Robust and Conjugate Gaussian Process Regression

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Gaussian process regression

- **Regression problem:** Let $f : \mathcal{X} \to \mathbb{R}$ be some unknown function of interest. we have access to data $\{x_i, y_i\}_{i=1}^n$ where:

$$y_i = f(x_i) + \epsilon_i$$

- Two main assumptions:

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

"Prior"

$$\epsilon_i \sim N(0, \sigma^2)$$

"Likelihood/ Observation Model"

Why Gaussian processes?

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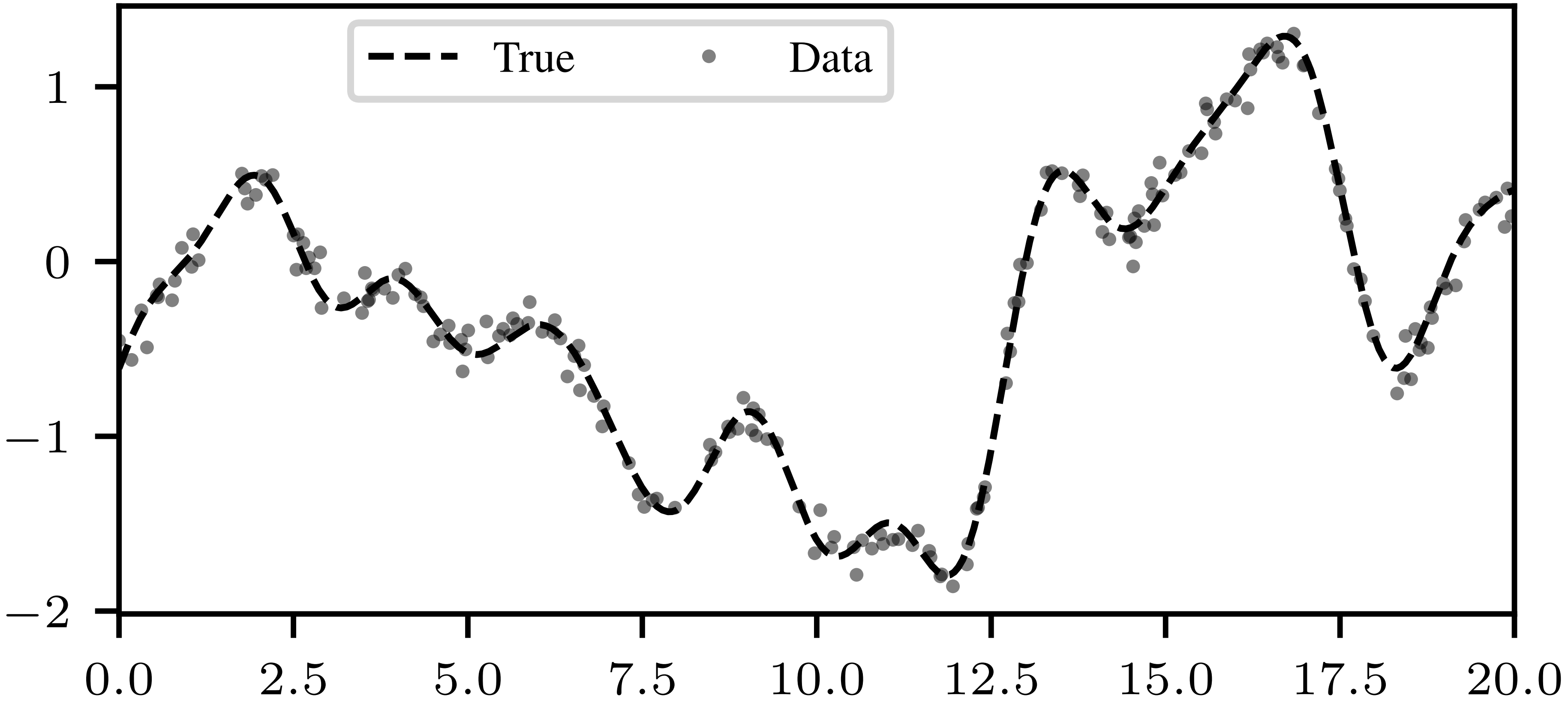
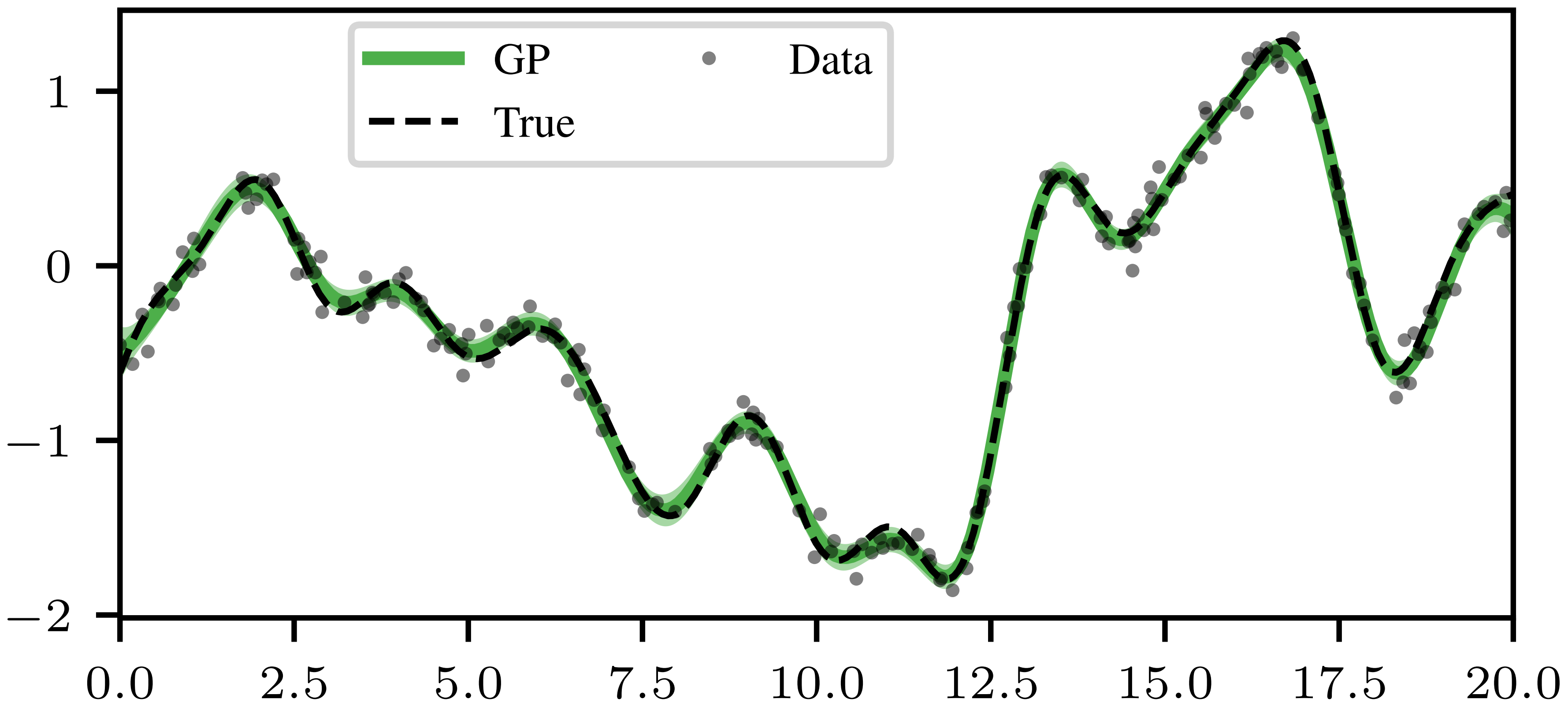
3. We can do **exact conditioning** through Gaussian conjugacy! We therefore don't need to do any approximation of the posterior!

