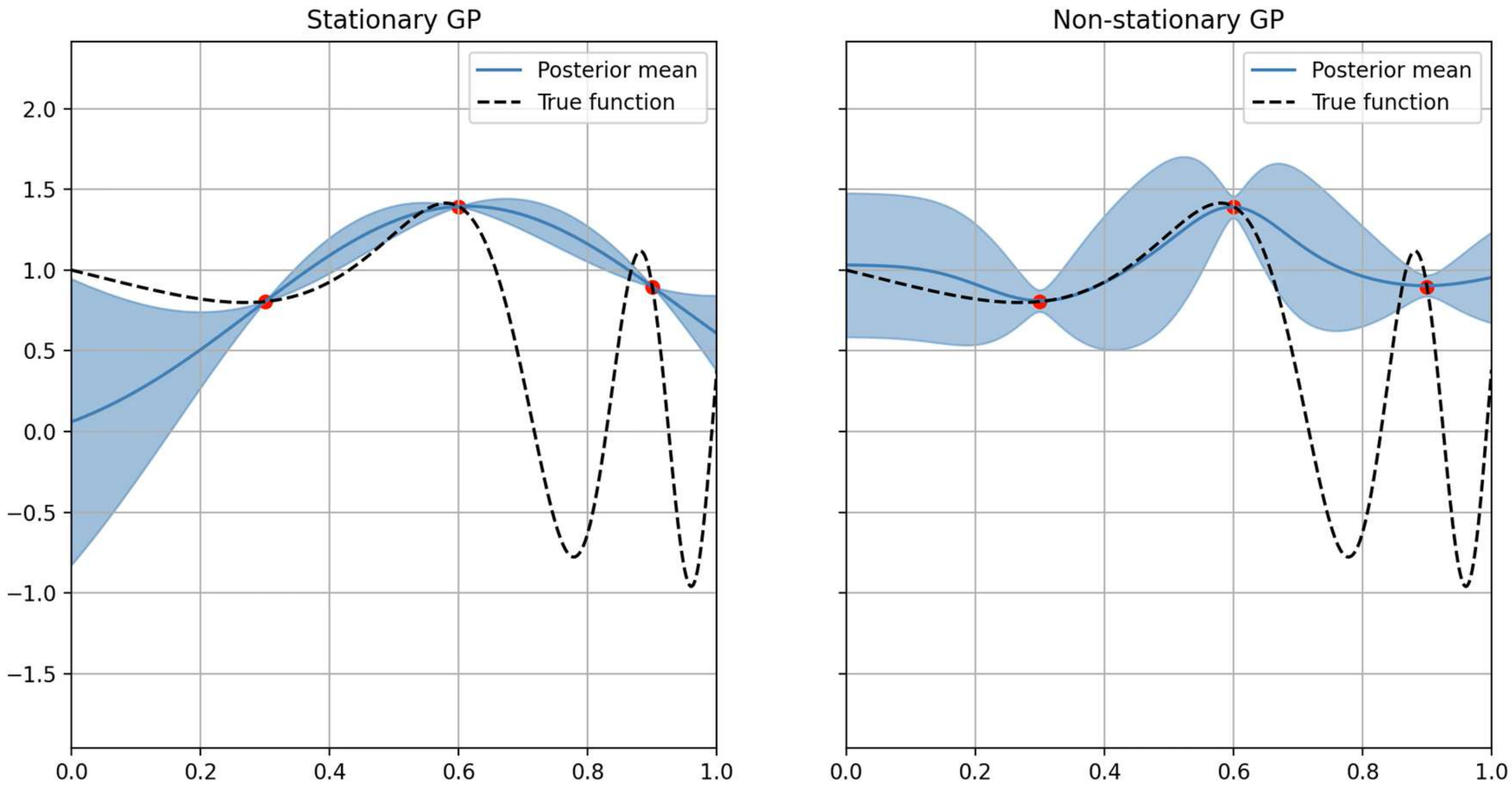
- Hyperparameters are global

Non-stationary GP:

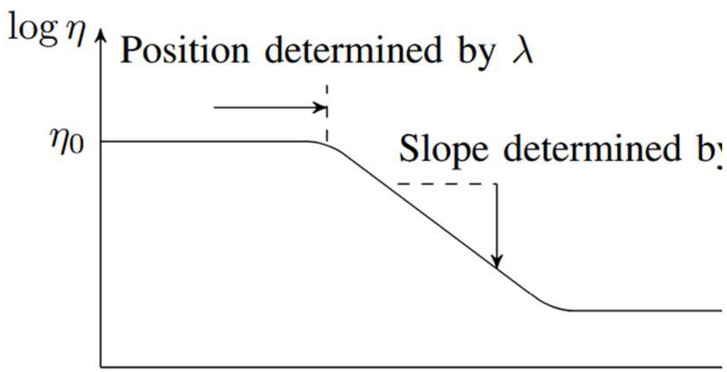
- Hyperparameters are local

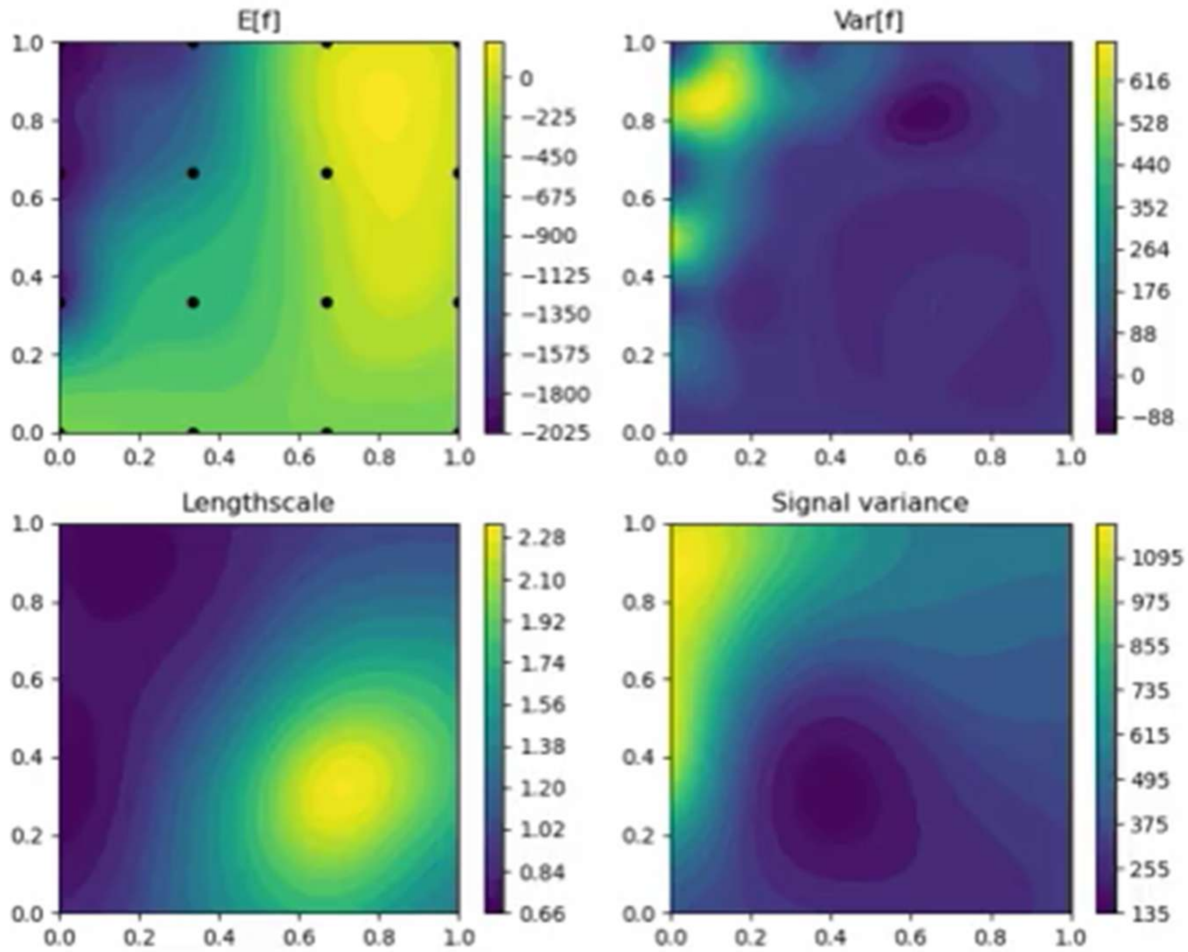


Example adaptive sampling – stat vs non-stat GP

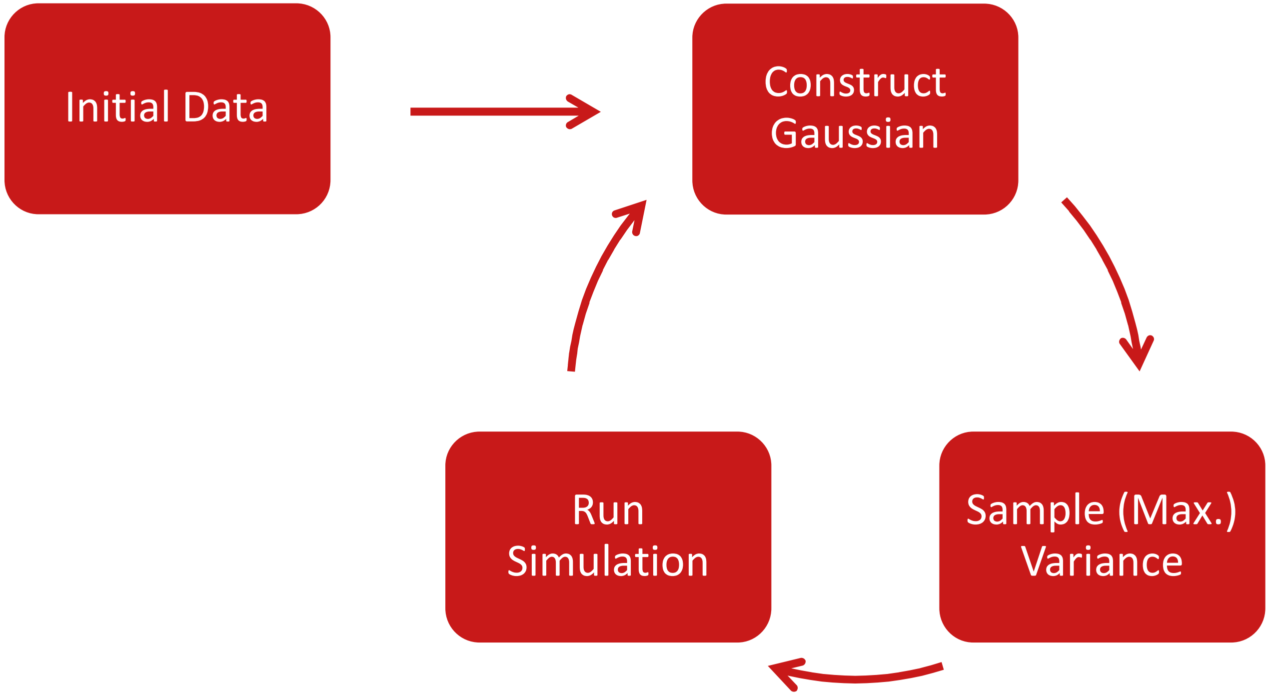


Adaptive sampling

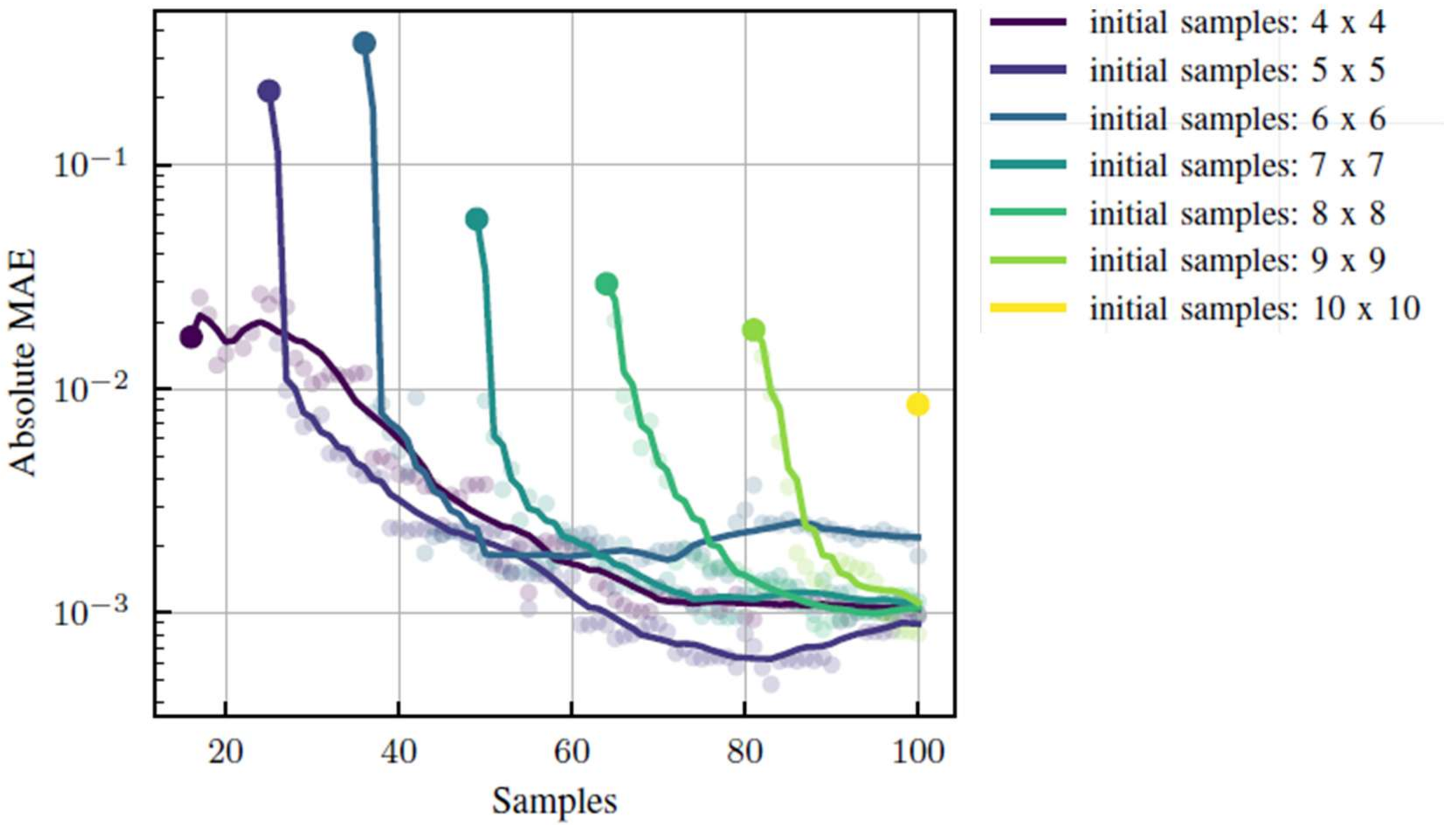




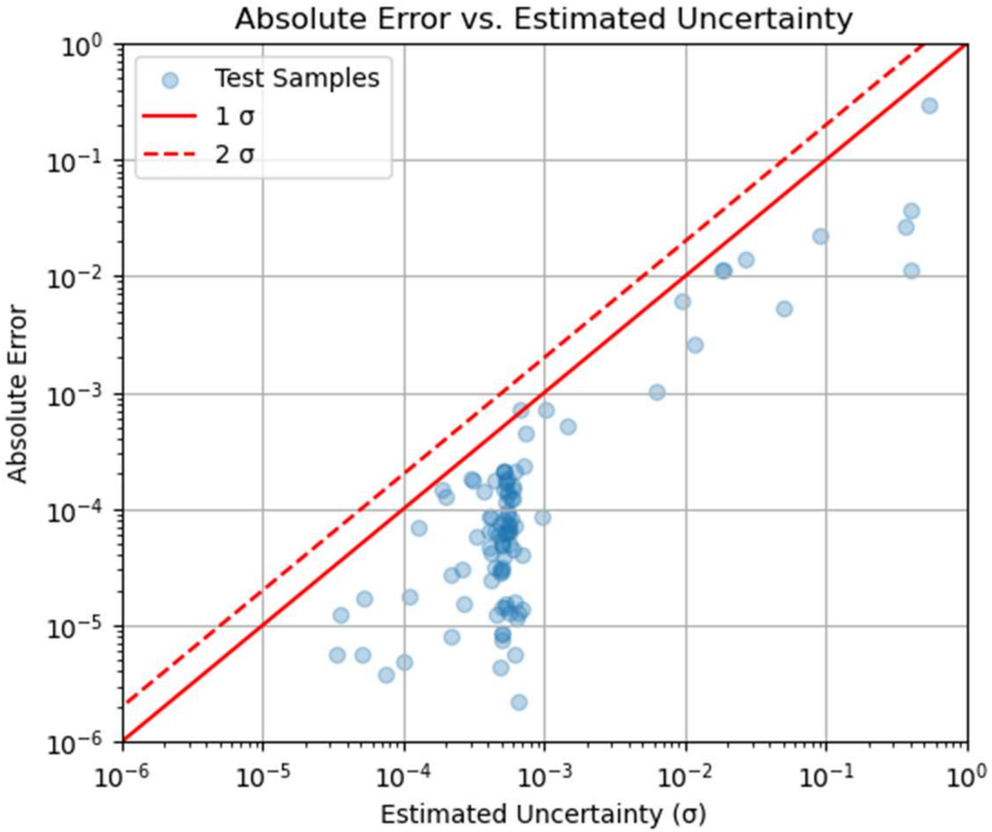
A Fully Automated Process



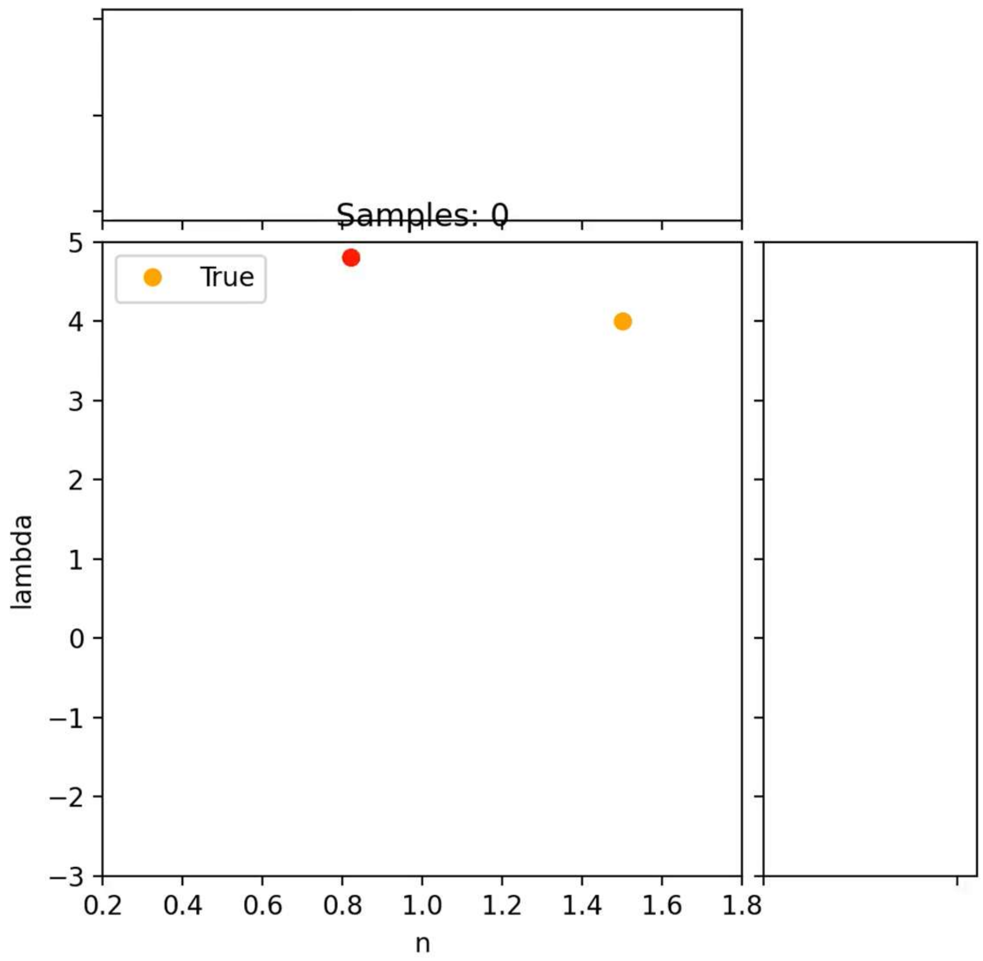
Results: Adaptive Sampling



