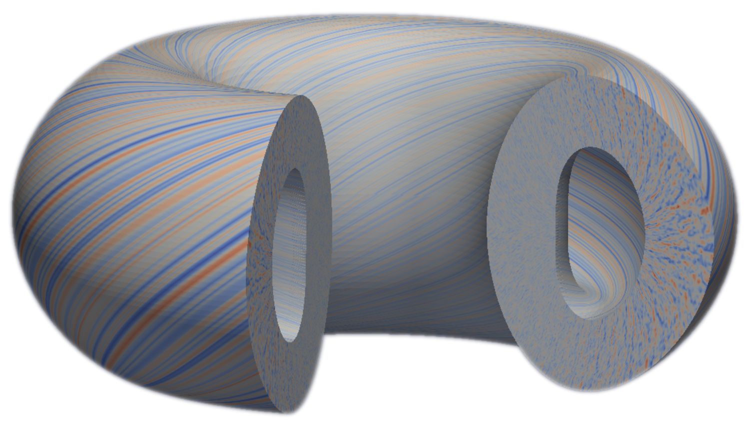
Evaluating imprecise probabilities in fusion plasma surrogates using conformal prediction



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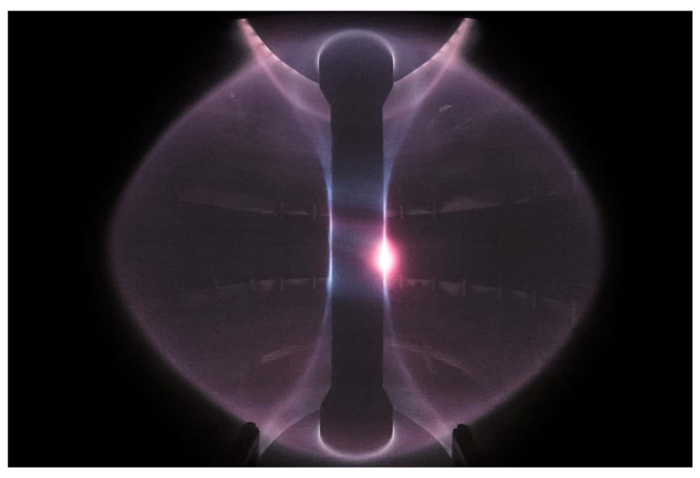
Motivation

Fusion plasmas are highly non-linear and turbulent systems, and often require many hours on high performance computers to evaluate. Reliable surrogate models are therefore a must for integrated modelling, design optimisation, and uncertainty quantification. Due to this cost, we must build surrogates with as few data points as possible, and models may struggle to fit accurately to these complicated physical responses. We therefore seek reliable error estimation in surrogate modelling.

Instabilities in tokmak plasmas

Micro-tearing modes (MTMs) are a type of linear micro-instability that can grow in (mainly) spherical tokamaks. MTM Turbulence is highly detrimental to tokamak confinement and performance. Modelling required to understand and create scenarios to mitigate their effects. Needs to be fast (ms query time).



A simulation database of ∼3000 data points - Total: ∼1M CPUhrs

	Variable	Min	Max
inputs	k_y	0	1
	Safety factor	2	9
	Magnetic shear	0	5
	Electron density gradient	0	10
	β	0	0.3
	Electron collisionality	0	0.1
	Electron tempurature gradient	0	0.1
outputs	MTM classification label	0	1
	Frequency of dominant mode	-	-
	Growth rate of dominant mode	-	-

Surrogacy tasks:

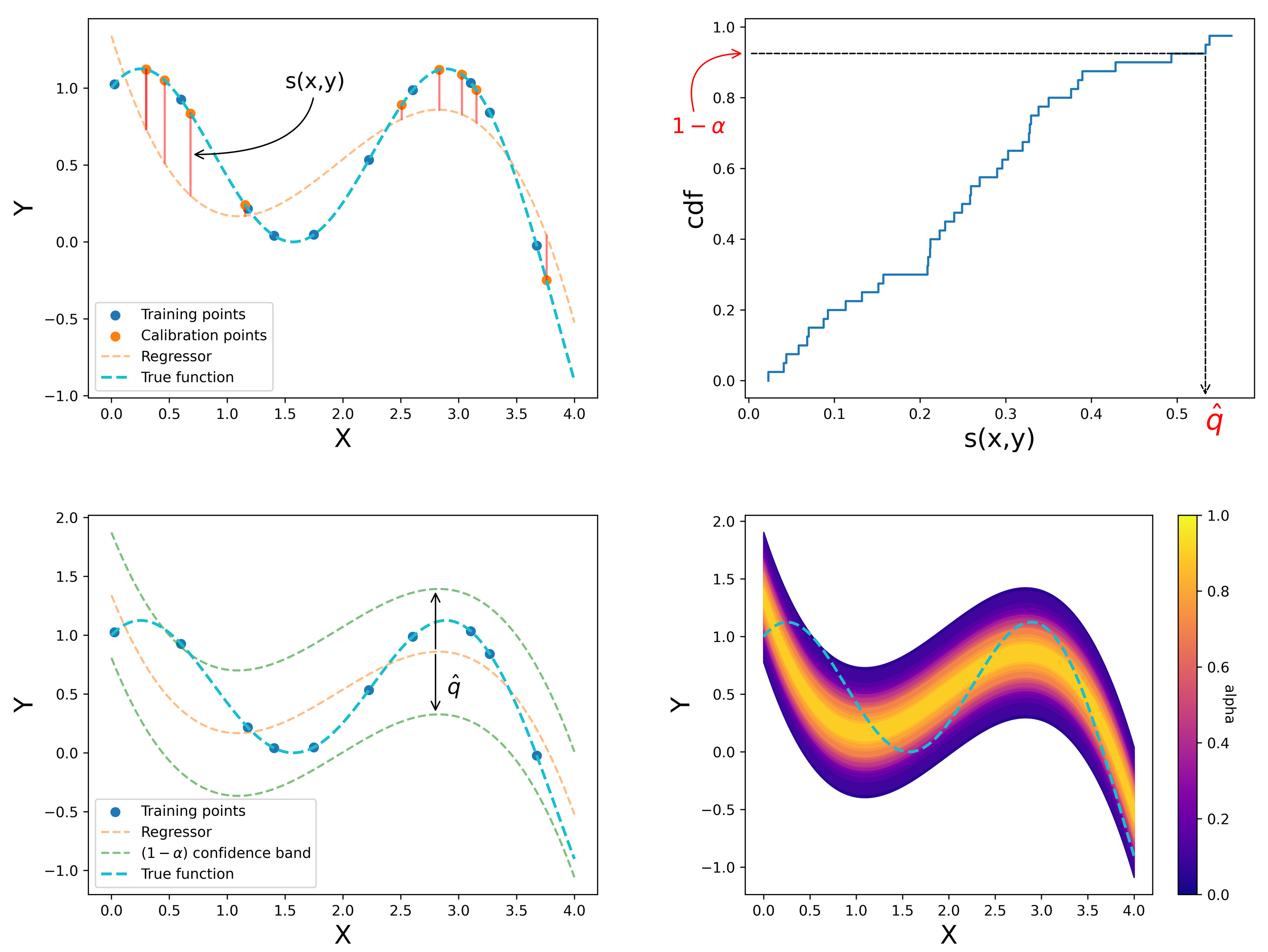
- Classify stability boundary of MTM and non-MTM
- In instable region, predict frequency and growth rates

Inductive conformal prediction (ICP)

Conformal prediction extends the point prediction $\hat{y}$ of a surrogate $\hat{f}$ to a prediction set $\mathbb{C}^\alpha$, giving the following marginal coverage guaranteed:

$$\mathbb{P}(Y_{n+1} \in \mathbb{C}^\alpha) \geq 1 - \alpha. \quad (1)$$

Under some assumptions, the method works irrespective of the selected machine learning model, data-set, and sample size. ICP also allows us to apply CP to pre-trained surrogate models.