A synthetic problem

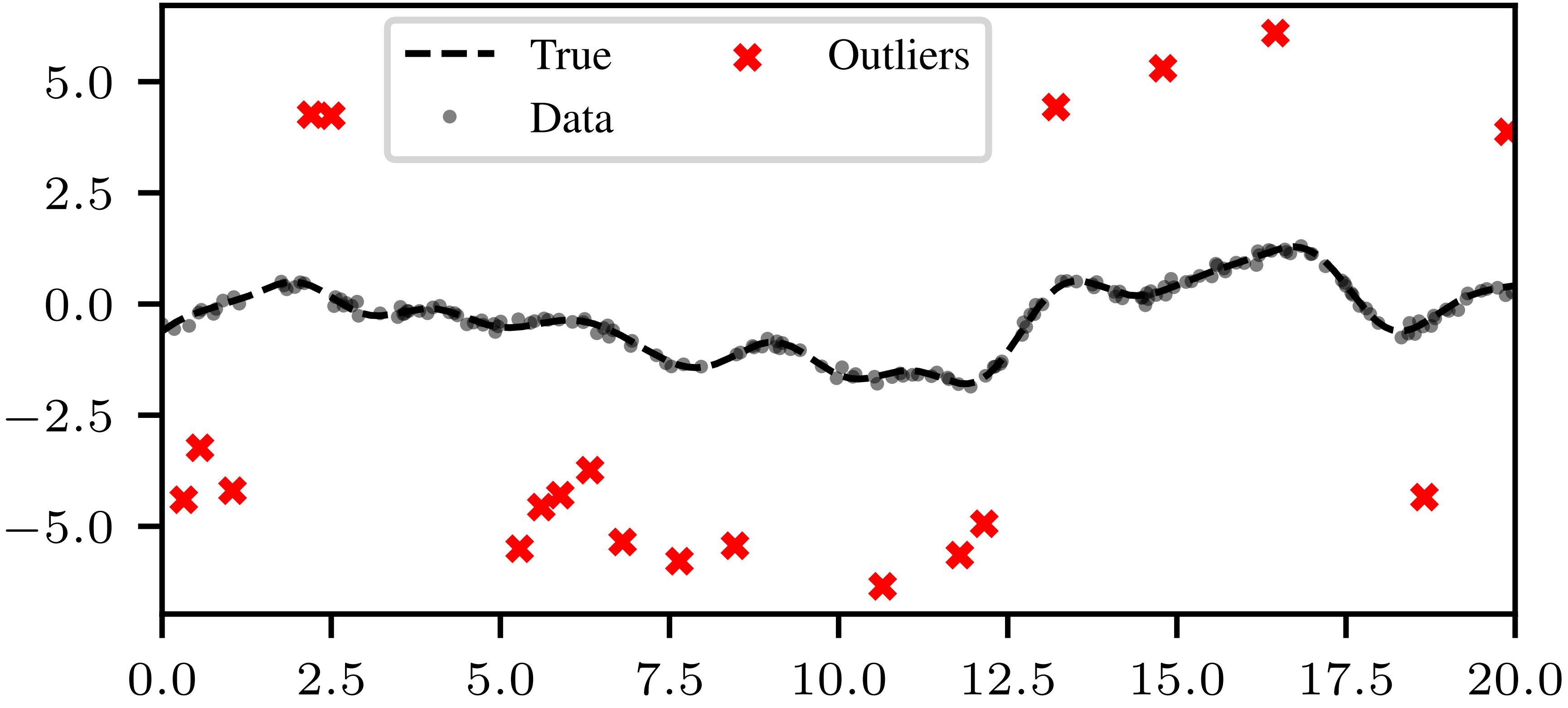


GP regression on the synthetic problem



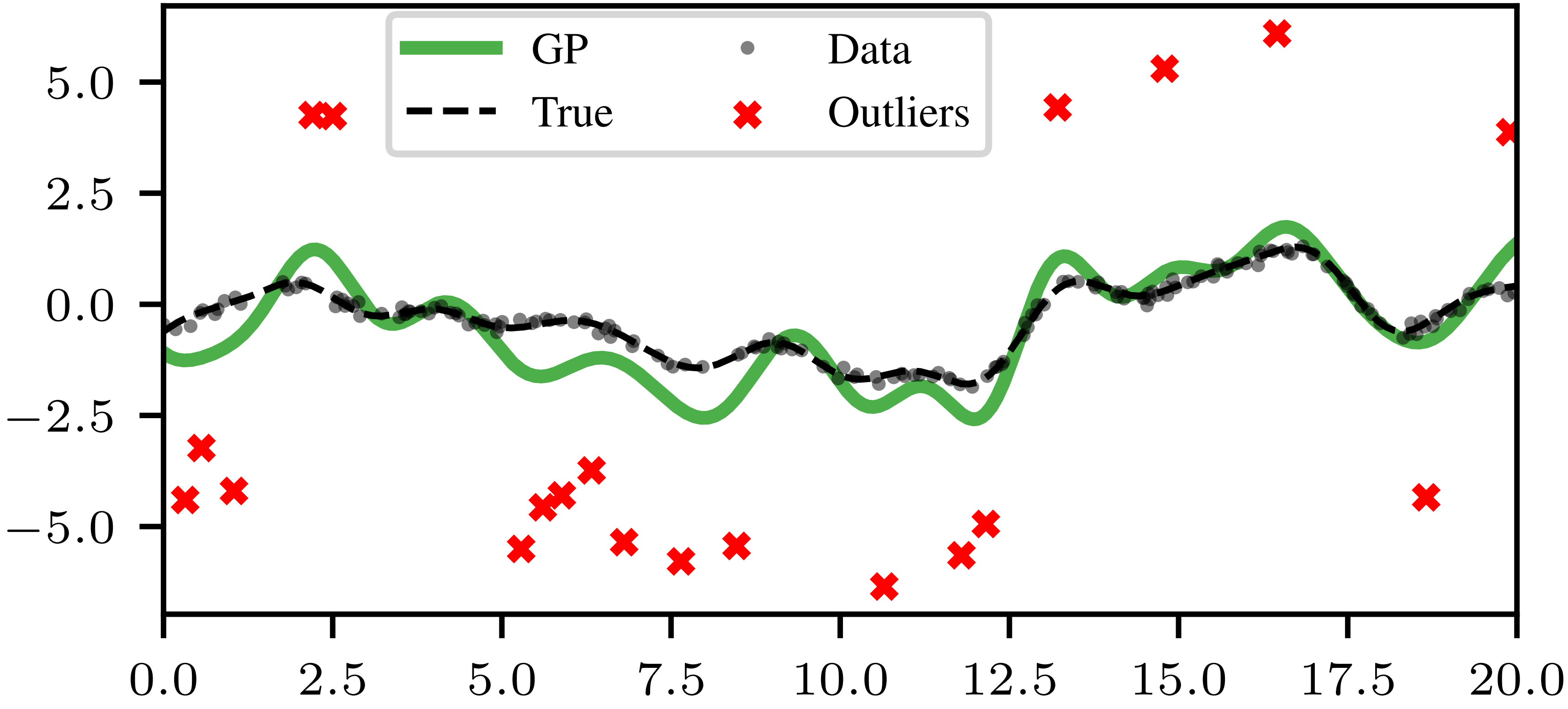
[I am being a bad Bayesian by plotting only the mean… sorry….]