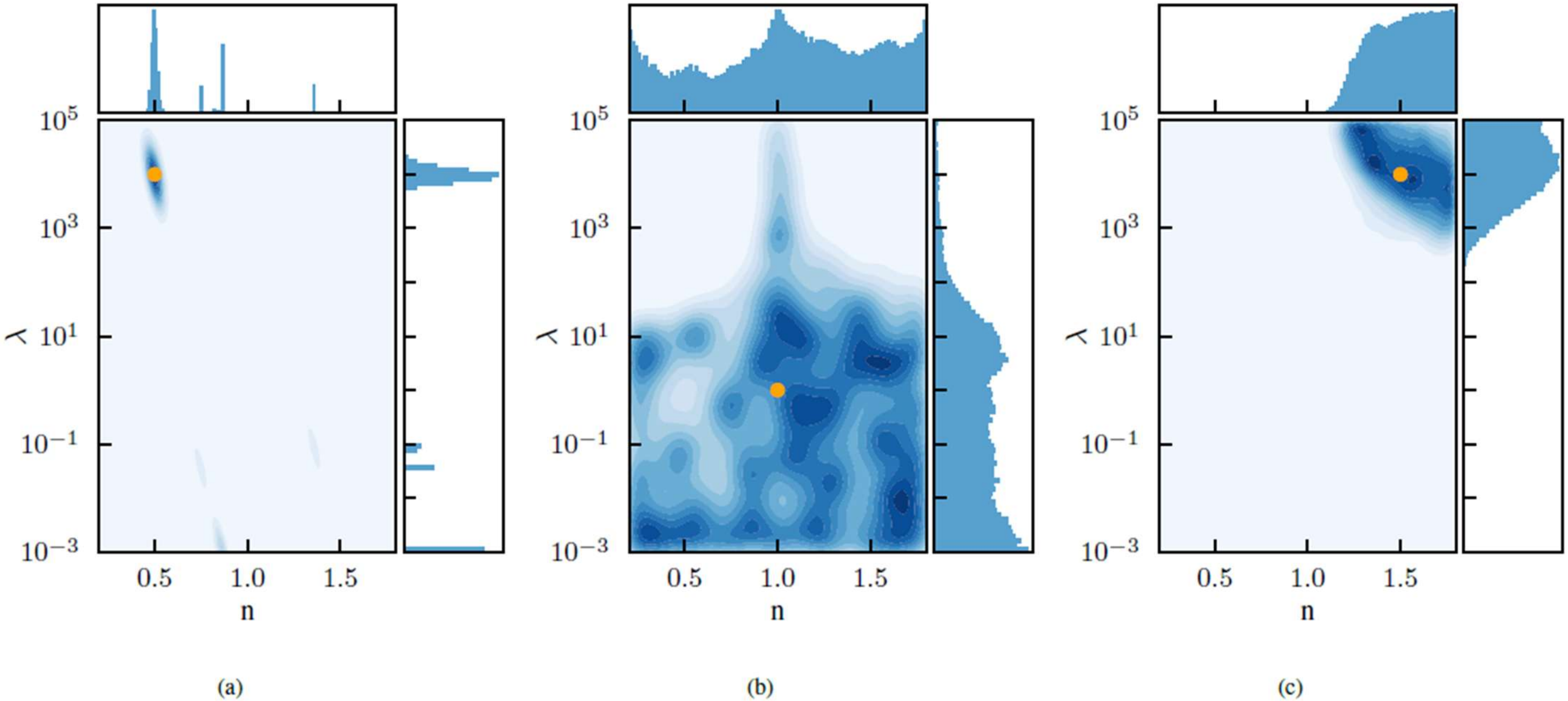
Gaussian process uncertainty



Demonstration:



Results: Inverse problem



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Discussion

- GP scales badly
- NSGP package is not yet fully optimized

Conclusion & Recommendations

- NSGPs in combination with adaptive sampling very effective
- NSGP package created for Python
- Numerical error correlates well with uncertainty
- ROM with BI is a viable way to obtain rheological parameters in complex flow settings
- Future work: generalization of framework

Feedback

- Incentive could have been clearer, also why and for whom we are doing it can be emphasized more. Put more focus on the importance on uncertainty.
- Add some words to the slides with only animations to support the explanation to support the people who are unfamiliar with the concepts.
- Simplify the GP explanation to ‘mapping of input to output parameters with uncertainty measure.
- Explain the inverse problem as the backward mapping of the problem.
- Good to not discuss the ROM part of the problem. Good to use simplified function for the explanation of GP.
- General set-up for the final presentation: Slide with approach, GP, Sampling and inverse problem
- Fix coloring to be the same in the FEM slide.

