Robust and Conjugate Spatio-Temporal Gaussian Processes

William Laplante
University College London

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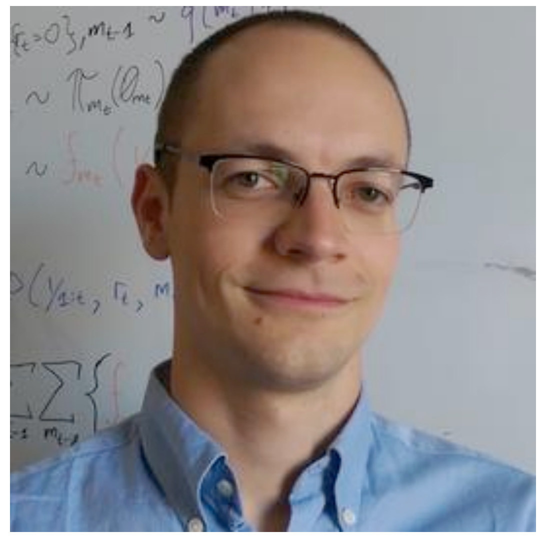
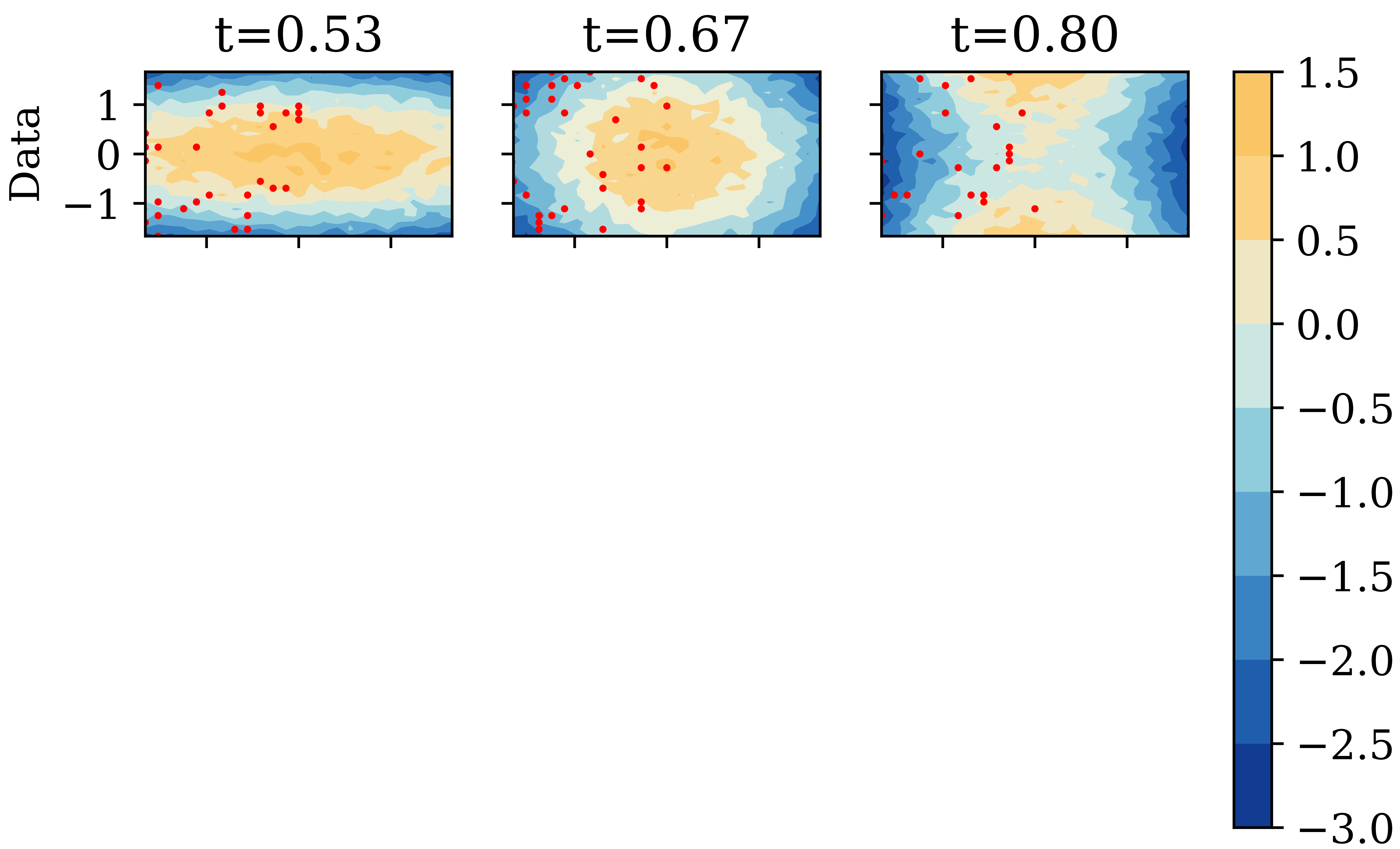


Jeremias Knoblauch
University College London

François-Xavier Briol
University College London

Preview...



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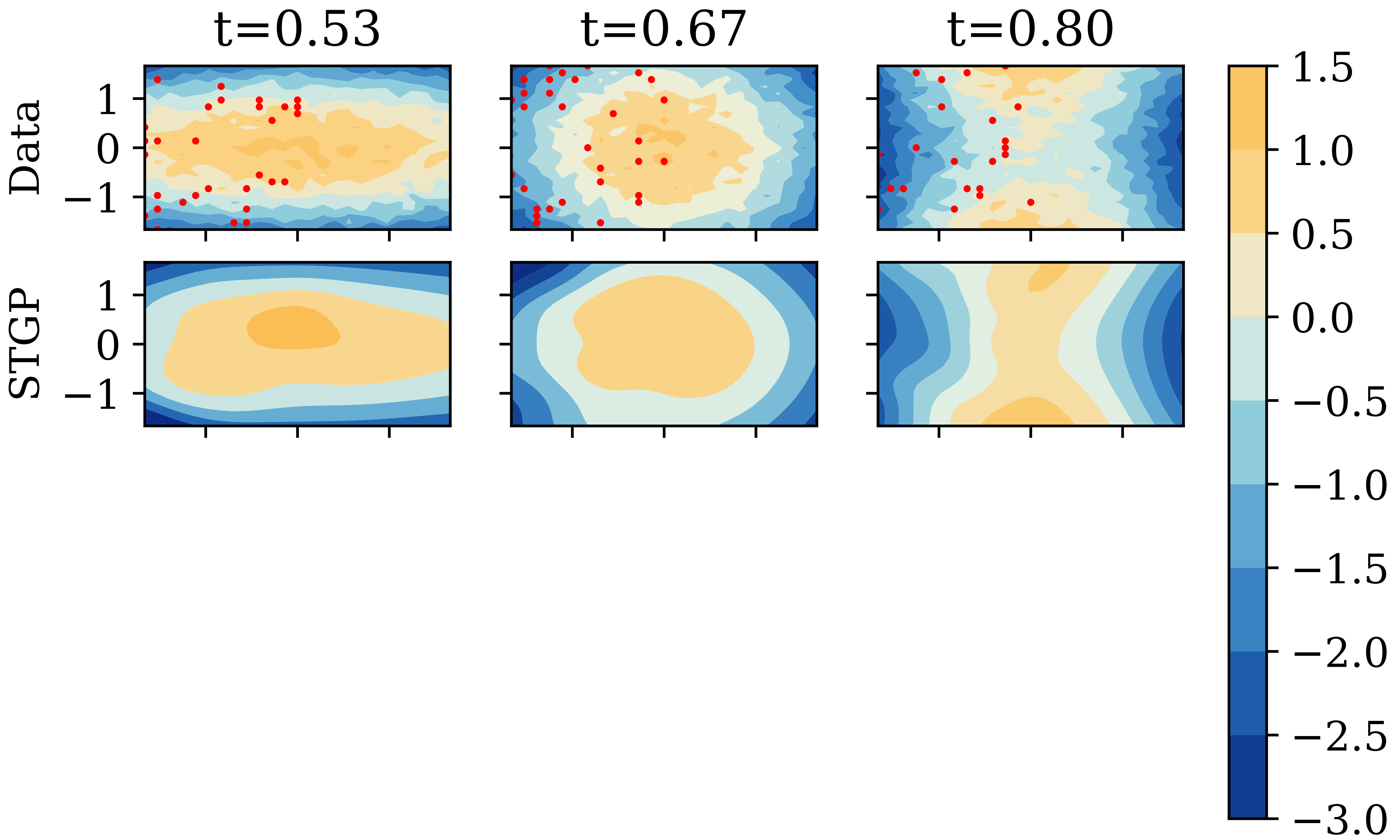
Baseline Method



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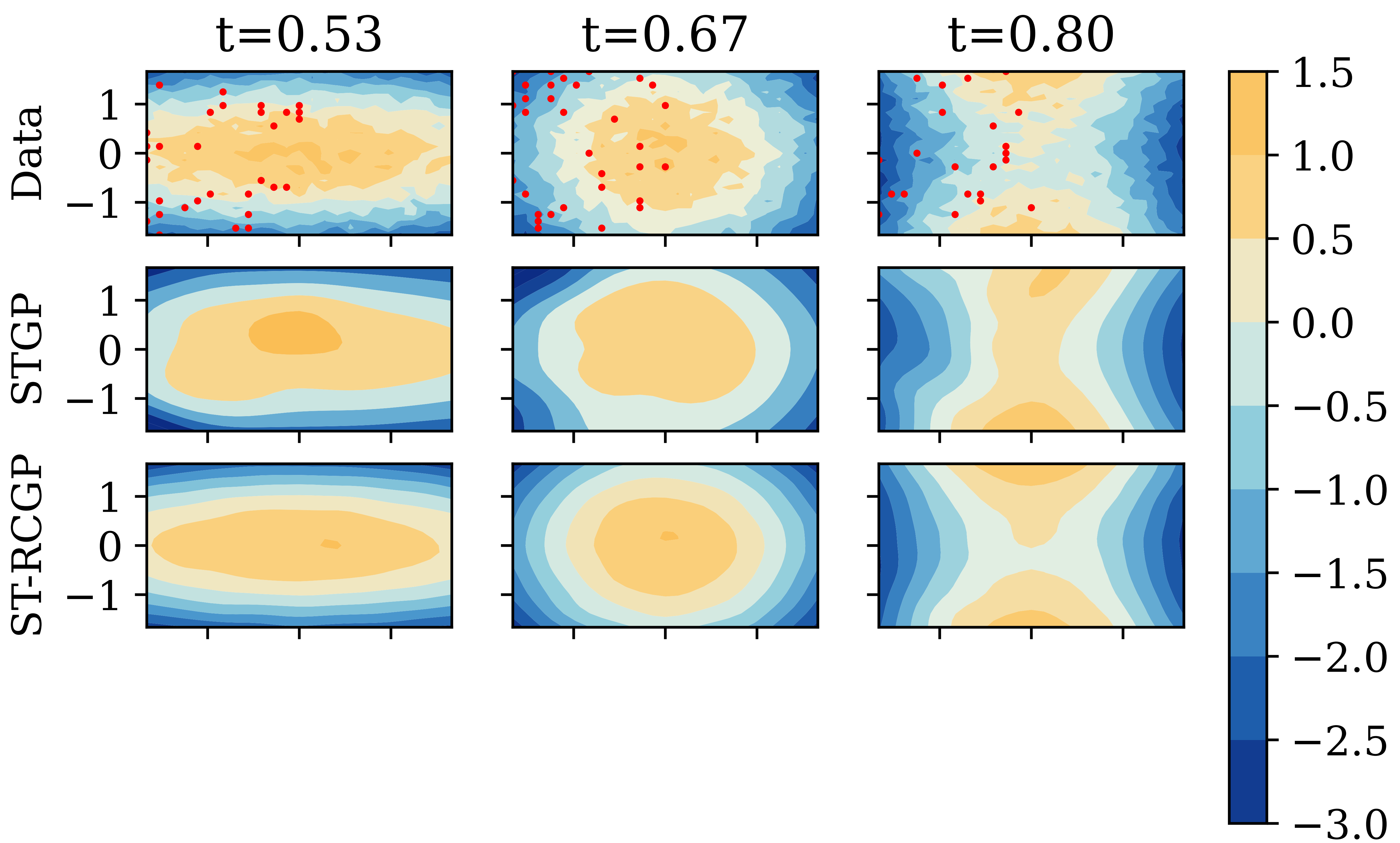

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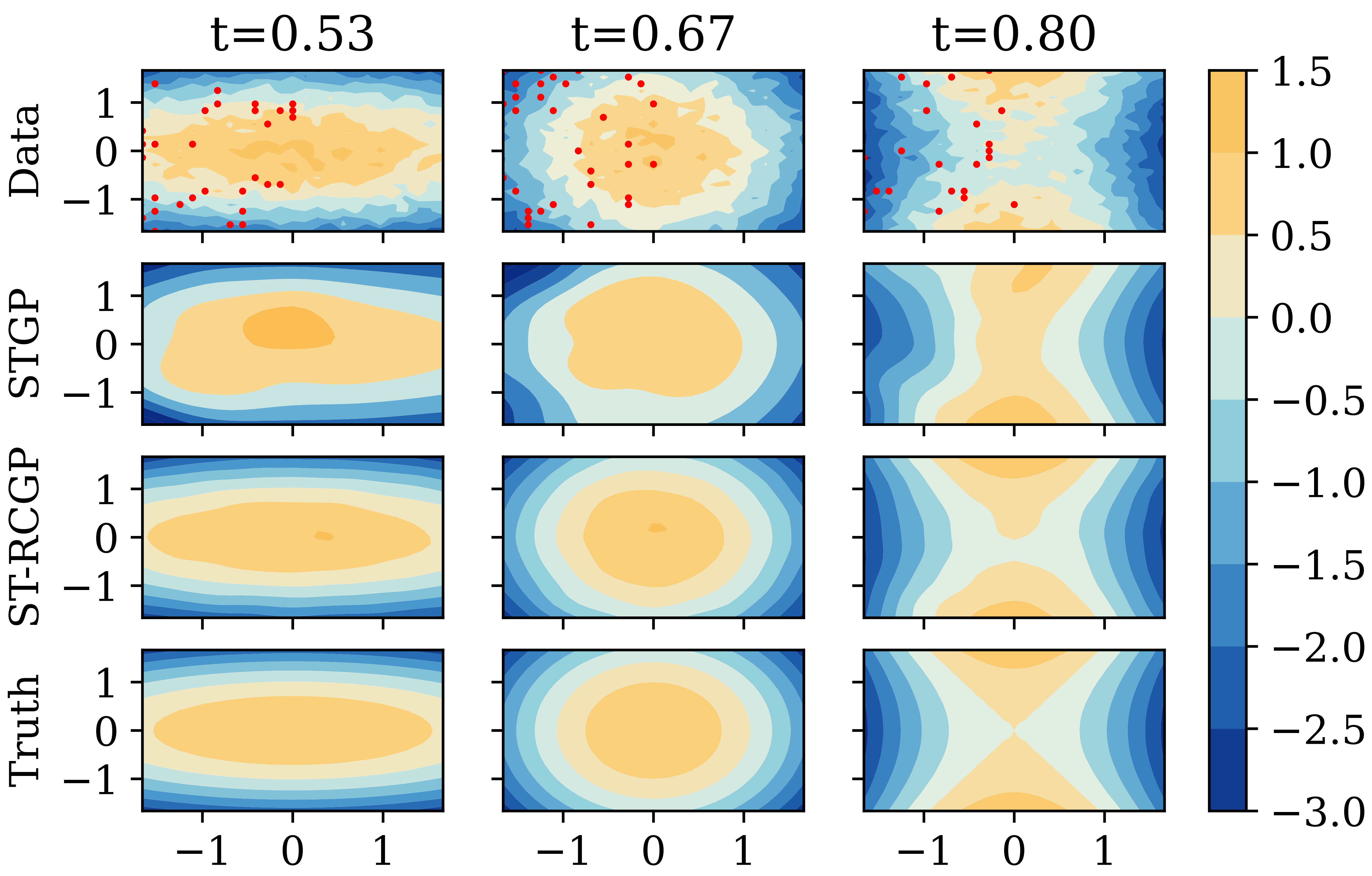