Regression in the “real world”



$\epsilon_i \sim \cancel{N(0, \sigma^2)}$

GP regression in the "real world"



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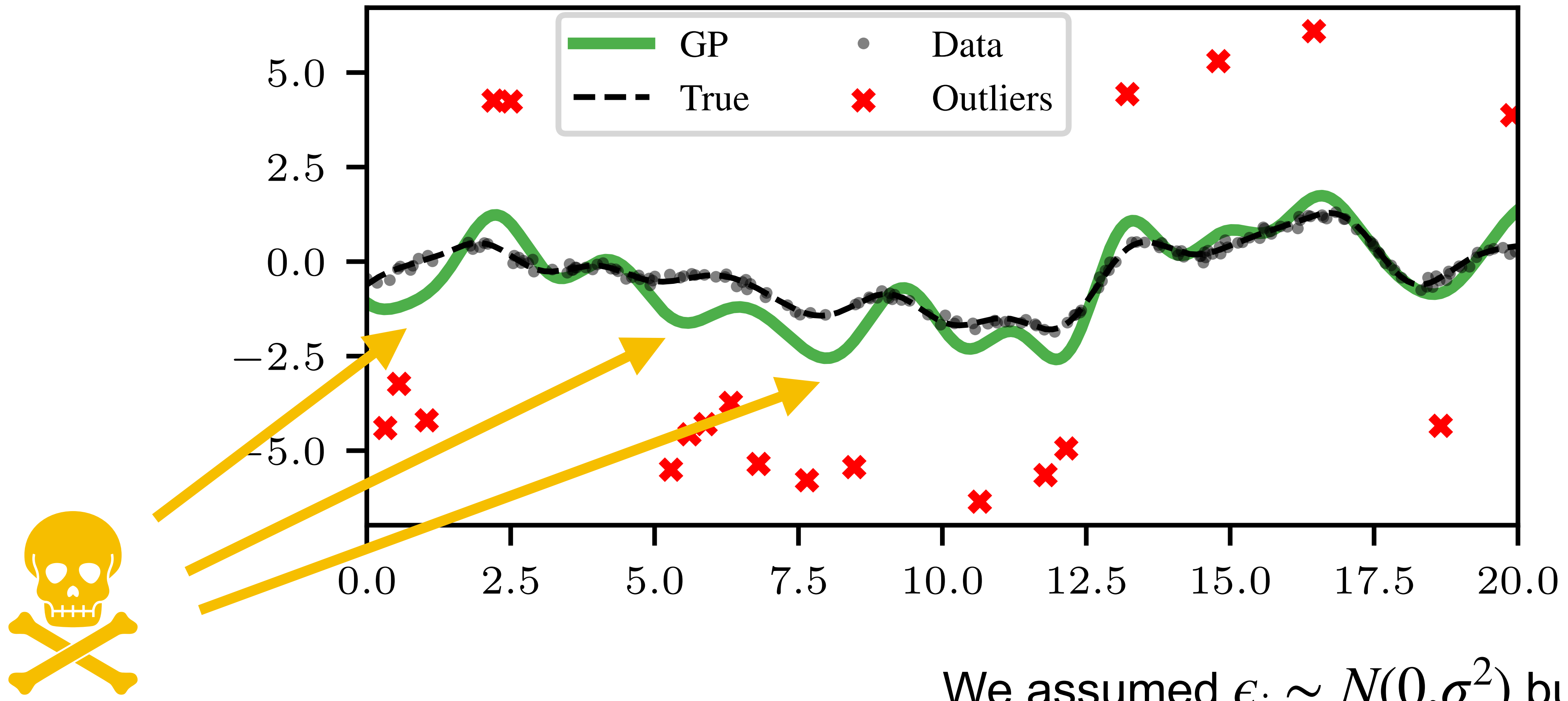