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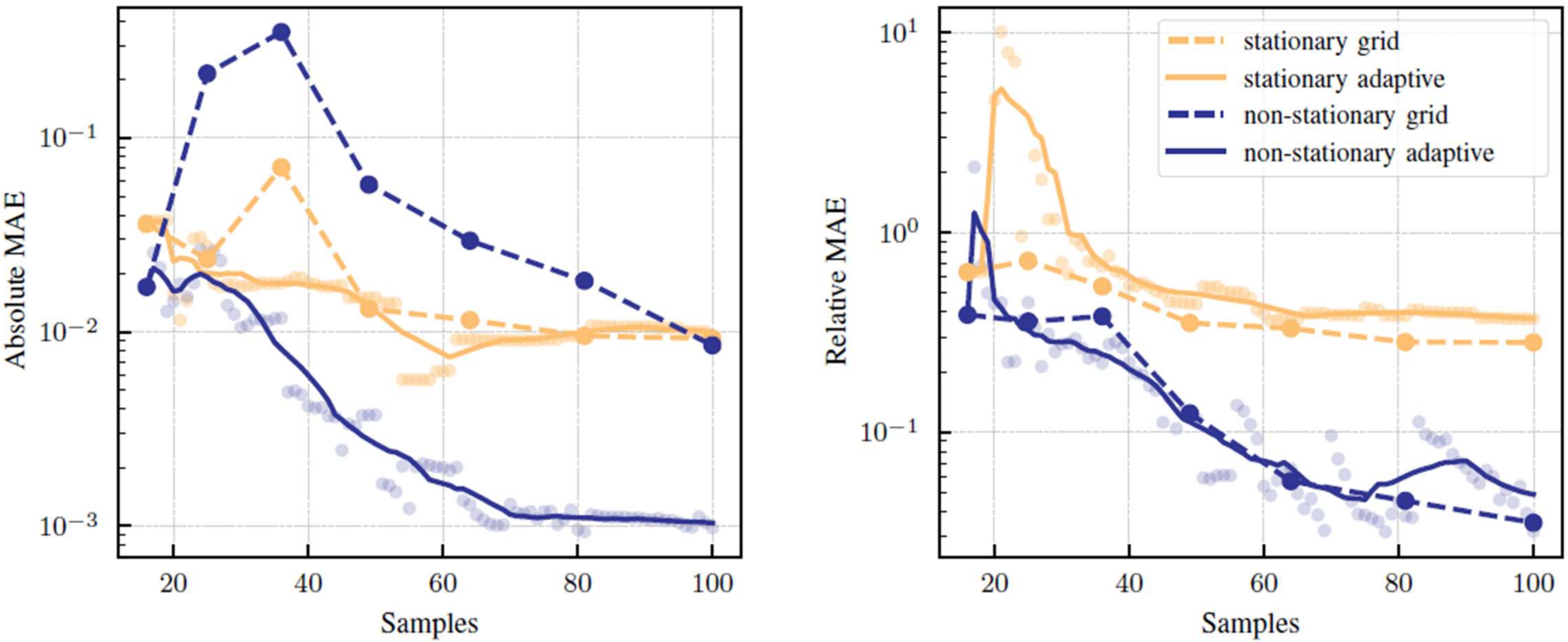