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Observations

$\mathcal{D} := \{\mathbf{x}_k, y_k\}_{k=1}^{N} \subseteq \mathcal{X} \times \mathcal{Y}$

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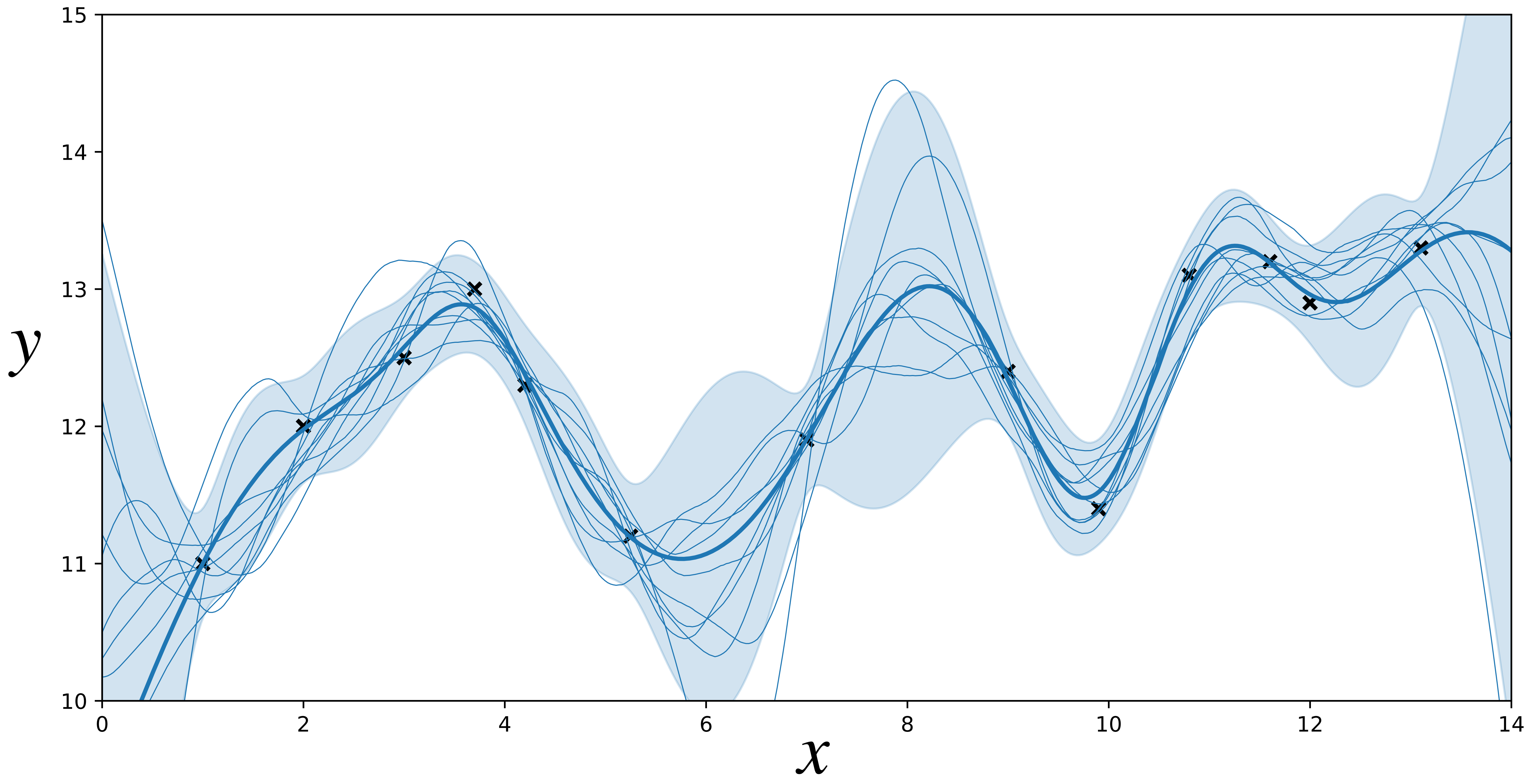

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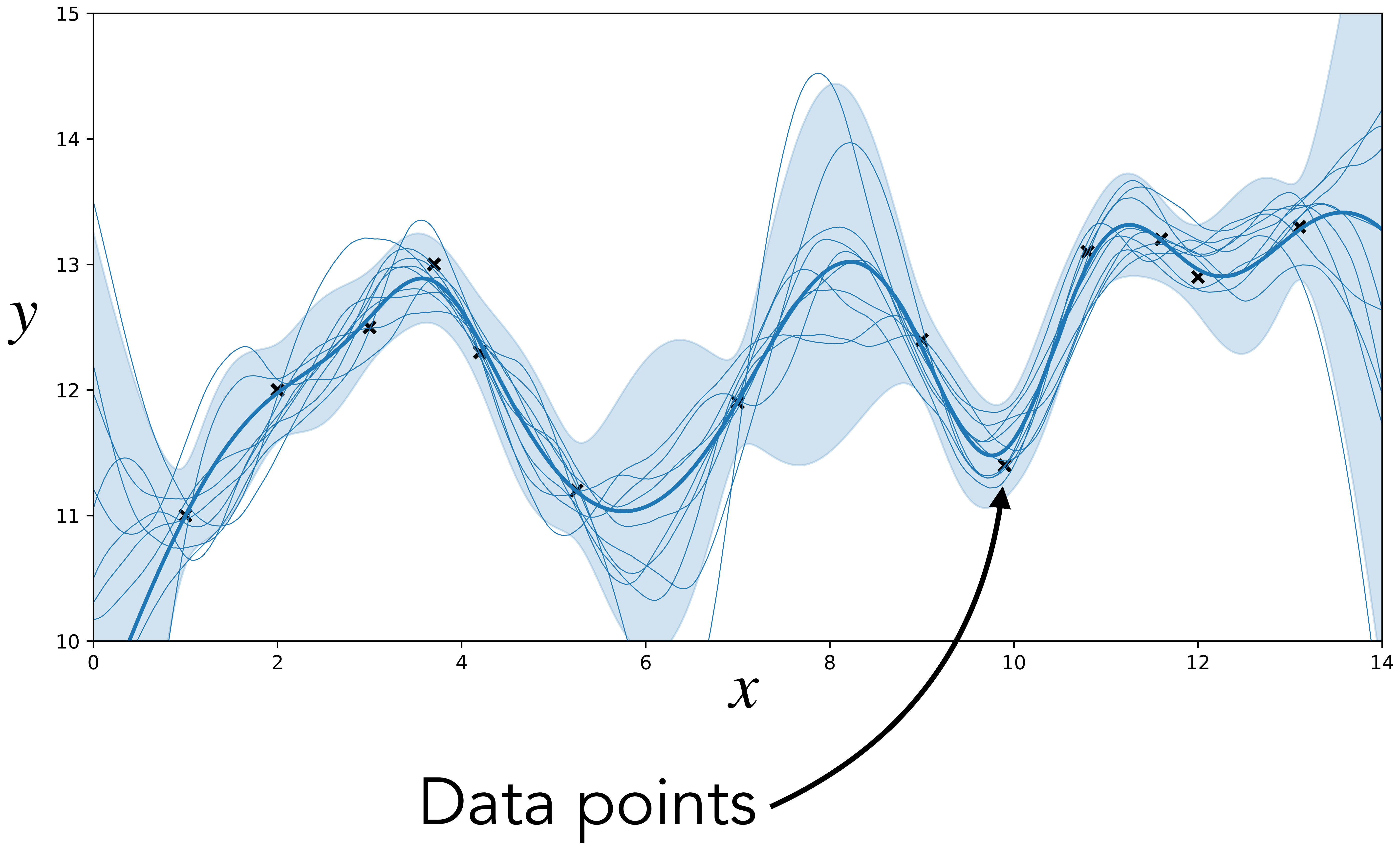

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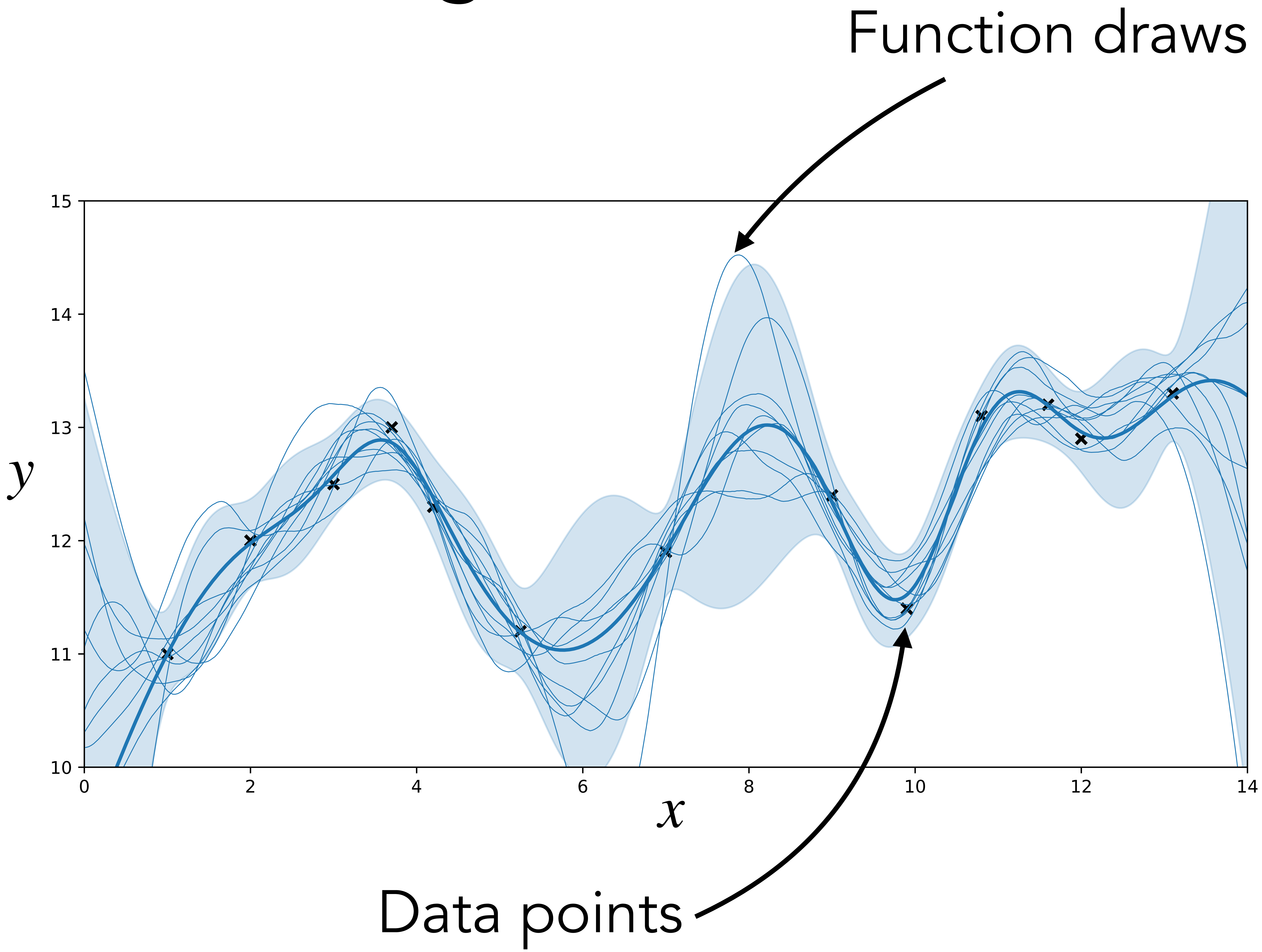

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Problem! $\mathcal{O}(N^3)$ cost…

Solution to GP Cost for Spatio-Temporal Inputs?

KALMAN FILTERING AND SMOOTHING SOLUTIONS TO TEMPORAL GAUSSIAN PROCESS REGRESSION MODELS

Jouni Hartikainen and Simo Särkkä

Aalto University
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ABSTRACT

In this paper, we show how temporal (i.e., time-series) Gaussian process regression models in machine learning can be reformulated as linear-Gaussian state space models, which can be solved exactly with classical Kalman filtering theory. The result is an efficient non-parametric learning algorithm, whose computational complexity grows linearly with respect to number of observations. We show how the reformulation can be done for Matérn family of covariance functions analytically and for squared exponential covariance function by applying spectral Taylor series approximation. Advantages of the proposed approach are illustrated with two numerical experiments.

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The underlying idea of efficient inference of Gaussian processes using a state space formulation is not new, because the contribution of Kalman's original 1960's article [3] was exactly this kind of re-formulation of the filtering problem of Wiener [4]. The idea of Bayesian modeling of unknown processes as Gaussian processes has also been widely utilized in communications theory [5, 6], but the philosophy differs slightly from that of Gaussian process regression in machine learning [7]. The idea of approximating

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Result: $\mathcal{O}(N^3)$ **cost becomes** $\mathcal{O}(N)$**!**

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State-Space Model

$$\mathbf{z}_0 \sim \mathcal{N}(\mathbf{0}, \mathbf{\Sigma}_0)$$
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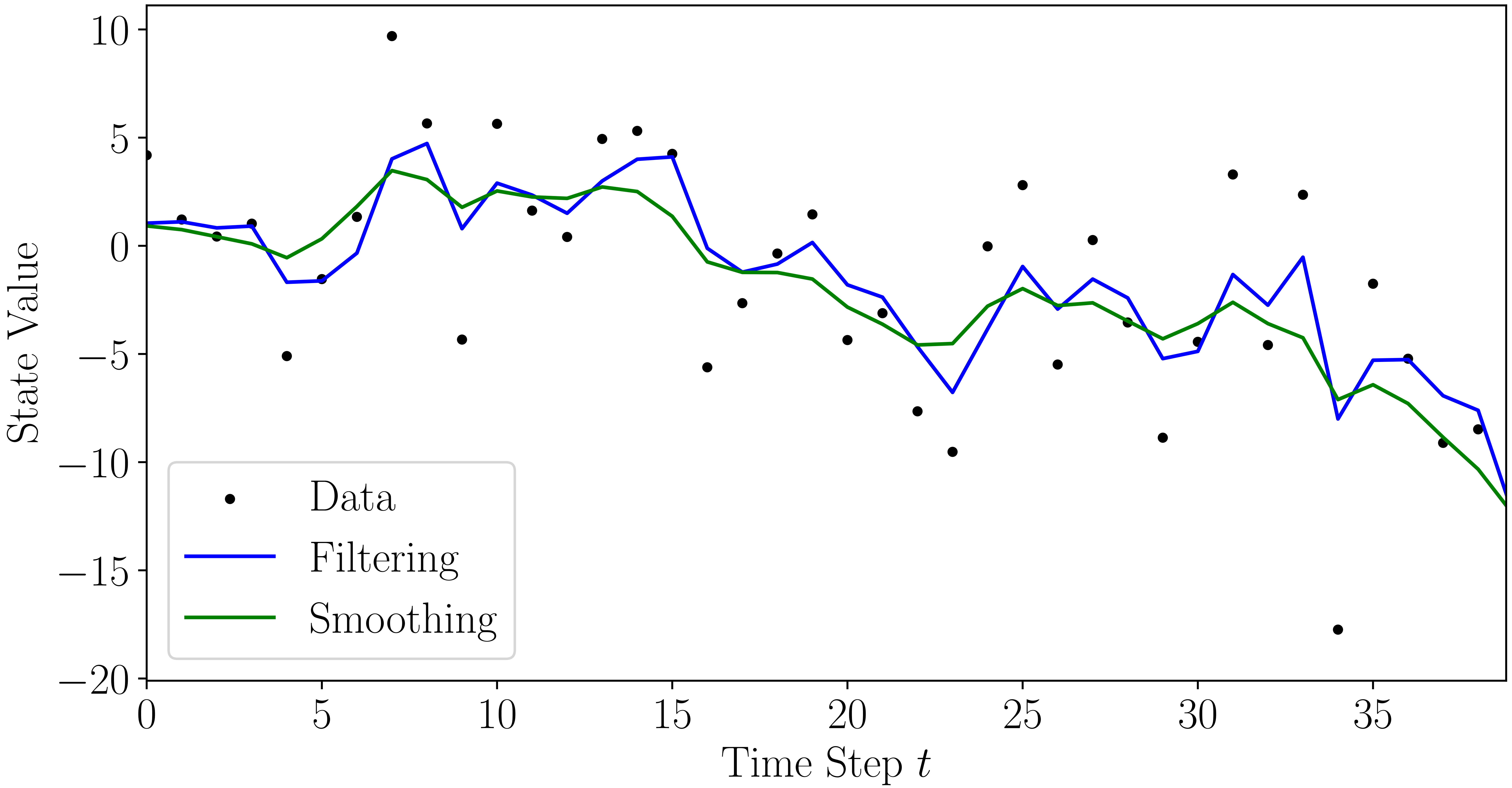
Obtain posterior predictive via **filtering & smoothing.**