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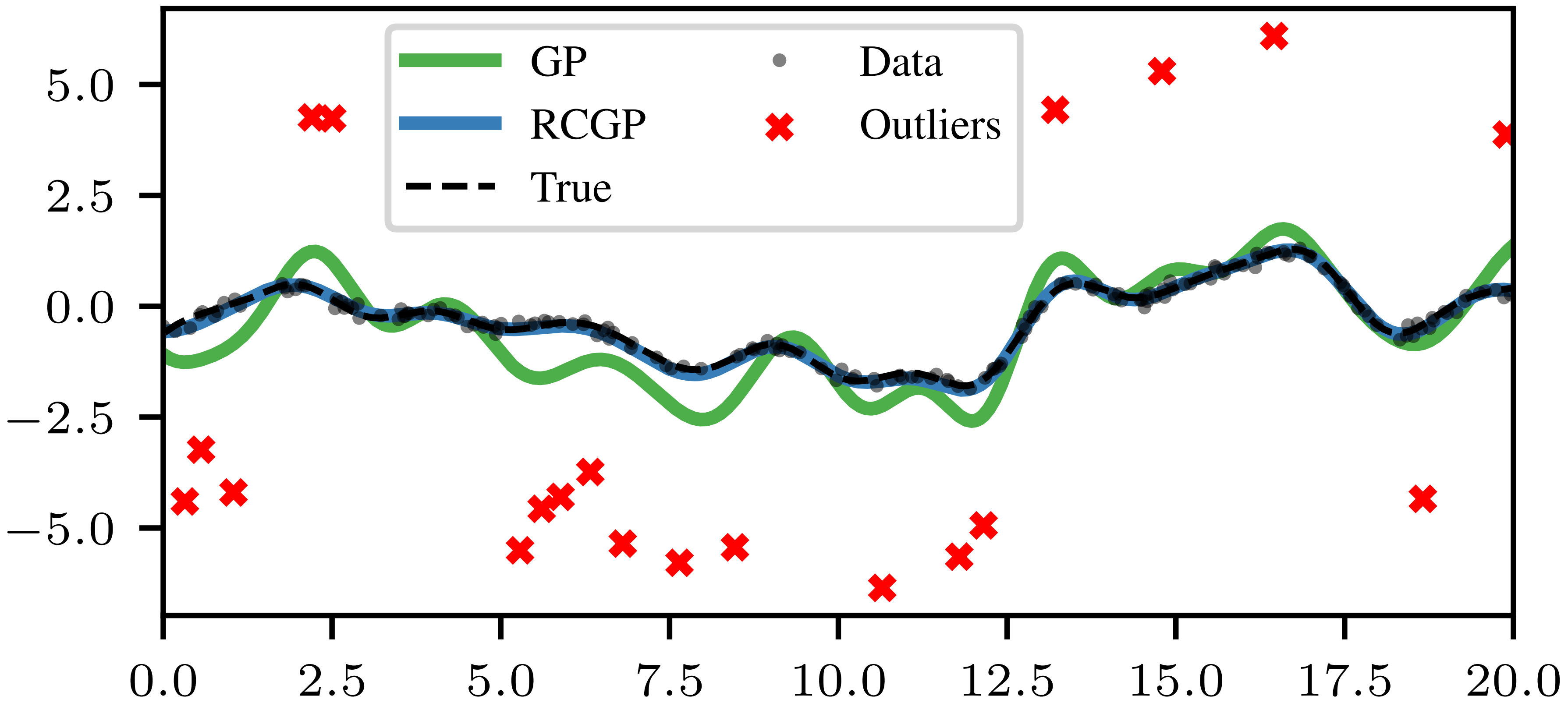

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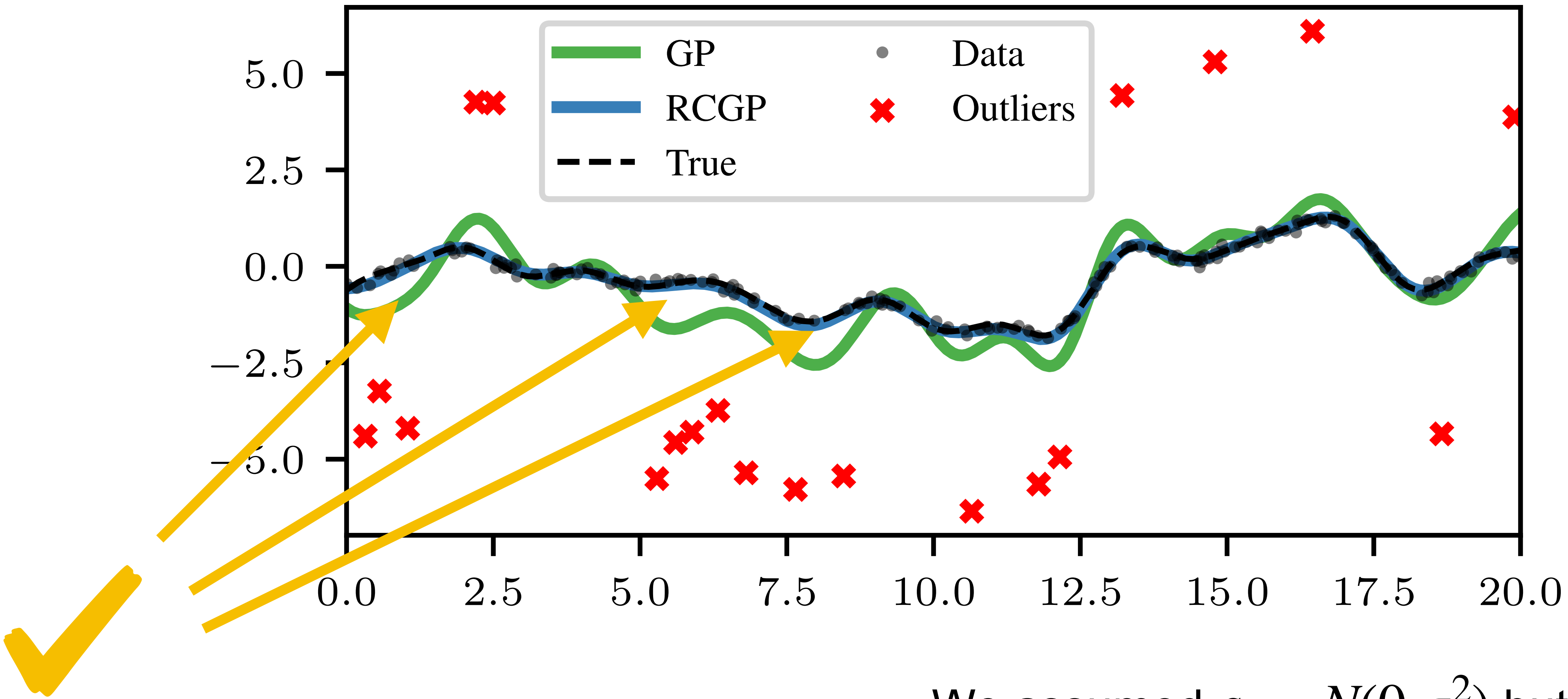