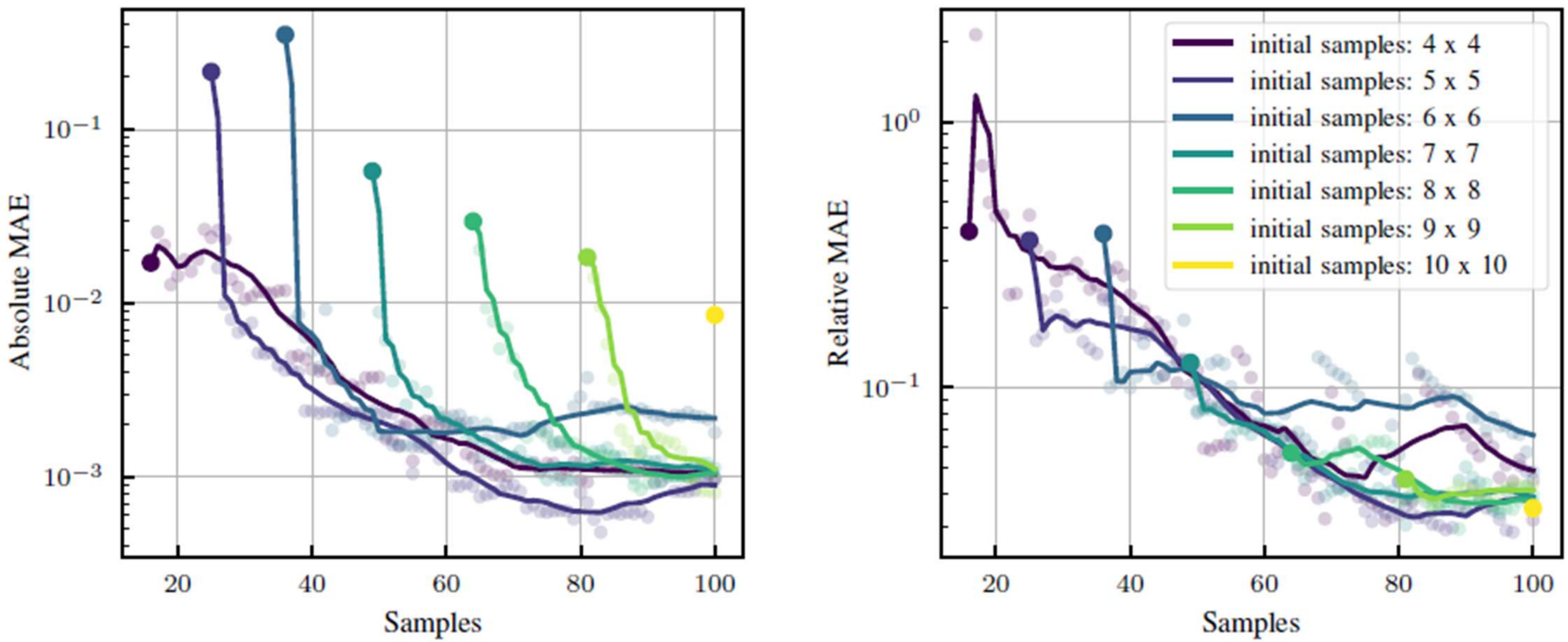
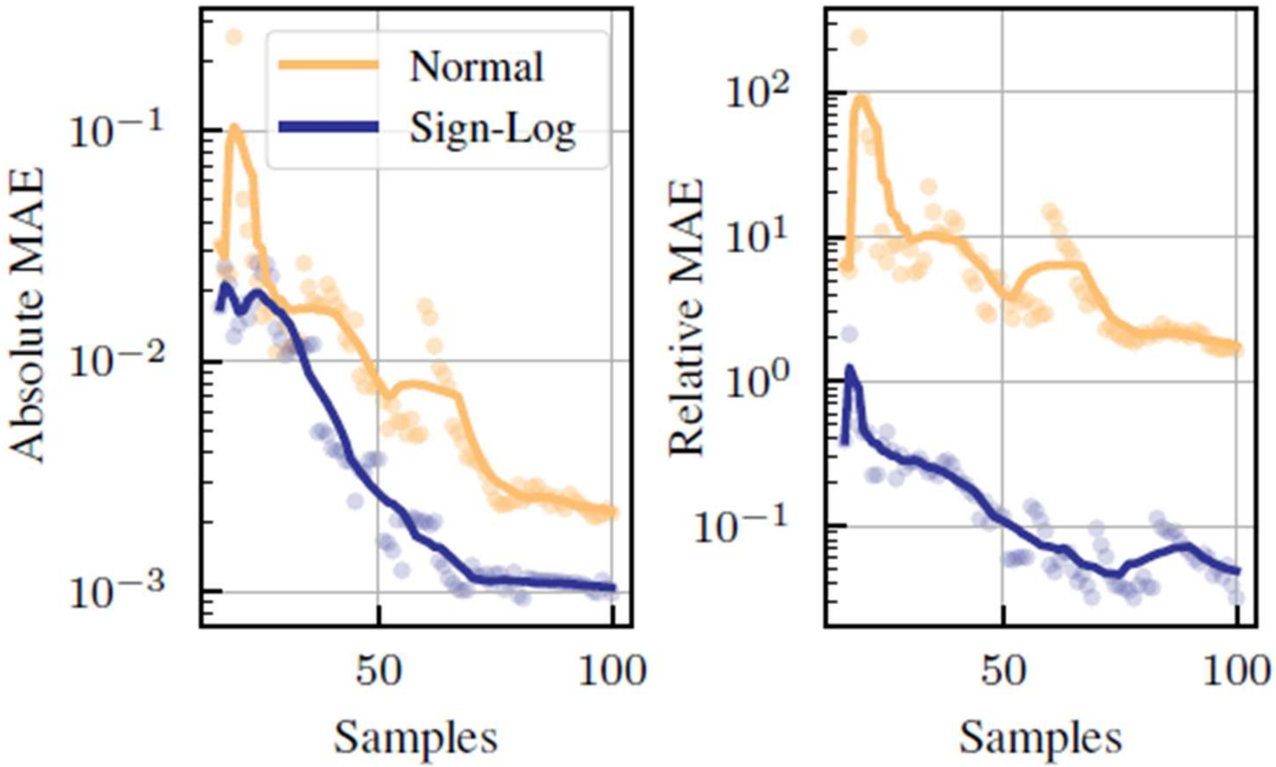
Results forward problem