Filtering & Smoothing



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Note on Smoothing: Throughout we use the Rauch-Tung-Striebel (RTS) smoother. Closed-form, for linear Gaussian models

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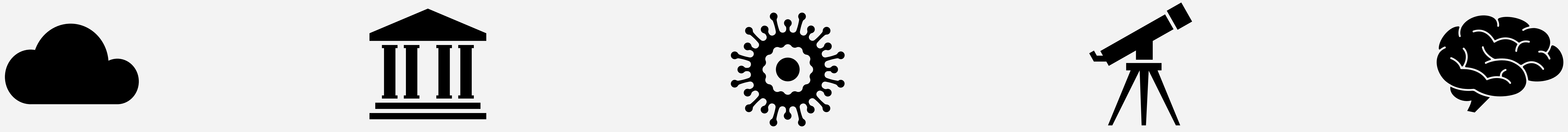
Applications



STGPs are great! What's the problem then?

Problems With STGPs

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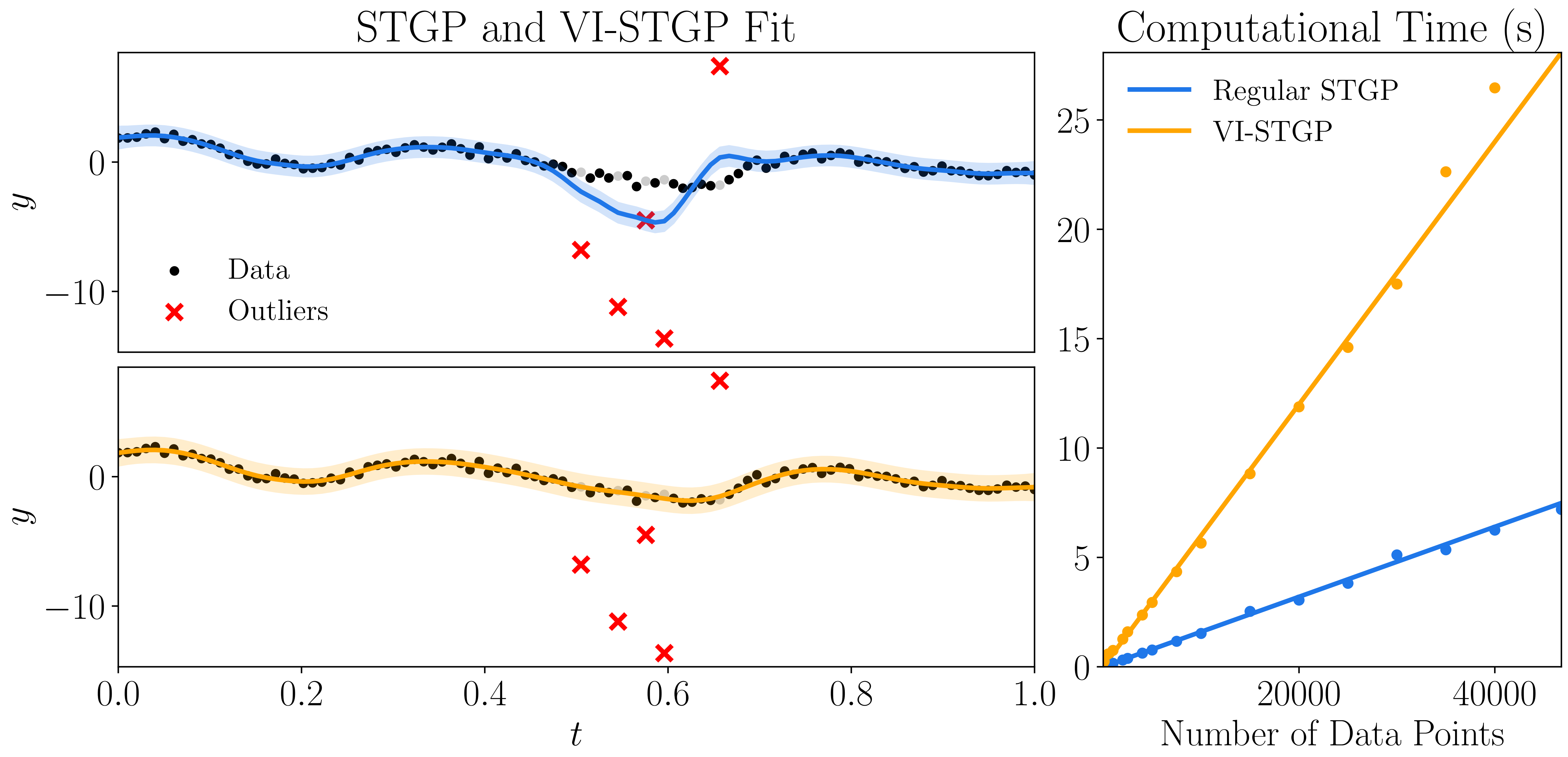
Tradeoff between robustness & comp. cost



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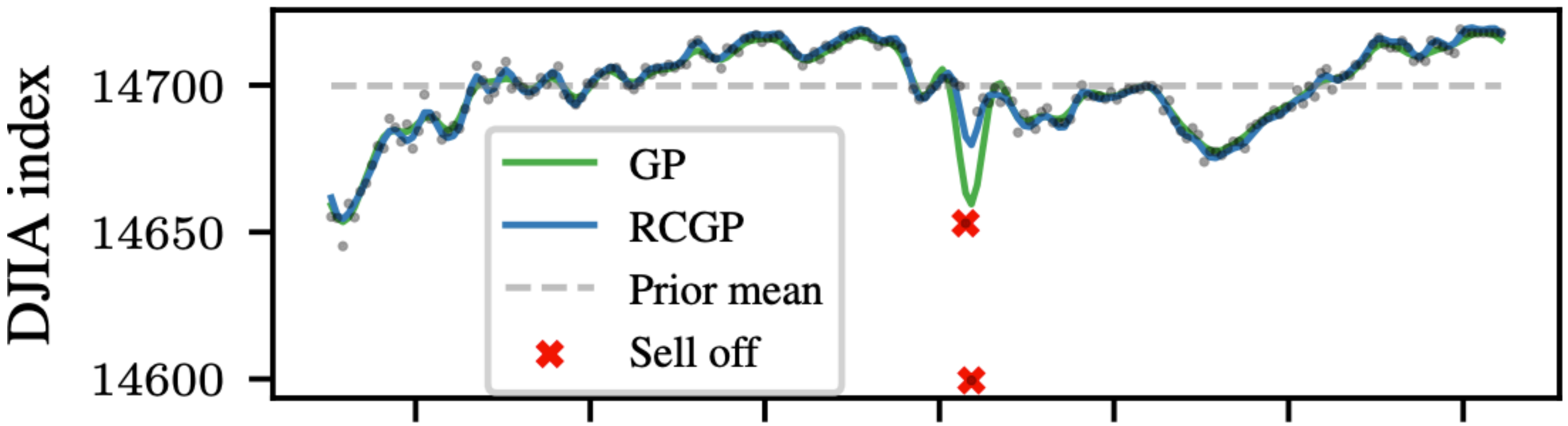

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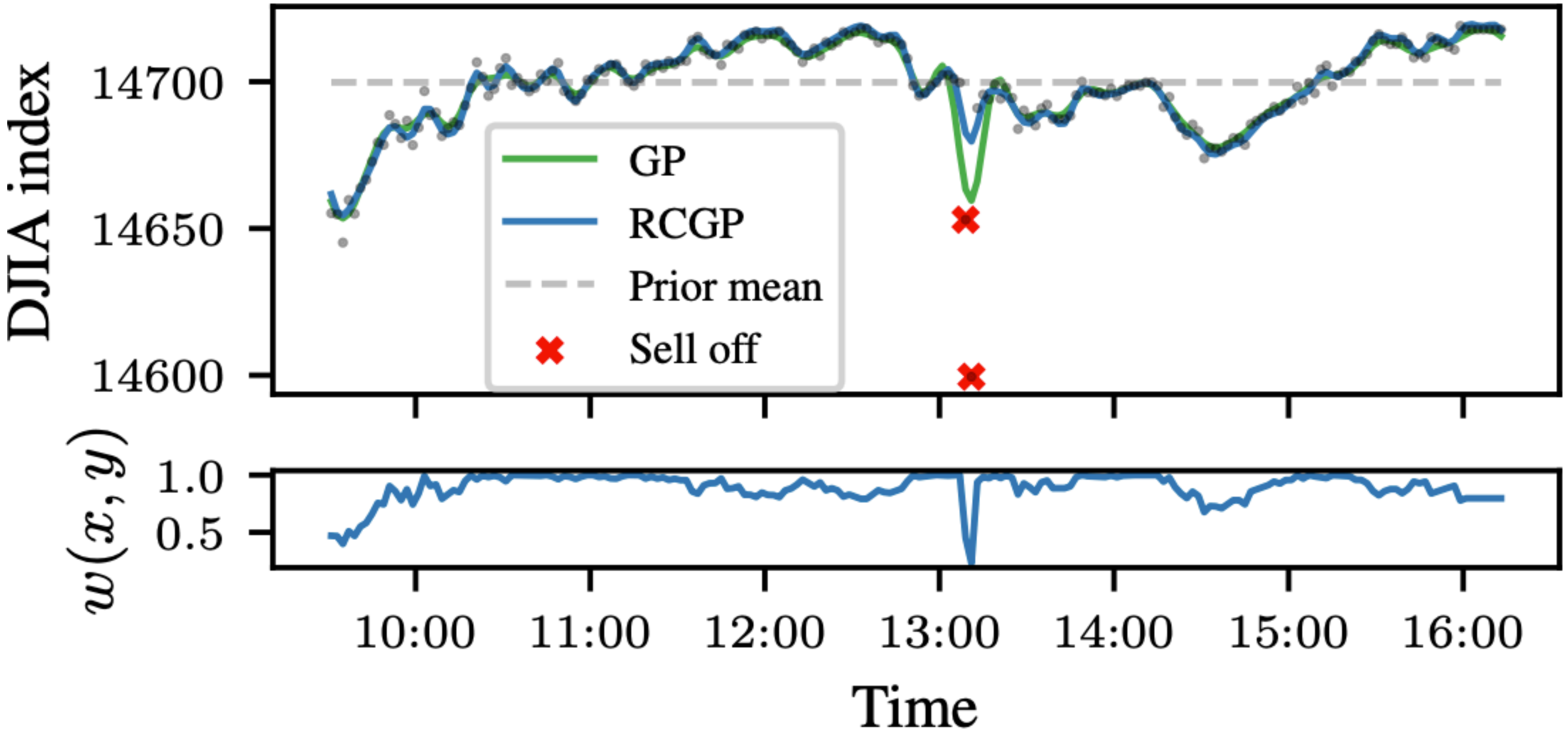

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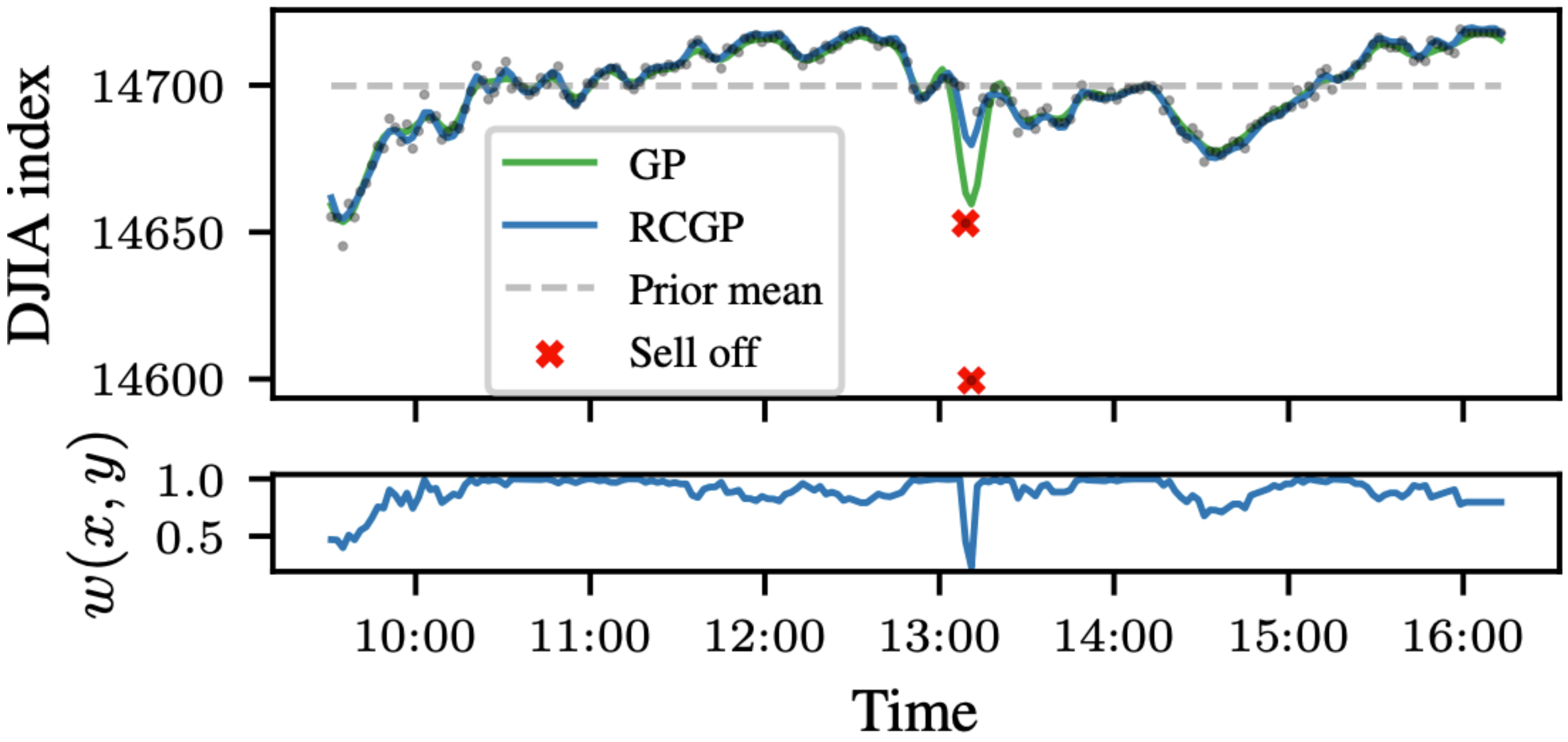