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Existing work

Existing work

Gaussian process regression with Student-t likelihood

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Gaussian Process Robust Regression for Noisy Heart Rate Data

Oliver Stegle*, Sebastian V. Fallert, David J. C. MacKay, and Søren Brage

Identification of robust Gaussian Process Regression with noisy input using EM algorithm

Atefeh Daemi, Yousef Alipouri, Biao Huang *
Department of Chemical and Materials Engineering, University of Alberta, Edmonton, Alberta, T6G 1H9, Canada

Corruption-Tolerant Gaussian Process Bandit Optimization

Ilija Bogunovic
ETH Zürich

Andreas Krause
ETH Zürich

Jonathan Scarlett
National University of Singapore

Robust Gaussian process modeling using EM algorithm

Rishik Ranjan[a], Biao Huang[a,*], Alireza Fatehi[a,b]
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[b] APAC Research Group, Industrial Control Center of Excellence, Faculty of Electrical Engineering, K.N. Toosi University of Technology, Tehran 16317-14191, Iran

Robust Bayesian Optimization with Student-t Likelihood

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Michael McCourt MCCOURT@SIGOPT.COM
Kevin Tee KEVIN@SIGOPT.COM
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Robust Gaussian Process Regression with a Bias Model

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Tallahassee, FL 32310, USA

Robust and Scalable Gaussian Process Regression and Its Applications

Yifan Lu[1], Jiayi Ma[1*], Leyuan Fang[2], Xin Tian[1], and Junjun Jiang[3]
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Robust Regression with Twinned Gaussian Processes

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ROBUST GAUSSIAN PROCESS REGRESSION WITH HUBER LIKELIHOOD *

By Pooja Algikar[1,a], Lamine Mili[2,b]

Robust Gaussian Process Regression with the Trimmed Marginal Likelihood

Daniel Andrade[1] Akiko Takeda[2,3]

Robust Gaussian process regression with G-confluent likelihood

Martin Lindfors *,** Tianshi Chen ** Christian A. Naesseth ***

Robust Gaussian process regression based on iterative trimming

Zhao-Zhou Li [a,*], Lu Li [b,c], Zhengyi Shao [b,d]

Existing work

- There are two main categories:

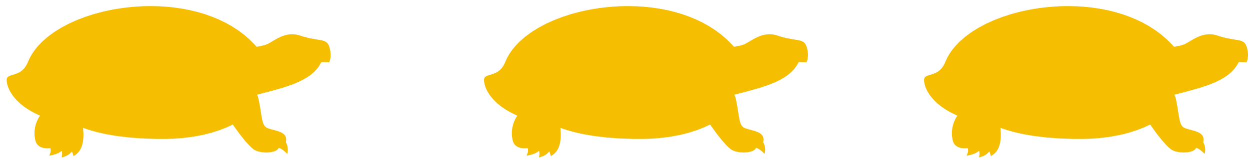
1. **Extended models:** i.e. use more flexible likelihood model to ensure that the outliers are well modelled. Examples include Student-t, mixtures, Laplace, etc…

$$\epsilon \sim P \neq N(0,\sigma^2)$$

2. **Outlier detection/removal:** i.e. find the outliers, remove them, then fit a standard GP model (with Gaussian observations) to the rest of the data.

Issues with existing work

- The main issue with all of the methods above is that they are **very slow**!
- This is because they all **break Gaussian conjugacy** and so we must resort to approximate methods such as MCMC, Laplace or Variational Bayes.



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Boston	1.9 (0.5)	30.7 (6.1)	16.7 (1.7)	$n = 506, d = 13$
Energy	3.8 (0.9)	34.0 (11)	33.8 (0.3)	$n = 768, d = 8$
Yacht	1.6 (0.3)	5.6 (0.7)	4.5 (0.4)	$n = 308, d = 6$

Table: Fitting time in second, including time for hyper parameter optimisation.

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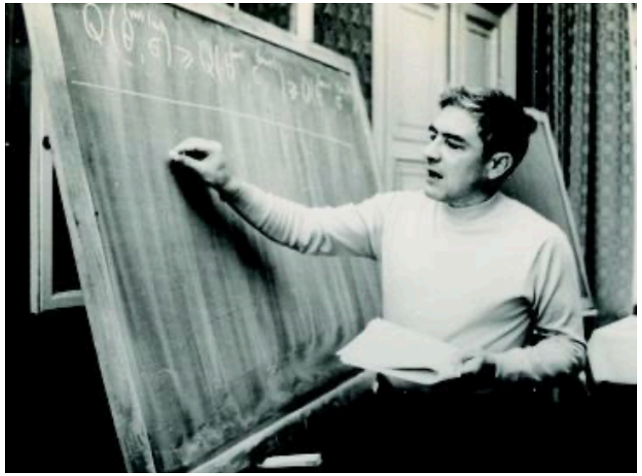
“Gauss was fully aware that his main reason for assuming an underlying normal distribution […] was mathematical, **i.e. computational, convenience**”

“This raises a question which could have been asked by Gauss […] **What happens if the true distribution deviates slightly from the assumed normal one?**”



Huber, P. J. (1964). Robust estimation of a location parameter. *The Annals of Mathematical Statistics*, *35*(1), 73–101.