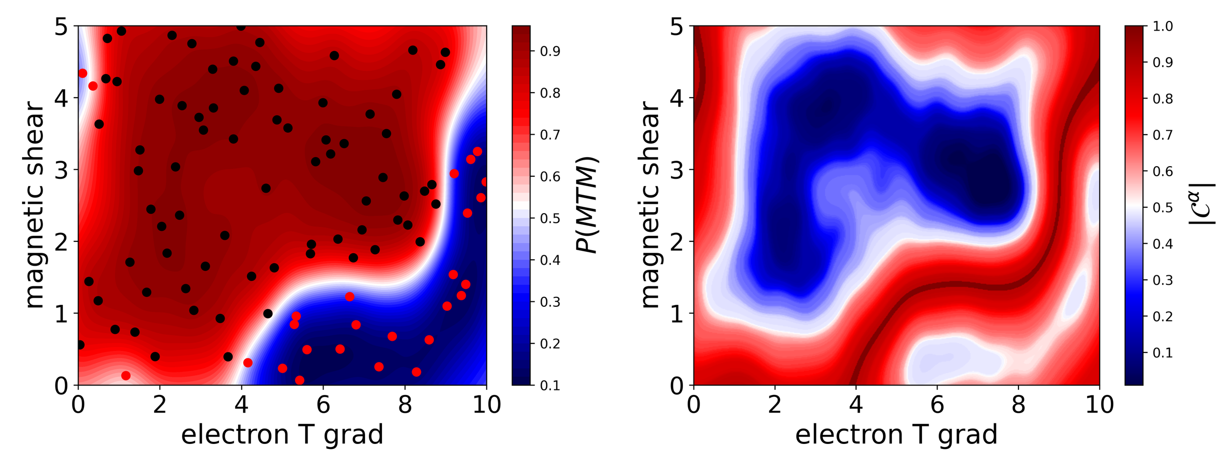
The above is a pictoral example of applying ICP to a simple regresson task. Panel a) Regressor (orange) compared to the true function at calibration points using a non-conformity score $s(x, y) = |y - \hat{f}(x)|$. Panel b) Distribution of non-conformity scores, and inverse evaluated at $1 - \alpha$. Panel c) Attained $(1 - \alpha)$ prediction set. Panel d) Nested prediction sets at all α-levels.

Surrogate before and after calibration

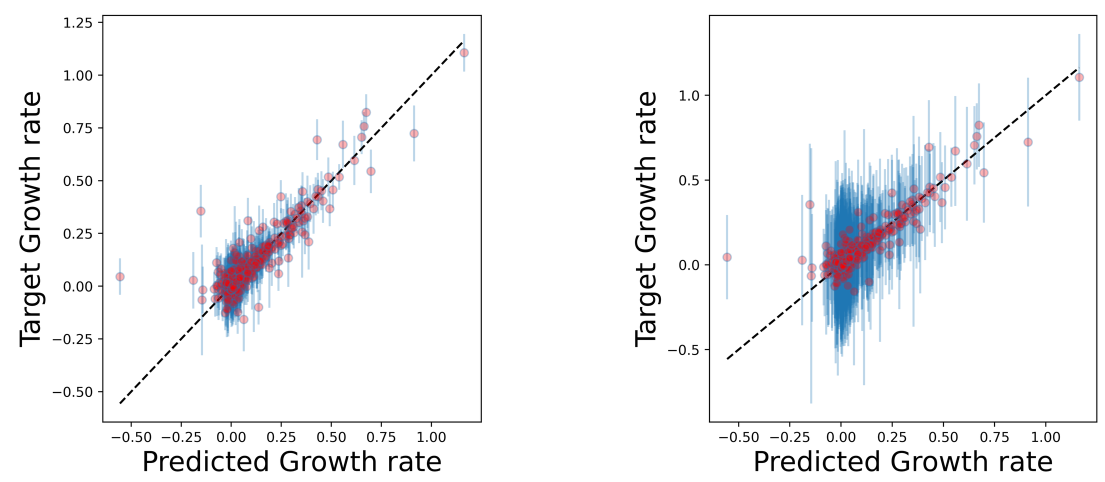
A Gaussian process is used throughout as the base machine learning model, for regression using a 1/2 Matern kernel, and a Bernoulli GP with 5/2 Matern kernel for classification. Data split: $n_{\text{train}} = 2000, n_{\text{cal}} = 500, n_{\text{val}} = 500$.