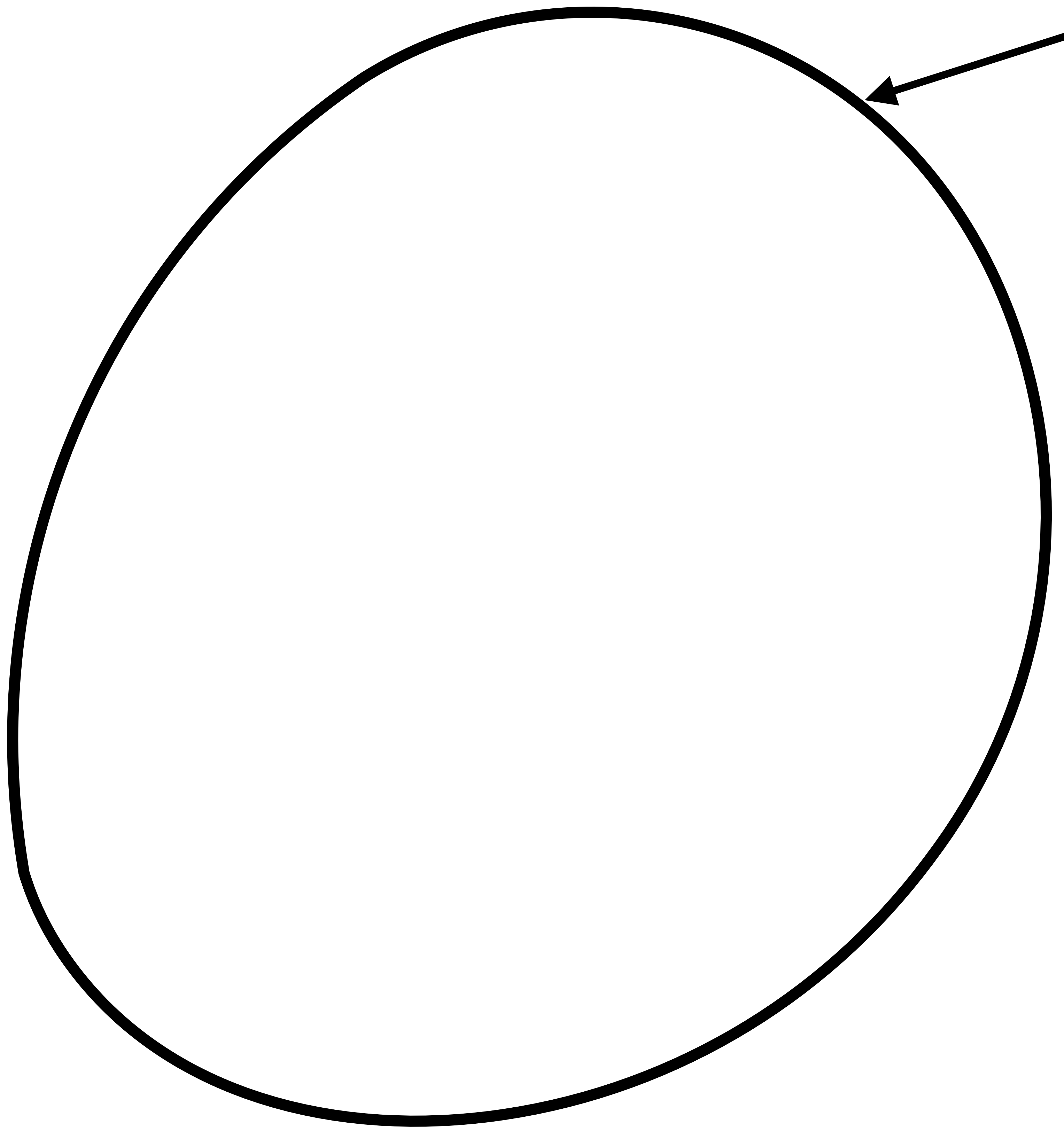
"Weight Function"

Key Idea: Introduce a weight function $w : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}^+$ that **downweights outliers**

RCGP's backbone: Generalised Bayesian Inference

$$\{\mathscr{B} : \underbrace{\mathscr{P}(\mathscr{F})}_{\text{space of priors}} \times \overbrace{\mathbb{R}^N}^{\text{data space}} \to \underbrace{\mathscr{P}(\mathscr{F})}_{\text{space of posteriors}}\}$$

Possible belief updates



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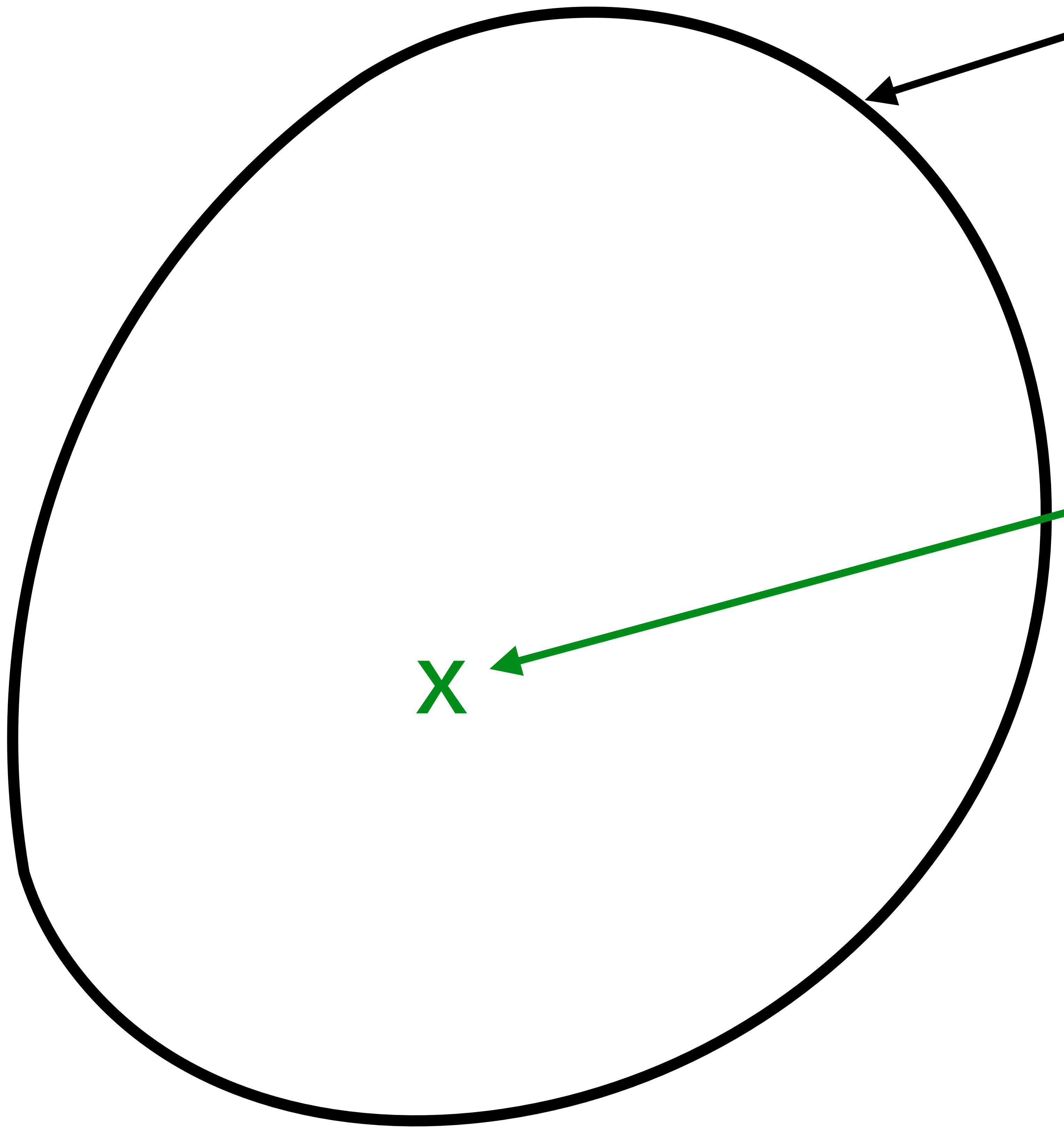

Standard Bayes' Posterior

$$\boxed{p(\mathbf{f} \,|\, \mathbf{y}, \mathbf{x}) \propto p(\mathbf{y} \,|\, \mathbf{f}, \mathbf{x}) \cdot p(\mathbf{f} \,|\, \mathbf{x})}$$

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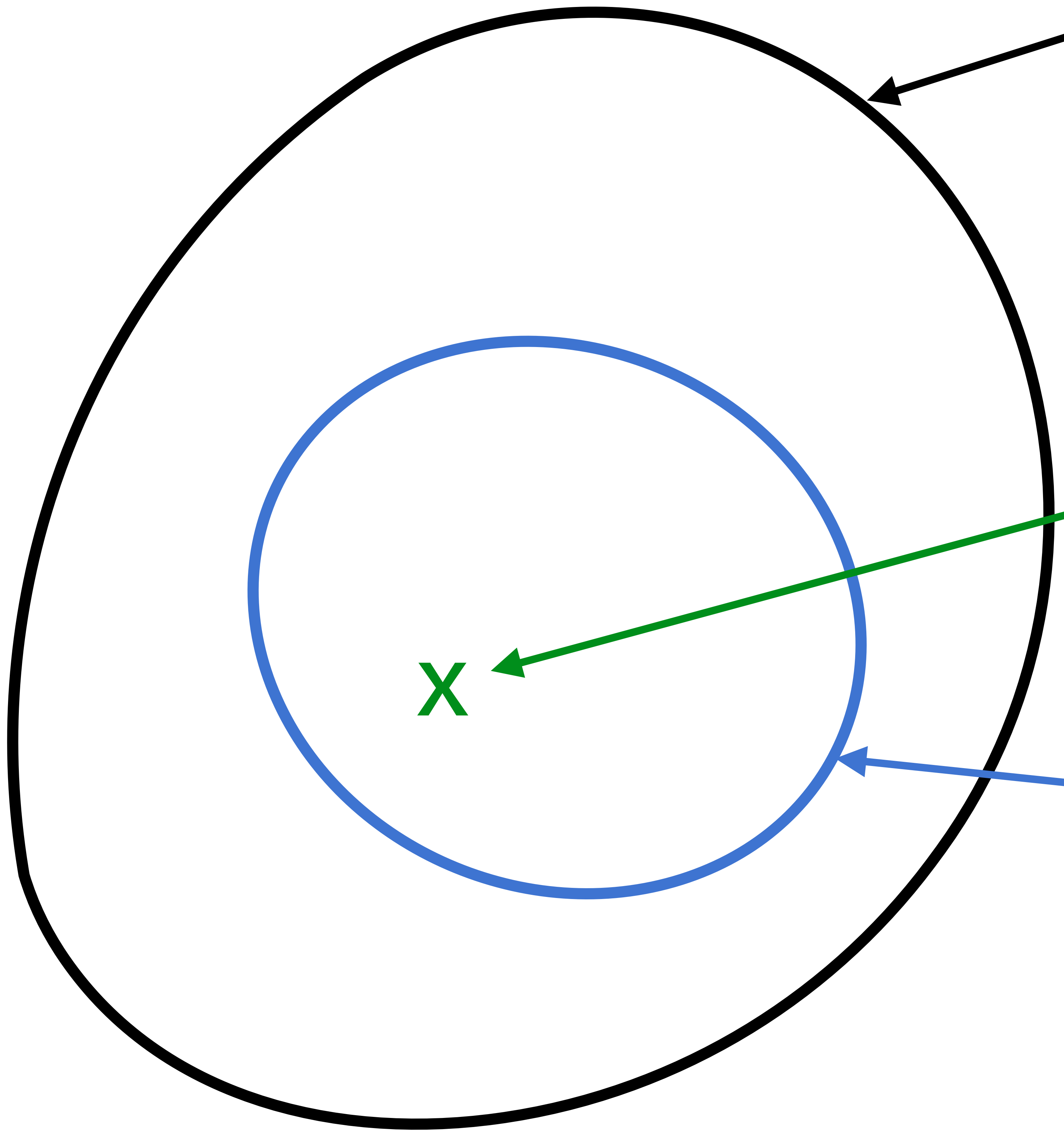

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Divergence-based losses are a good option! $D(\mathbb{P}, \mathbb{Q}) \geq 0$ $D(\mathbb{P}, \mathbb{Q}) = 0 \iff \mathbb{P} = \mathbb{Q}$

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Divergence Used in RCGP: (Weighted) Score-matching

Hyvärinen, A. (2006). Estimation of non-normalized statistical models by score matching. *Journal of Machine Learning Research*, *6*, 695–708.

Barp, A., Briol, F.-X., Duncan, A. B., Girolami, M., & Mackey, L. (2019). Minimum Stein discrepancy estimators. *Neural Information Processing Systems*, 12964–12976.

Altamirano, M., Briol, F.X. and Knoblauch, J. (2023). Robust and scalable bayesian online changepoint detection. *International Conference on Machine Learning* 642-663.

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Therefore, $p(\mathbf{f} \mid y_{1:N}, \mathbf{x}_{1:N})$ depends on weights (robust), and is conjugate with GP prior!

Key Idea of RCGPs: The Weight Function

Weight function used is the Inverse Multi-Quadratic (IMQ) kernel

$$w_{IMQ}(\mathbf{x}, y) := \beta\left(1 + \frac{(y - \gamma(\mathbf{x}))^2}{c(\mathbf{x})^2}\right)^{-1/2} \quad \longleftrightarrow \quad \text{“Statistically efficient”}$$

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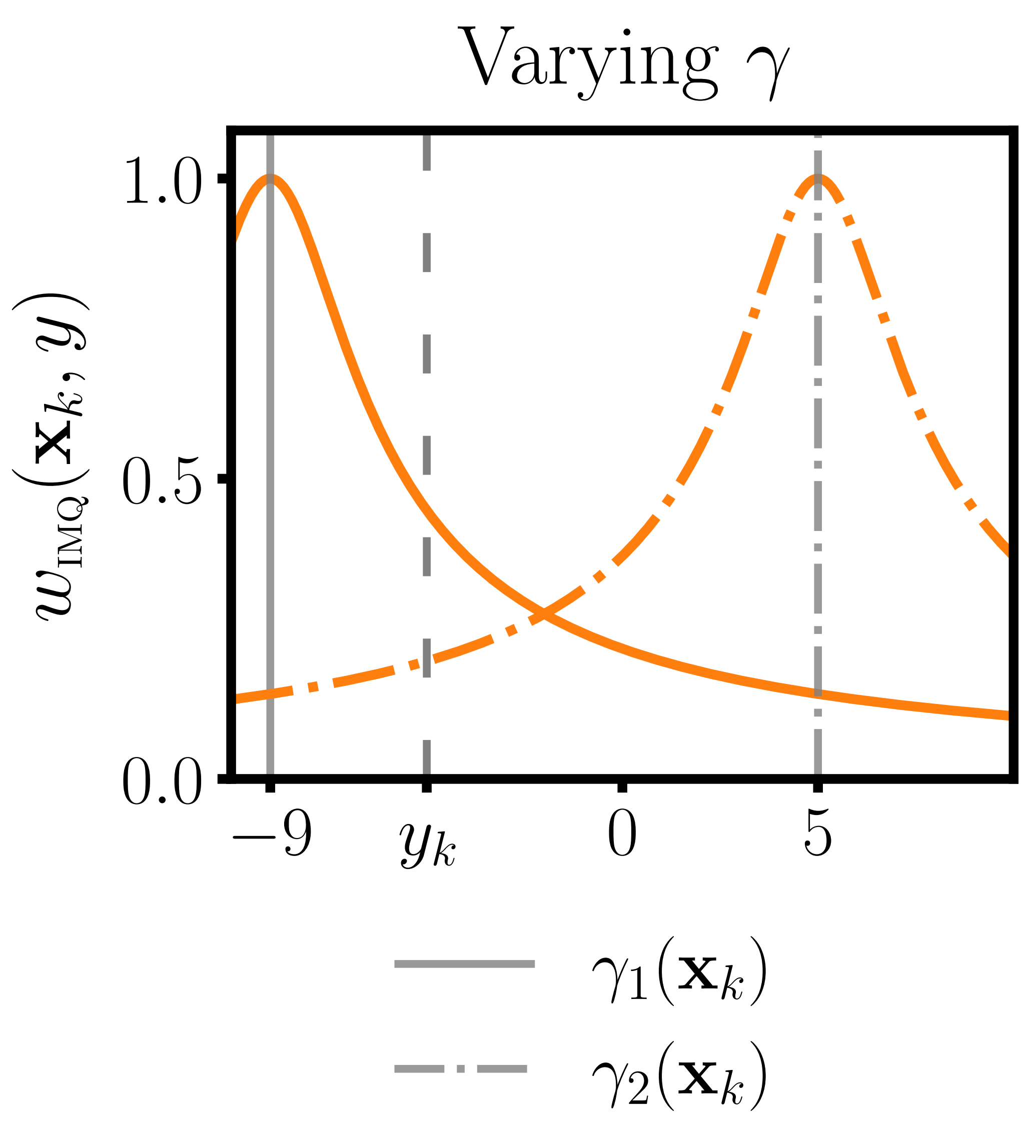