Full adaptive sampling



Signed log


Normal
Sign-Log
Absolute MAE
10^{-1}
10^{-2}
10^{-3}
50
100
Samples
Relative MAE
10^{2}
10^{1}
10^{0}
10^{-1}
50
100
Samples

Gaussian Process Formulas

$$f(\mathbf{x}) \sim \mathrm{GP}(\mu(\mathbf{x}), \Sigma(\mathbf{x}, \mathbf{x}')), \text{with} \tag{15}$$

$$\mu(\mathbf{x}) = \mathbb{E}(f(\mathbf{x})) \tag{16}$$

$$\Sigma(\mathbf{x}, \mathbf{x}') = K(\mathbf{x}, \mathbf{x}') + \mathbf{I}\omega \tag{17}$$

$$K(\mathbf{x}, \mathbf{x}') = \sigma^2 \exp(-\frac{1}{2l^2}(\mathbf{x} - \mathbf{x}')^2), \tag{18}$$

Non-Stationary Gaussian Process Formulas

$$K_f(\mathbf{x}, \mathbf{x}') = \sigma(\mathbf{x})\sigma(\mathbf{x}')\sqrt{\frac{2l(\mathbf{x})l(\mathbf{x}')}{l(\mathbf{x})^2 + l(\mathbf{x}')^2}} \times \exp\left(-\frac{(\mathbf{x}-\mathbf{x}')^2}{l(\mathbf{x})^2 + l(\mathbf{x}')^2}\right). \tag{23}$$

$$\log(l(\mathbf{x})) \equiv \tilde{l}(\mathbf{x}) \sim \mathrm{GP}(\mu_l, K_l(\mathbf{x}, \mathbf{x}')) \tag{19}$$

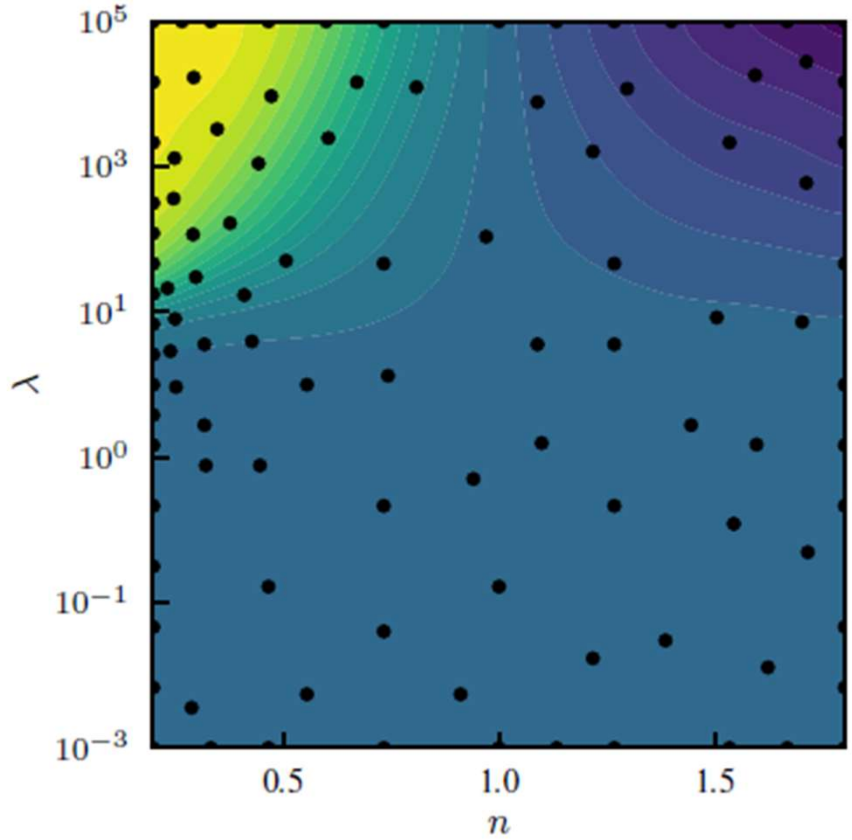
$$\log(\sigma(\mathbf{x})) \equiv \tilde{\sigma}(\mathbf{x}) \sim \mathrm{GP}(\mu_\sigma, K_\sigma(\mathbf{x}, \mathbf{x}')) \tag{20}$$

$$\log(\omega(\mathbf{x})) \equiv \tilde{\omega}(\mathbf{x}) \sim \mathrm{GP}(\mu_\omega, K_\omega(\mathbf{x}, \mathbf{x}')) \tag{21}$$

$$K_c(\mathbf{x}, \mathbf{x}') = \alpha_c^2 \exp(-\frac{1}{2\beta_c^2}(\mathbf{x}-\mathbf{x}')^2),$$
$$c \in \{l, \sigma, \omega\}$$

$$\boldsymbol{\theta} = (\mu_l, \mu_\sigma, \mu_\omega, \alpha_l, \alpha_\sigma, \alpha_\omega, \beta_l, \beta_\sigma, \beta_\omega)$$

Adaptive Sampling run



Total error

$$\sigma^2 = \sigma^2_{\text{Carreau}} + \sigma^2_{\text{FEM}} + \sigma^2_{\text{GP}} + \sigma^2_{\text{experiment}}.$$

$$\sigma^2_{\text{experiment}} = \frac{\sum_i (v_i - \bar{v})^2}{n-1}.$$

$$\sigma^2_{\text{FEM}} = (v_{\text{fine}} - v_{\text{inverse}})^2,$$

$$\text{MAE} = \frac{1}{N}\sum_{i=1}^{N} |\mathbf{y}_{\text{true}}(\mathbf{x}) - \mathbf{y}_{\text{pred}}(\mathbf{x})|,$$