Before: After:

Classifier:



Regressor:

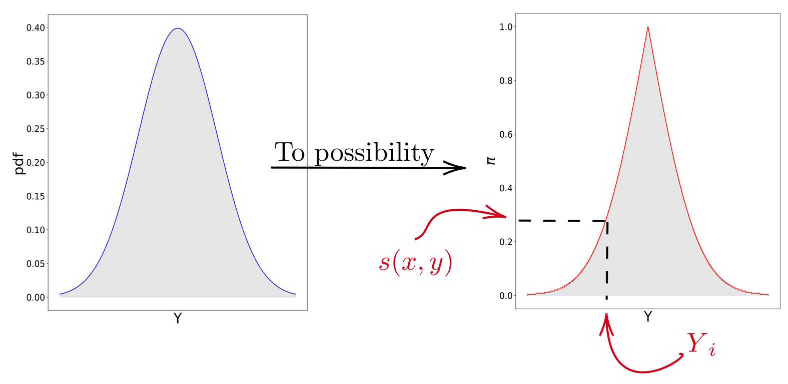


Classifier ($\hat{f} : \mathbb{R}^7 \to [0, 1]$):

$$s(x, y) = |y - \hat{f}(x)|$$

Regressor ($\hat{f} : \mathbb{R}^7 \to \mathrm{N}(\mu_X, \sigma_X)$):

$$s(x, y) = \begin{cases} 2F_Y(y|x) & \text{if } y \leq \mu(x) \\ 1 - 2F_Y(y|x) & \text{if } \mu(x) < y \end{cases}$$



How to deploy? Imprecise probabilities can help

But how do we use this for, e.g., uncertainty propagation, sensitivity analysis, reliability analysis, design optimisation, and coupled surrogates.

Drawbacks of CP for surrogate modelling

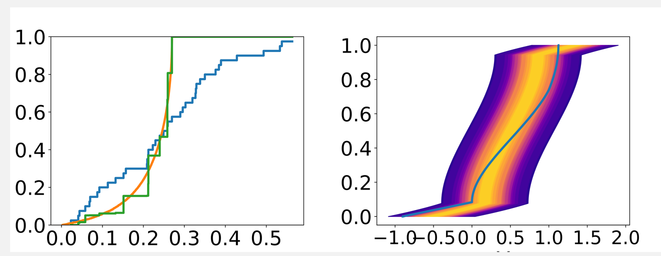
- No conditional coverage: $\mathbb{P}(Y_{n+1} \in \mathbb{C}^\alpha | X_{n+1}) \geq 1 - \alpha$ is not possible.
- Exchangeablity: training distribution and data uncertainty may be different. Uncertainty propagation and SA not obvious.
- No predictive distribution: how we compute with confidence intervals?

Possibility theory

- Nested prediction sets can be interpreted as a possibility distribution
- $\mathbb{C}^\alpha$ are the focal elements of a nested random set, with plausability countour $\pi(y)$
- Could allow us to evaluate failure probabilities $\overline{\mathbb{P}}(U_f) = \sup_{x \in U_f} \pi_X(x)$

Covariate shifting

If relative likelihoods are known, we can evaluate a different distribution



References

[1] Leonardo Cella and Ryan Martin. Valid inferential models for prediction in supervised learning problems. In ISIPTA, pages 72–82. PMLR, 2021

[2] Ryan J Tibshirani, Rina Foygel Barber, Emmanuel Candes, and Aaditya Ramdas. Conformal prediction under covariate shift. In NEURIPS, volume 32, 2019.