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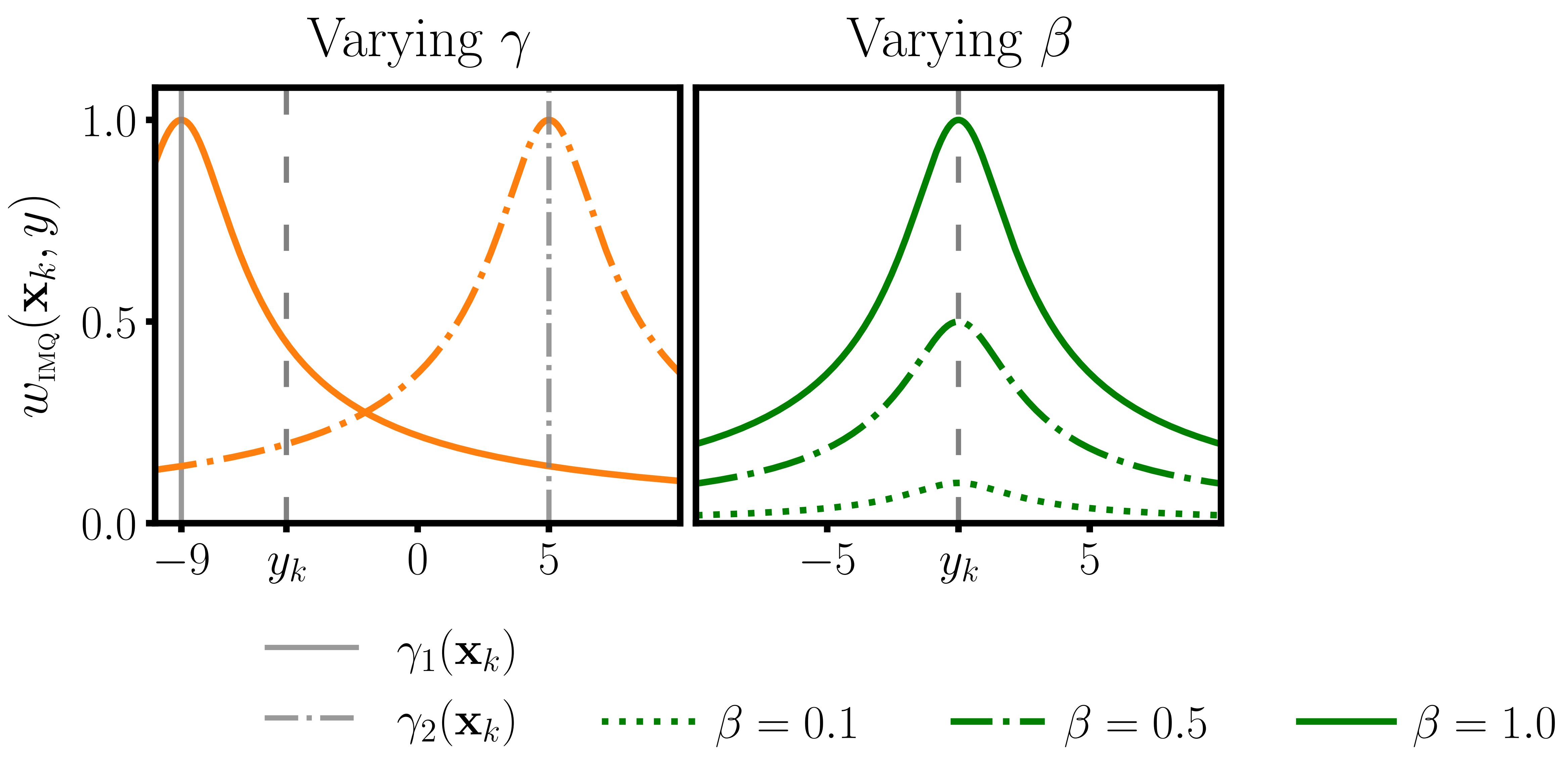

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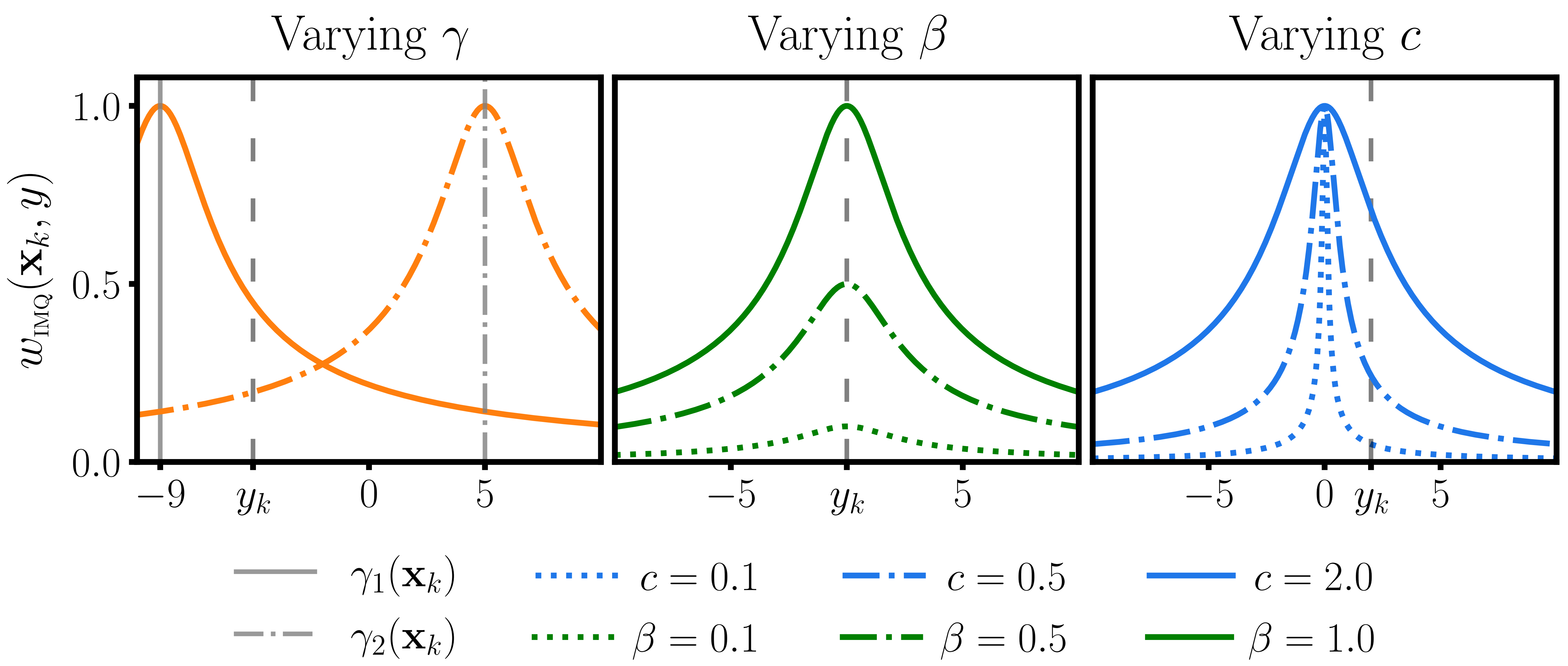

<u>Exact</u> Translation to State-Space Setting: ST-RCGP

Inference: Filtering Update Equations

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Before (STGP)

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Where $\mathbf{J}_{\mathbf{w}_k} := \operatorname{diag}\left(\frac{\sigma^2}{2}\mathbf{w}_k^{-2}\right)$ and $\hat{\mathbf{f}}_{w_k} := \hat{\mathbf{f}}_k + \sigma^2 \nabla_y \log(\mathbf{w}_k^2)$

For weights $\mathbf{w}_k = (w(\mathbf{x}_{k,1}, y_{k,1}), \ldots, w(\mathbf{x}_{k,n_s}, y_{k,n_s}))^\top$

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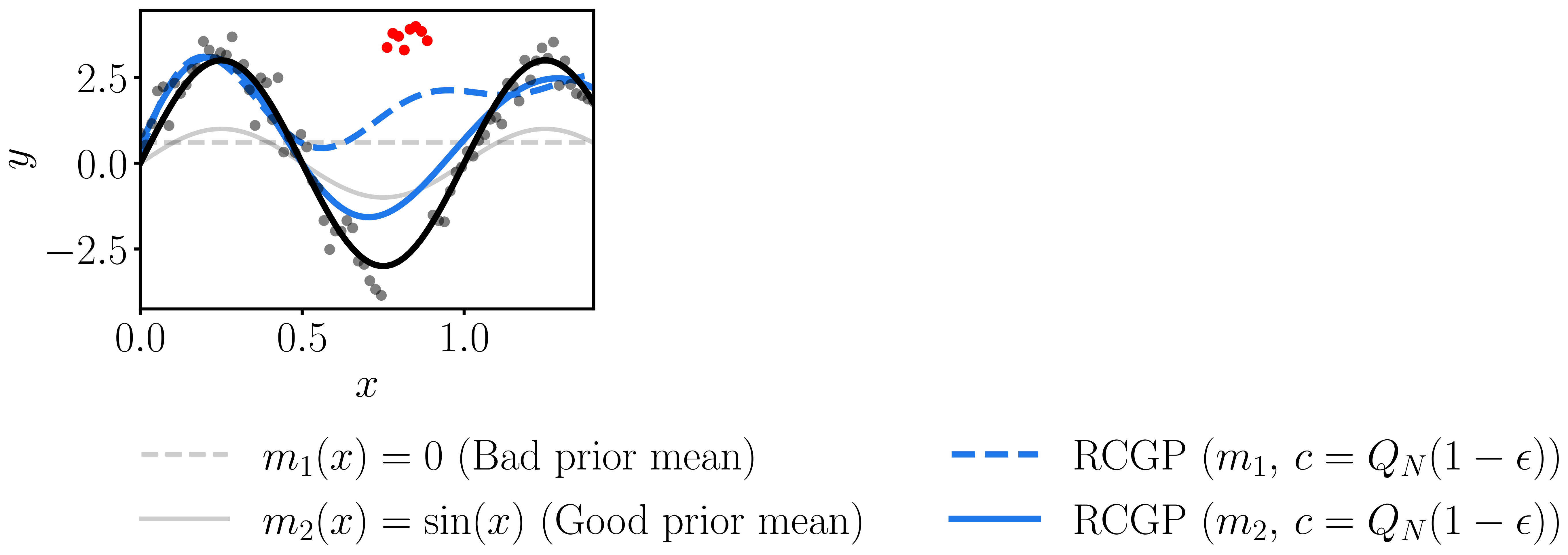

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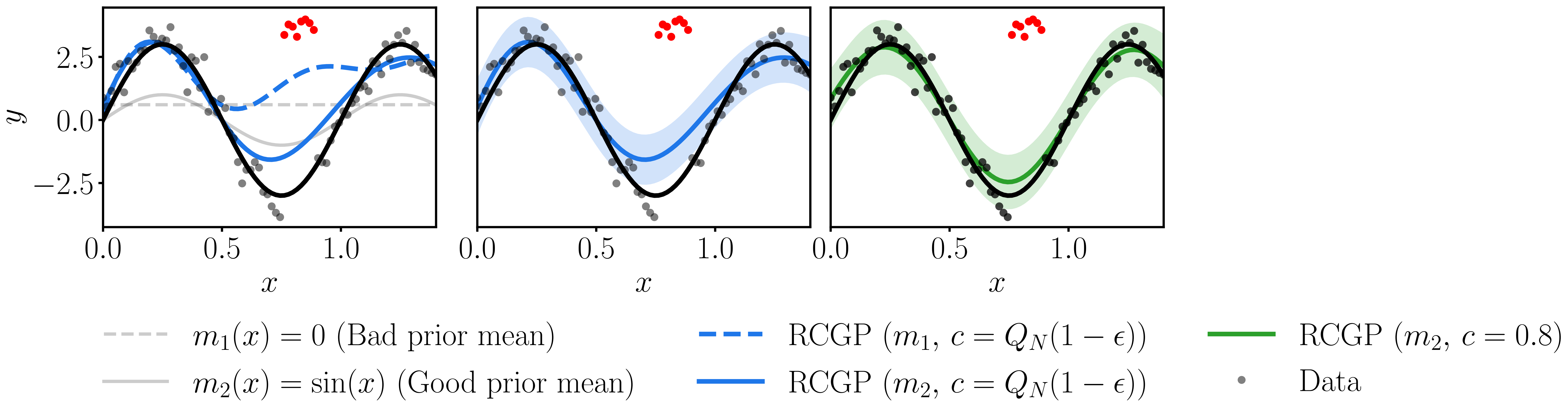

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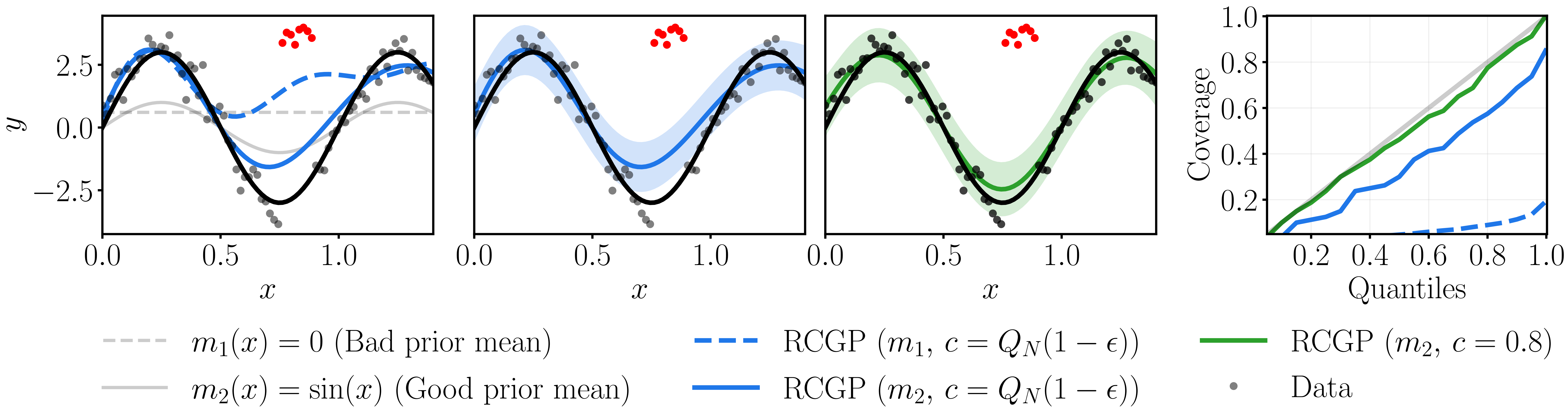
Issue #3: Poor uncertainty quantification (when parameters are wrongly specified)