This talk:

Robust and Conjugate Gaussian Process Regression

Matias Altamirano [1] François-Xavier Briol [1] Jeremias Knoblauch [1]

Appeared as a **spotlight paper** (top 3% of papers) at **ICML 2024**!

Bayesian inference for regression

- In standard GP regression, we do:

Posterior / Likelihood / Prior

$$p(\mathbf{f} \mid \mathbf{y}, \mathbf{x}) \propto p(\mathbf{y} \mid \mathbf{f}, \mathbf{x}) \times p(\mathbf{f} \mid \mathbf{x})$$

$$\mathbf{x} = (x_1, \ldots, x_n)^\top$$
$$\mathbf{f} = (f(x_1), \ldots, f(x_n))^\top$$
$$\mathbf{y} = (y_1, \ldots, y_n)^\top$$

Generalised Bayesian inference for regression

- In standard GP regression, we do:

$$\overbrace{p(\mathbf{f}\,|\,\mathbf{y},\mathbf{x})}^{\text{Posterior}} \propto \overbrace{p(\mathbf{y}\,|\,\mathbf{f},\mathbf{x})}^{\text{Likelihood}} \times \overbrace{p(\mathbf{f}\,|\,\mathbf{x})}^{\text{Prior}}$$

- We take a generalised Bayesian approach and do:

$$\underbrace{p^{L}(\mathbf{f}\,|\,\mathbf{y},\mathbf{x})}_{\text{Generalised Posterior}} \propto \exp\left(-n\underbrace{L_n(\mathbf{f},\mathbf{y},\mathbf{x})}_{\text{Loss function}}\right) \times \underbrace{p(\mathbf{f}\,|\,\mathbf{x})}_{\text{Prior}}$$

Standard vs Generalised Bayesian inference

$$p^L(\mathbf{f} \,|\, \mathbf{y}, \mathbf{x}) \propto \exp\left(-nL_n(\mathbf{f}, \mathbf{y}, \mathbf{x})\right) \times p(\mathbf{f} \,|\, \mathbf{x})$$

- Standard Bayes is recovered by taking

$$L_n(\mathbf{f}, \mathbf{y}, \mathbf{x}) = -\frac{1}{n} \log p(\mathbf{y} \,|\, \mathbf{f}, \mathbf{x})$$

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- This is **optimal**, but **only when the model is well-specified**; i.e. when $\epsilon \sim N(0,\sigma^2)$!

→ **Key Question:** What should we do when this is not the case??

Generalised Bayesian inference

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Bissiri, P., Holmes, C., & Walker, S. (2016). A general framework for updating belief distributions. *Journal of the Royal Statistical Society Series B: Statistical Methodology*, *78*, 1103–1130.

Knoblauch, J., Jewson, J., & Damoulas, T. (2022). An optimization-centric view on Bayes' rule: reviewing and generalizing variational inference. *Journal of Machine Learning Research*, *23*(132), 1–109.

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- We can choose the loss function to induce **robustness to mild model misspecification**.

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- Common choice is a loss based on a divergence:

$$\mathcal{D}\left(\frac{1}{n}\sum_{i=1}^{n} \delta_{y_i}, p_f\right)$$

Data-generating process; here a Gaussian

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  - In this talk, we will also choose the loss function for computational convenience!

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Score-matching and generalisations

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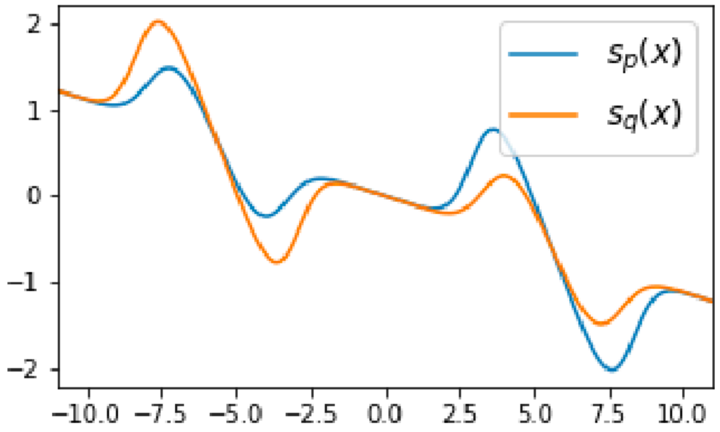
$$D(p\,||\,q) := \mathbb{E}_{Y\sim q}[\|\nabla_y \log p(Y) - \nabla_y \log q(Y)\|_2^2]$$