The Remedy Enabled by Sequential Inference

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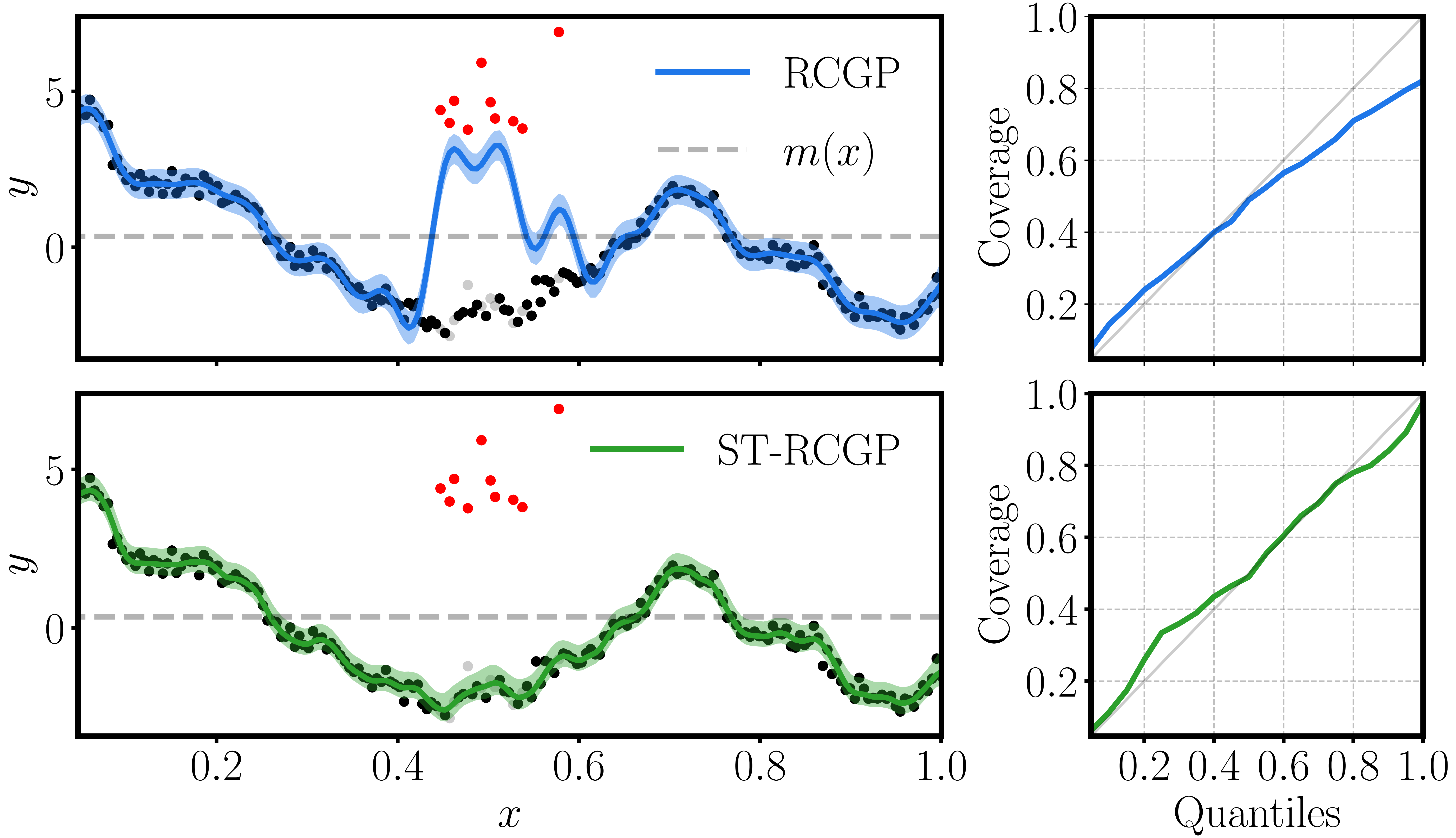
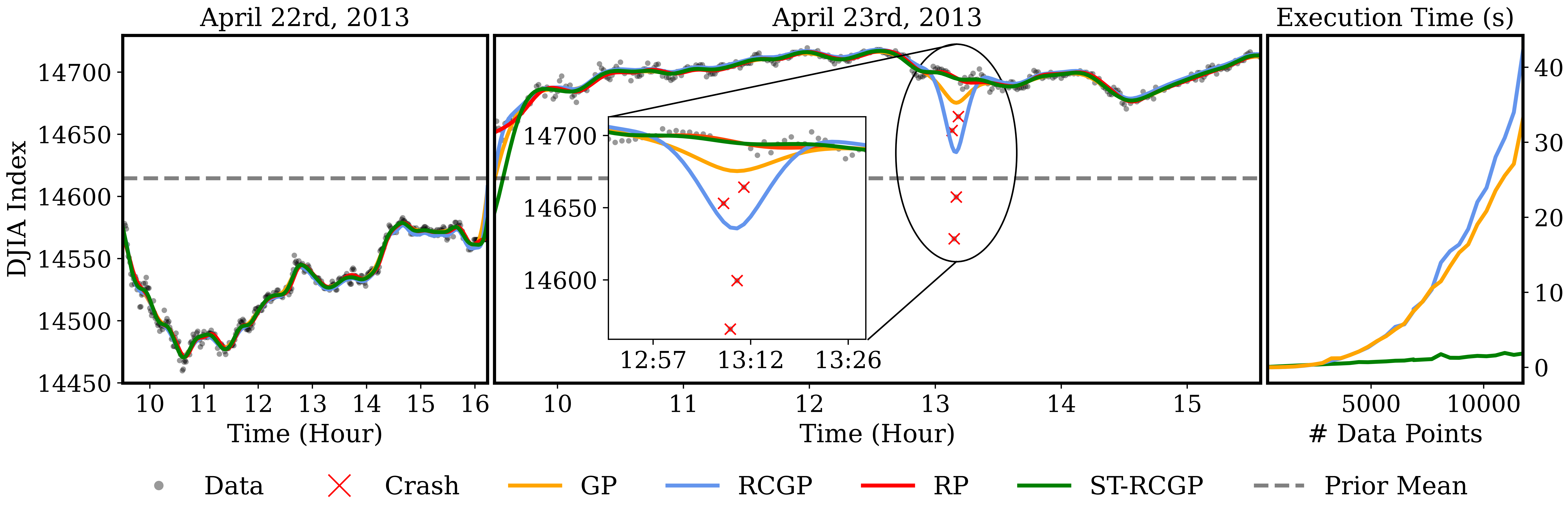
Result... Great!



Experiment 1: Robustness During Financial Crashes



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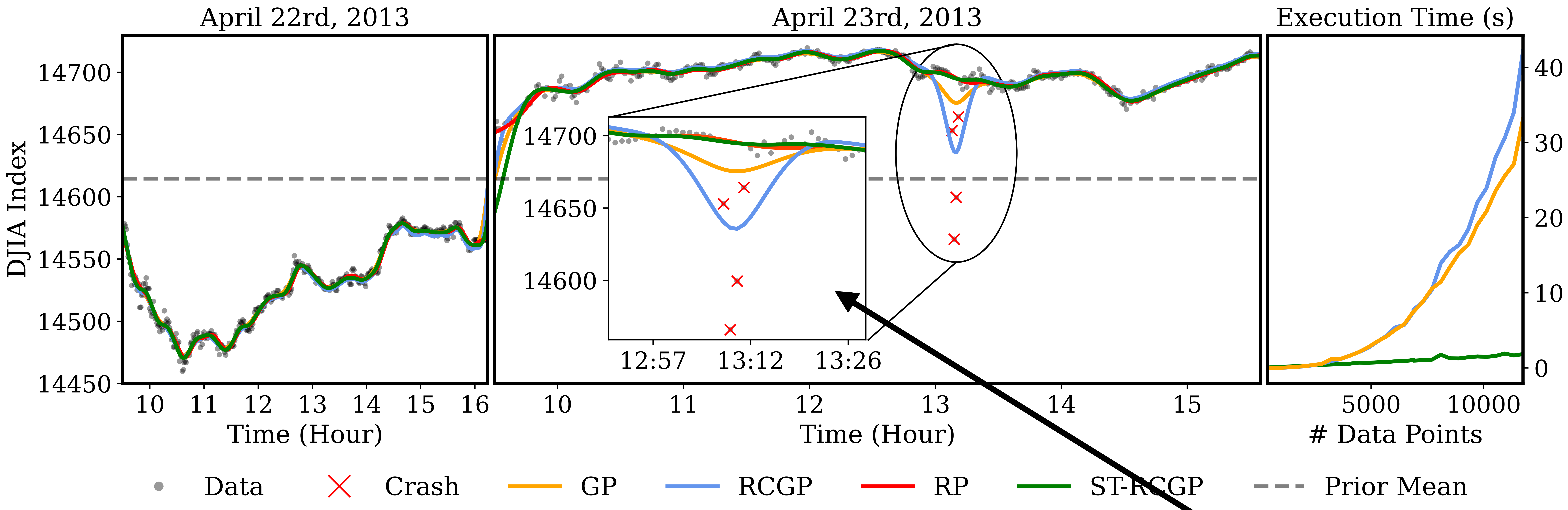

Associated Press's Twitter account **hacked!**

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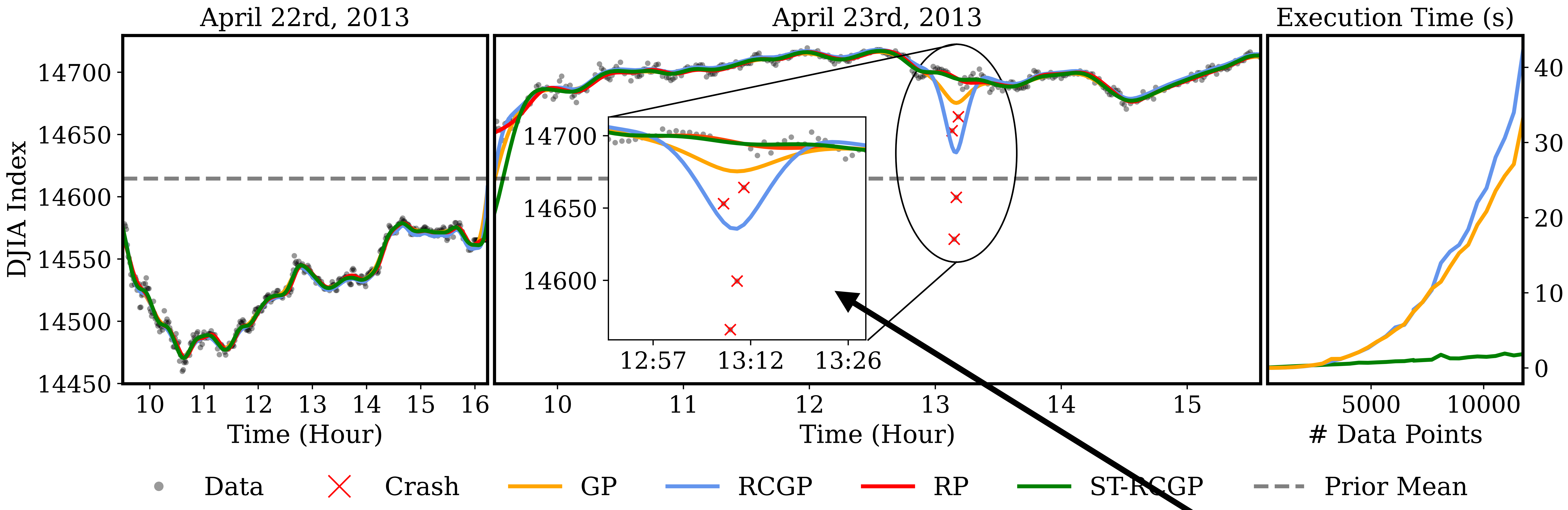

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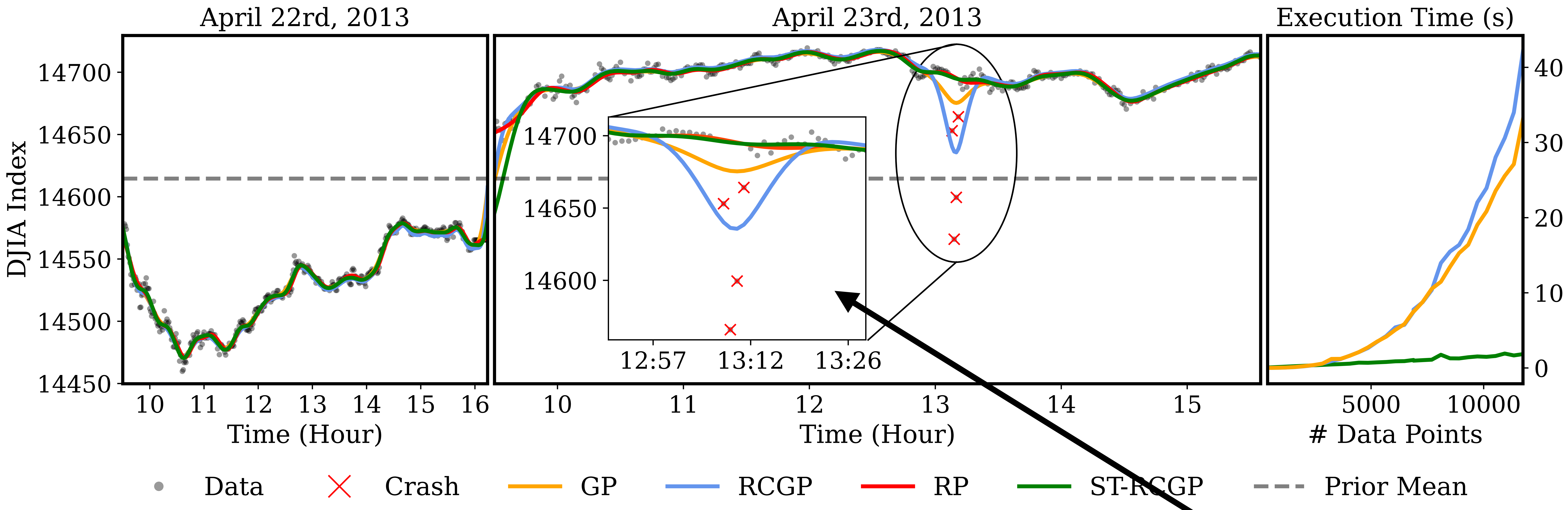

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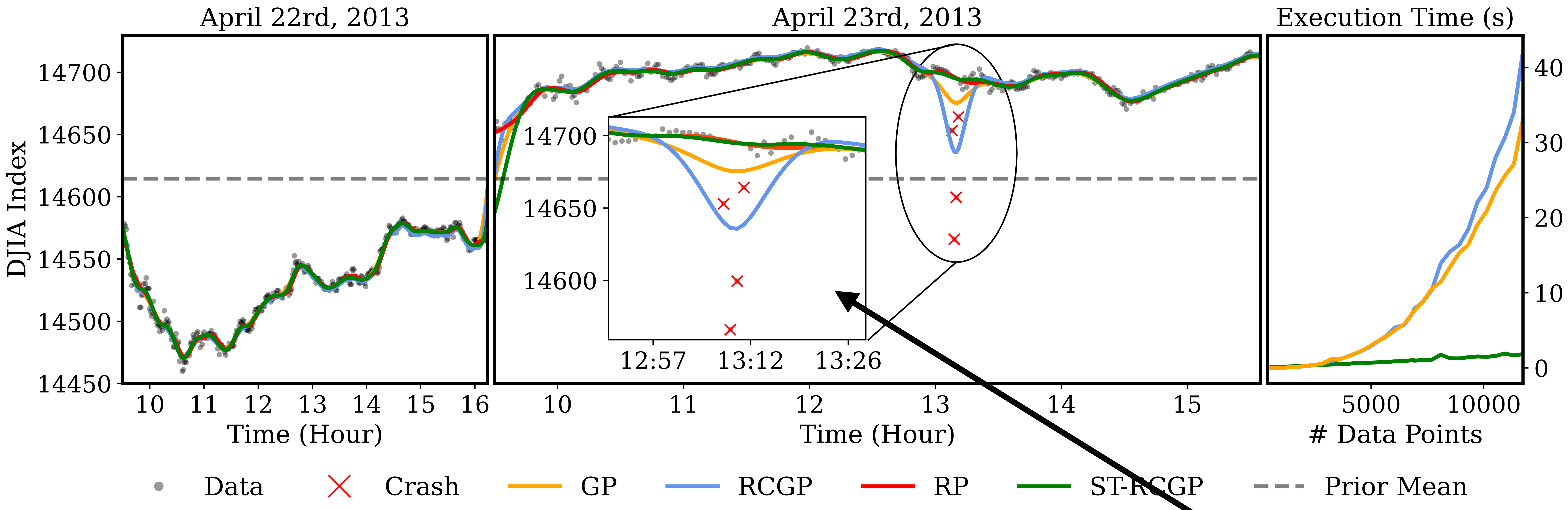

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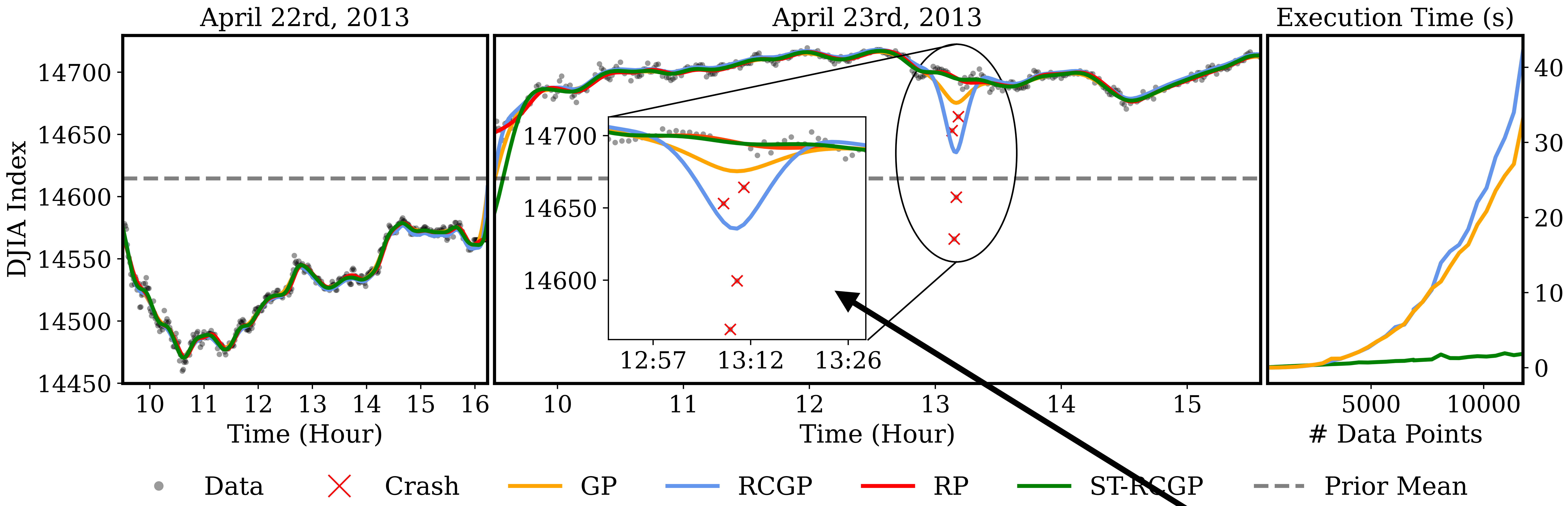
ST-RCGP: Robust AND fast! How? **Adaptive.**



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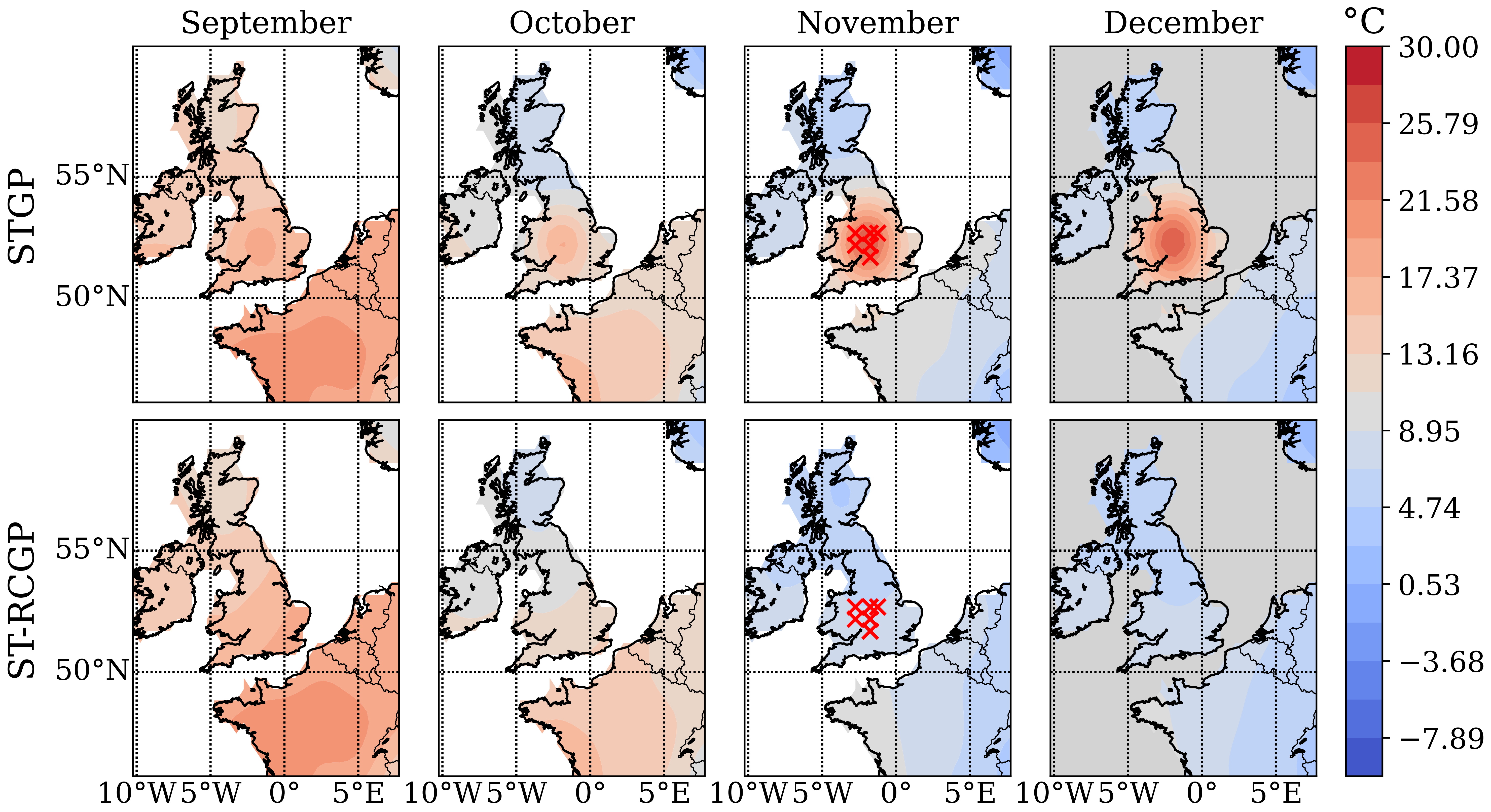

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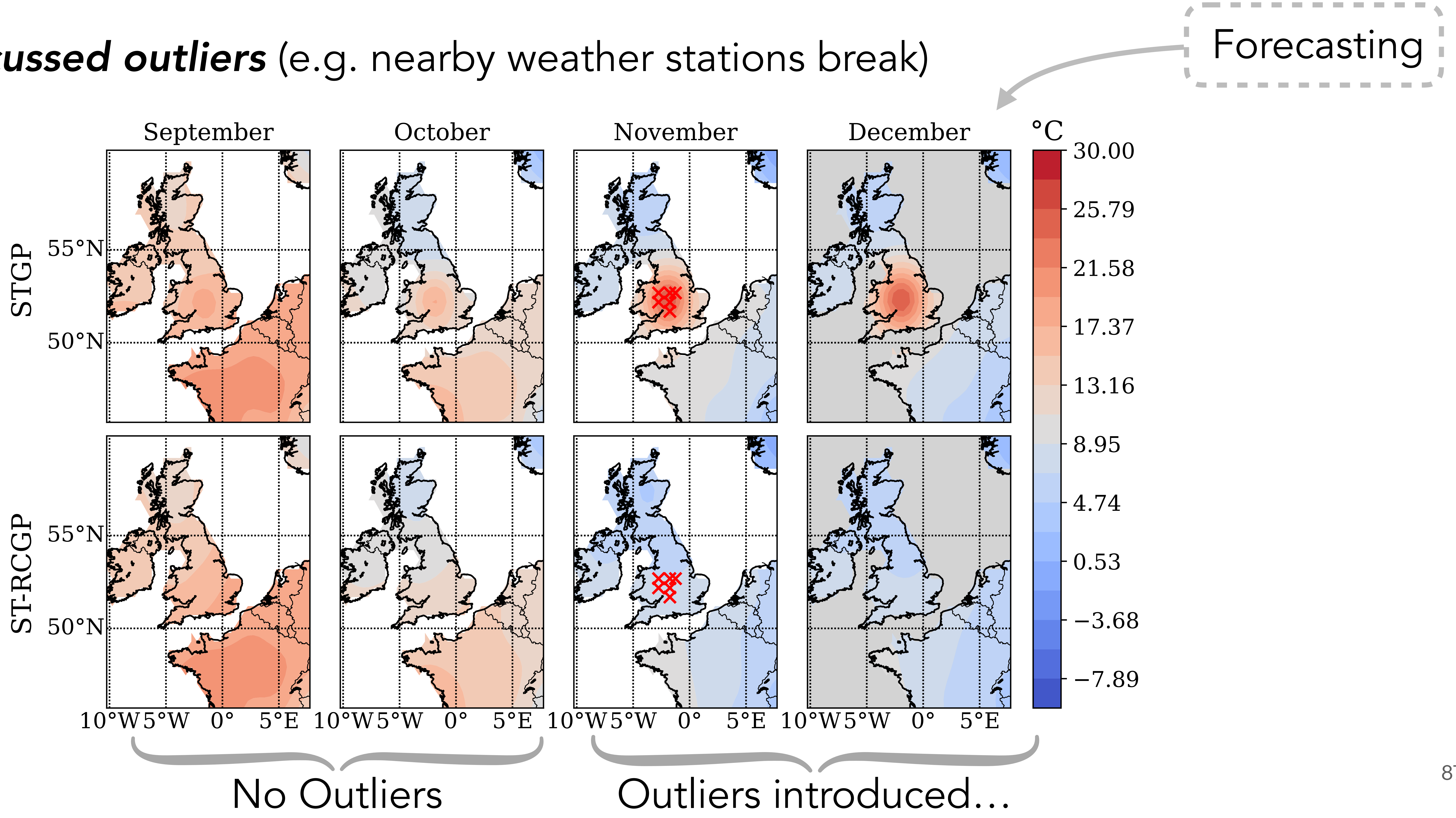

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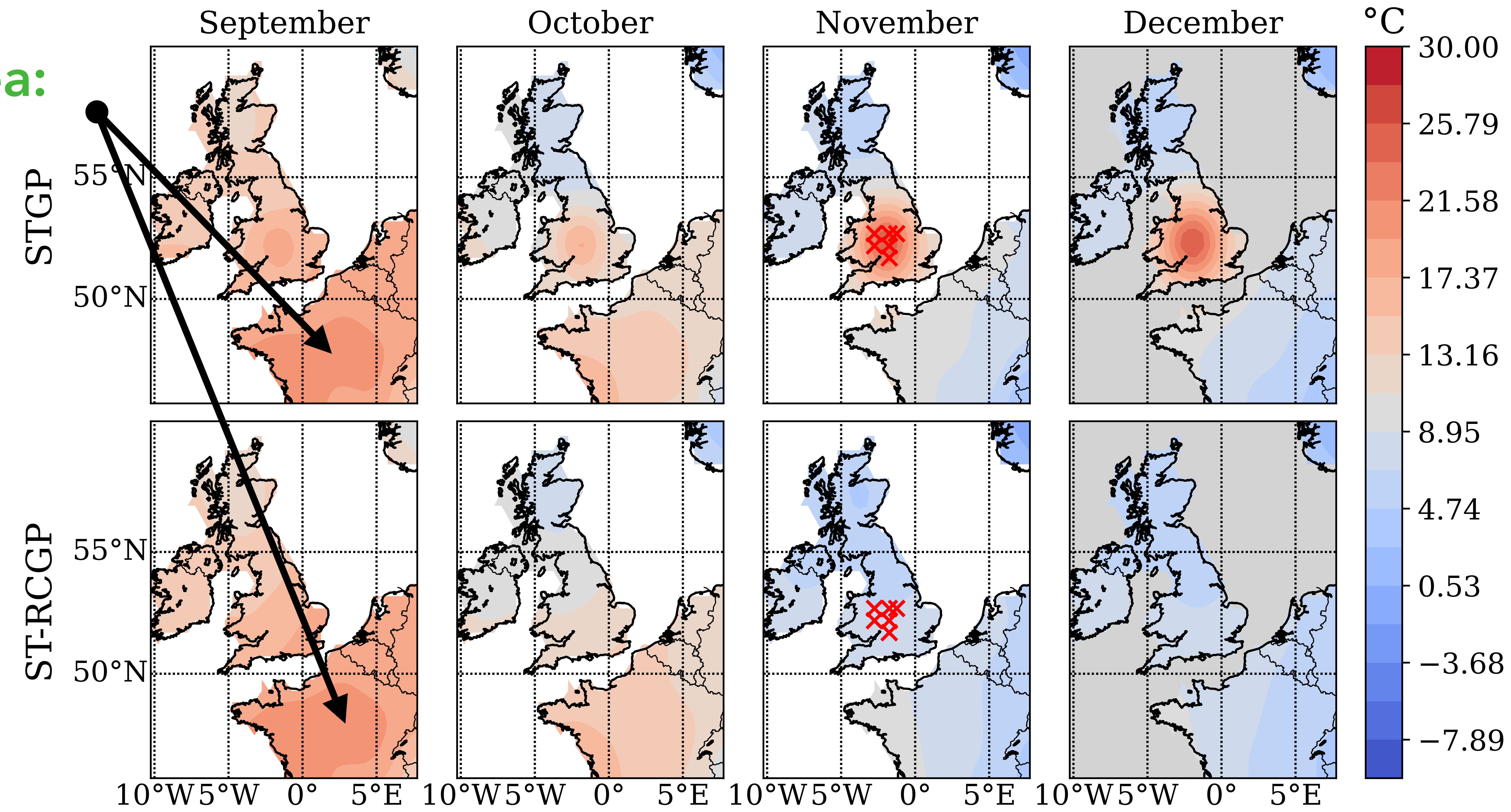

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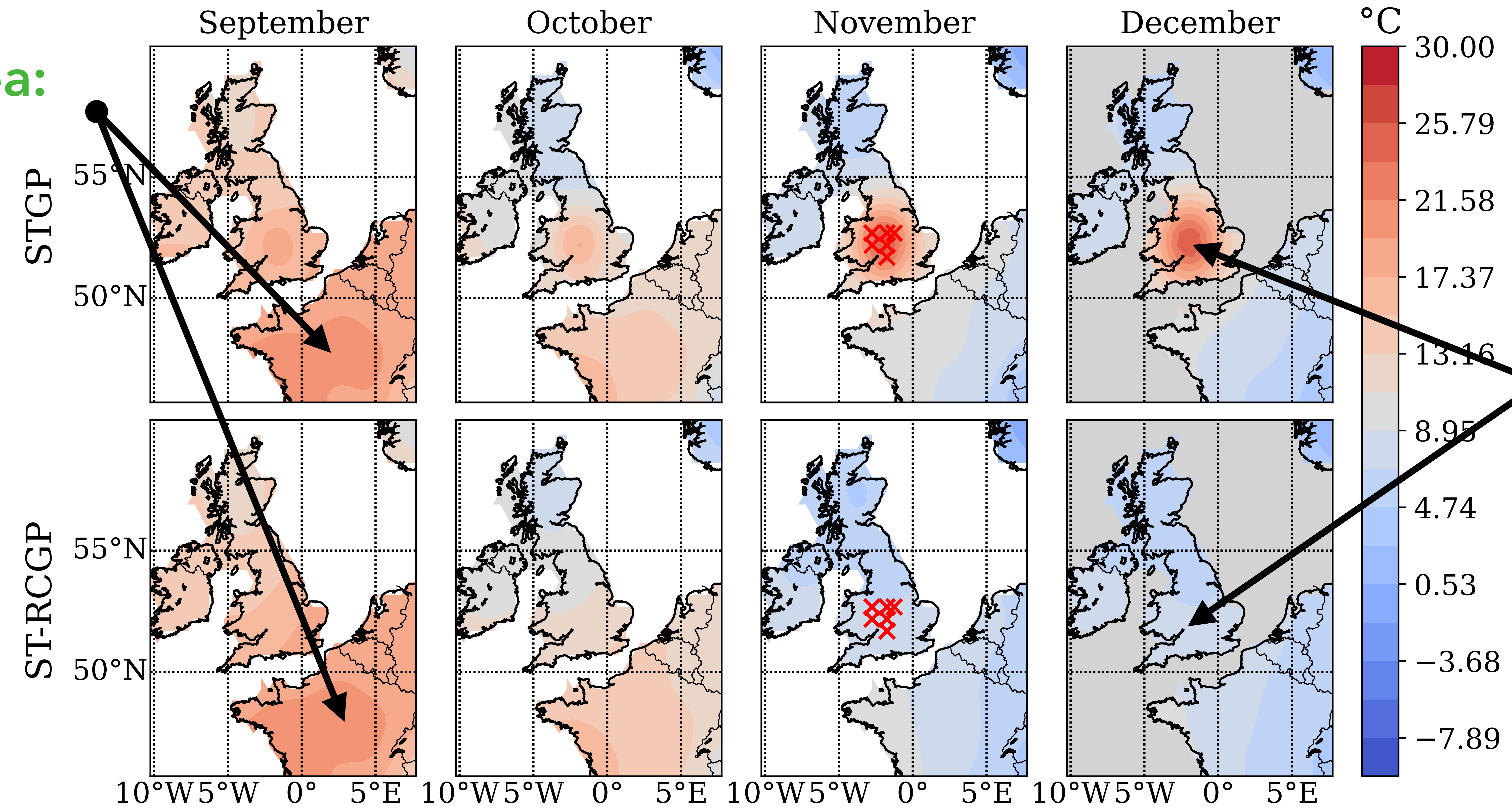

Outlier Area:

ST-RCGP ≫ STGP

$\mathcal{O}$(ST-RCGP) ≈ $\mathcal{O}$(STGP)

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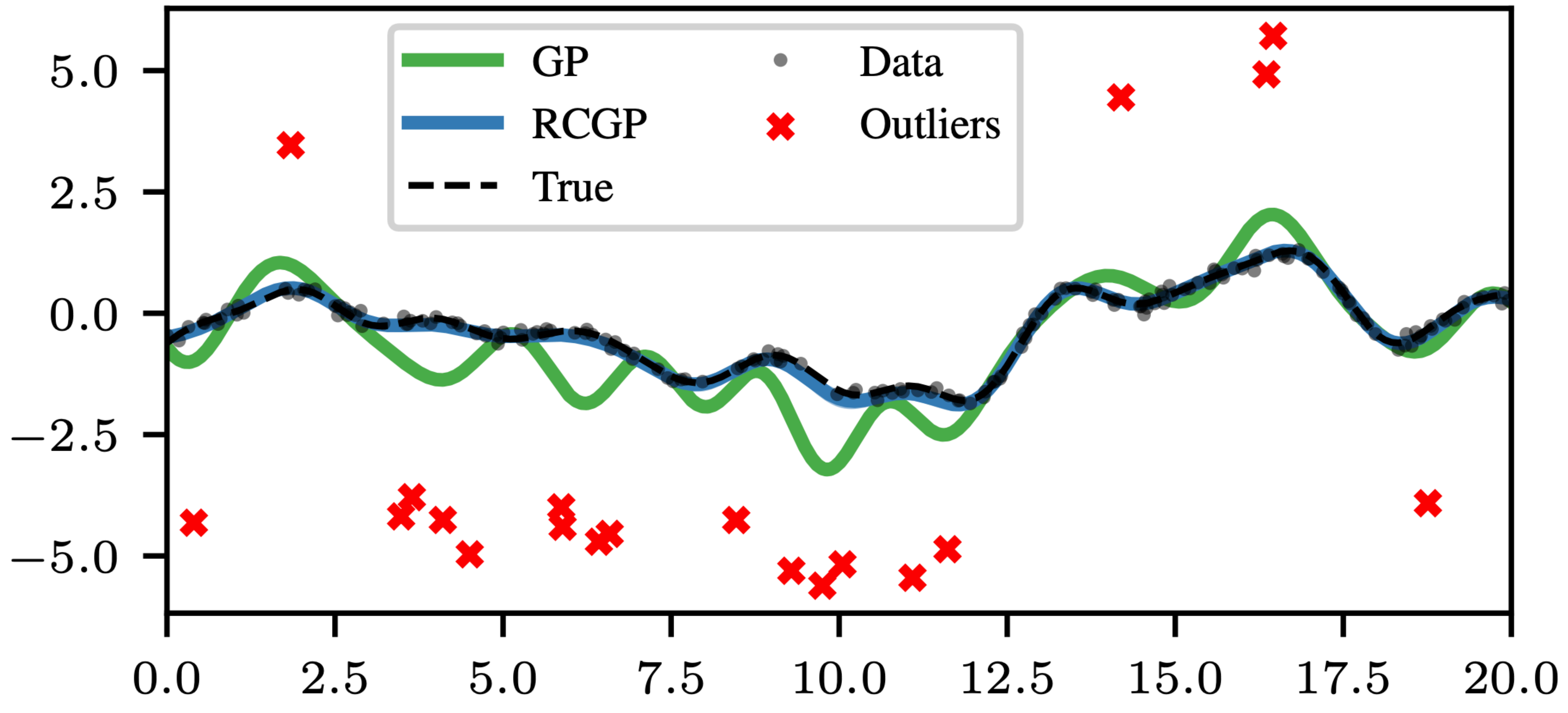
Related Work: RCGP

Robust and Conjugate Gaussian Process Regression

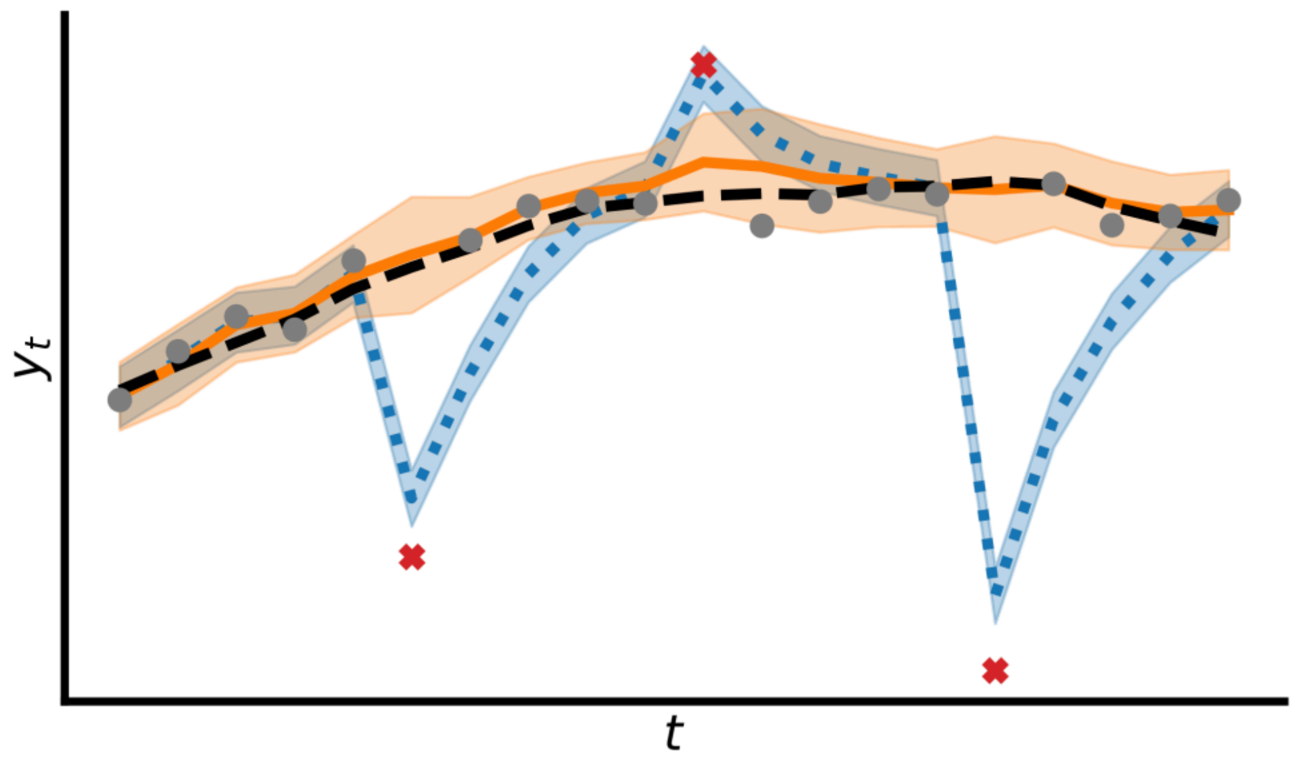


Scan to download RCGP paper!

See Altamirano, M., Briol, F.-X., Knoblauch,F. (2024). Robust and Conjugate Gaussian Process Regression in ICML

Related Work: Robust Kalman Filtering

Outlier-Robust Kalman Filter



Scan to download the full paper

See Also:
Towards Robust Inference for Bayesian Filtering of Linear Gaussian Dynamical Systems Subject to Additive Change

Scan to download the full paper

See Duran-Martin, G., Altamirano, M., Shestopaloff, A. Y., Sánchez-Betancourt, L., Knoblauch, J., Jones, M., ... & Murphy, K. (2024). Outlier-robust Kalman Filtering through Generalised Bayes In ICML

See Reimann H. (2024). Towards Robust Inference for Bayesian Filtering of Linear Gaussian Dynamical Systems Subject to Additive Change. (MSc thesis)

Related Work: Variational STGPs

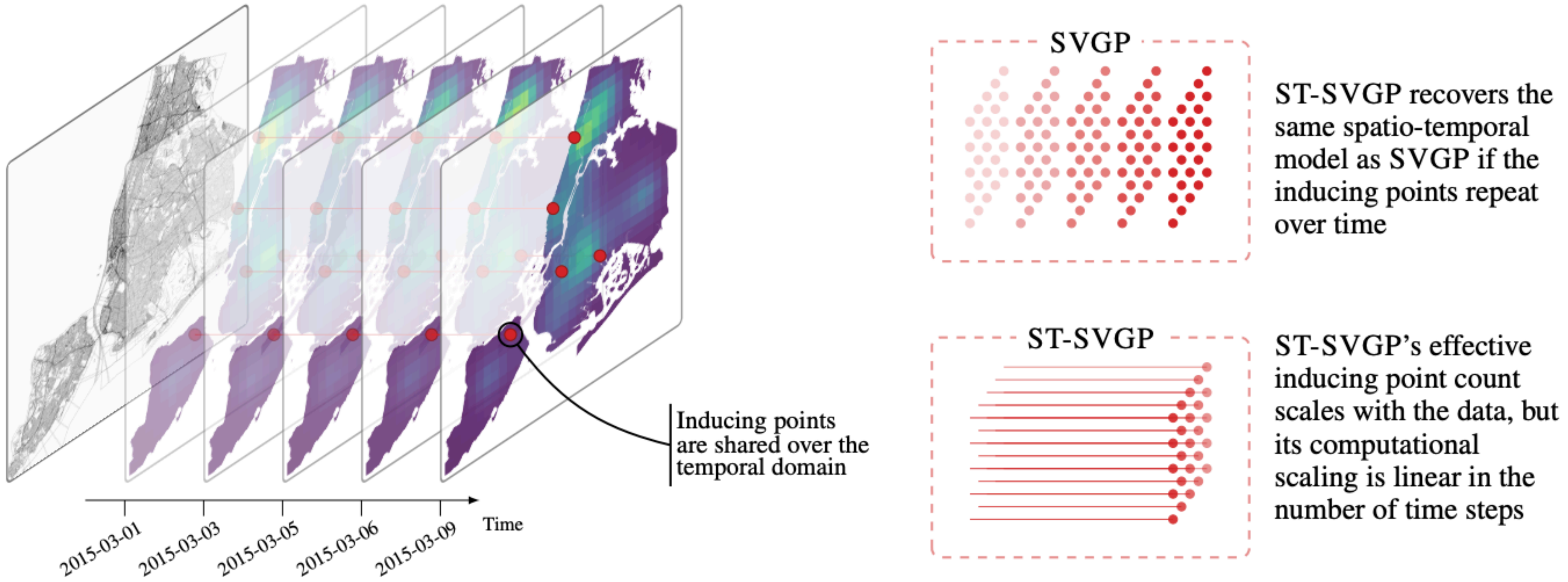


Figure 1: A demonstration of the spatio-temporal sparse variational GP (ST-SVGP) applied to crime count data in New York. ST-SVGP tracks spatial points over time via spatio-temporal filtering. The colourmap is the posterior mean, and the red dots are spatial inducing points. The diagram shows the difference between how inducing points are treated in ST-SVGP and SVGP.

Scan to download the full paper

See Hamelijnck, O., Wilkinson, William J., Loppi, Niki A., Solin, A., Damoulas, T. (2021). Spatio-Temporal Variational Gaussian Processes In NeurIPS

Summary

Scan to download
the ST-RCGP paper!

1. **Fix problematic issues with RCGPs in spatio-temporal settings**

2. **Provide an outlier-robust <u>and</u> efficient spatio-temporal GP**

See Laplante, W., Altamirano, M., Duncan, A., Knoblauch, J., Briol, F.-X. (2025). Robust and Conjugate Spatio-Temporal Gaussian Processes.

Any Questions?