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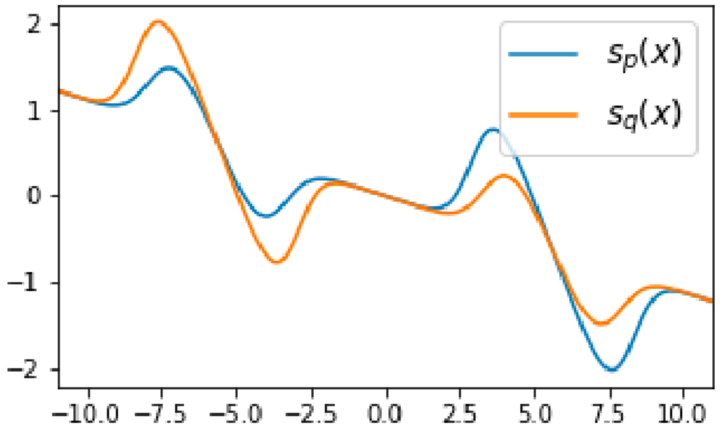
- We consider a weighted generalisation:

$$D(p\,||\,q) := \mathbb{E}_{Y\sim q}[\|{\color{blue}w(Y)}(\nabla_y \log p(Y) - \nabla_y \log q(Y))\|_2^2]$$



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

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

Score-matching and generalisations

- For regression setting, we need to extend this divergence (now $w : \mathcal{X} \times \mathbb{R} \to \mathbb{R}$):

$$D(p\,||\,q) := \mathbb{E}_{X \sim q_x}\left[\mathbb{E}_{Y \sim q(\cdot|X)}\left[\, \| \, w(X, Y)(\nabla_y \log p(Y|X) - \nabla_y \log q(Y|X)) \, \|_2^2 \right]\right]$$

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- With integration by part and replacing q by our samples, we get that:

$$D(p\,||\,q_n) = L_n^w(\mathbf{f}, \mathbf{y}, \mathbf{x}) + C$$

$$= \frac{1}{n}\sum_{i=1}^{n}\Big((w(x_i, y_i)\nabla_y \log p(y_i|x_i))^2 + 2\nabla_y (w(x_i, y_i)^2 \nabla_y \log p(y_i|x_i))\Big) + C$$

Likelihood

RCGPs are conjugate!

- Suppose $f \sim GP(m, k)$ and $\epsilon \sim N(0, \sigma^2 I_n)$, then the GP and RCGP posteriors are:

<u>Standard GP</u>

$$p(\mathbf{f} \mid \mathbf{y}, \mathbf{x}) = N(\mathbf{f}; \mu, \Sigma)$$

$$\mu = \mathbf{m} + K(K + \sigma^2 I_n)^{-1}(\mathbf{y} - \mathbf{m})$$

$$\Sigma = K(K + \sigma^2 I_n)^{-1}\sigma^2 I_n$$

$K_{ij} = k(x_i, x_j)$

Identity matrix

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RCGP

$$p^w(\mathbf{f} \,|\, \mathbf{y}, \mathbf{x}) = N(\mathbf{f}; \mu^R, \Sigma^R)$$

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Taking $w(x, y) = \sigma(x)/\sqrt{2}$ **recovers heteroscedastic GPs.**

We will choose $w(x, y)$ differently to induce robustness….

Down-weighting outliers

$$w(x, y) = \left(1 + \frac{(y - m(x))^2}{c^2}\right)^{-\frac{1}{2}}$$

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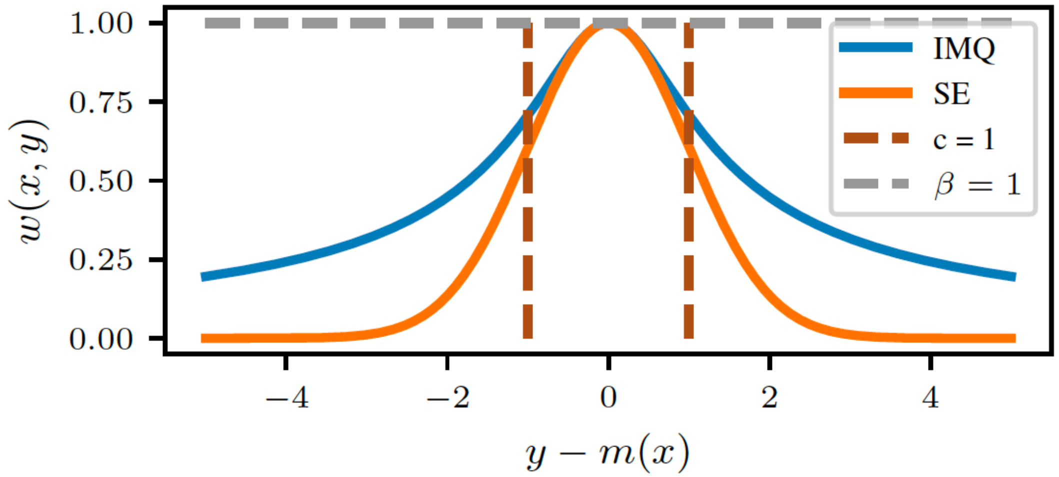

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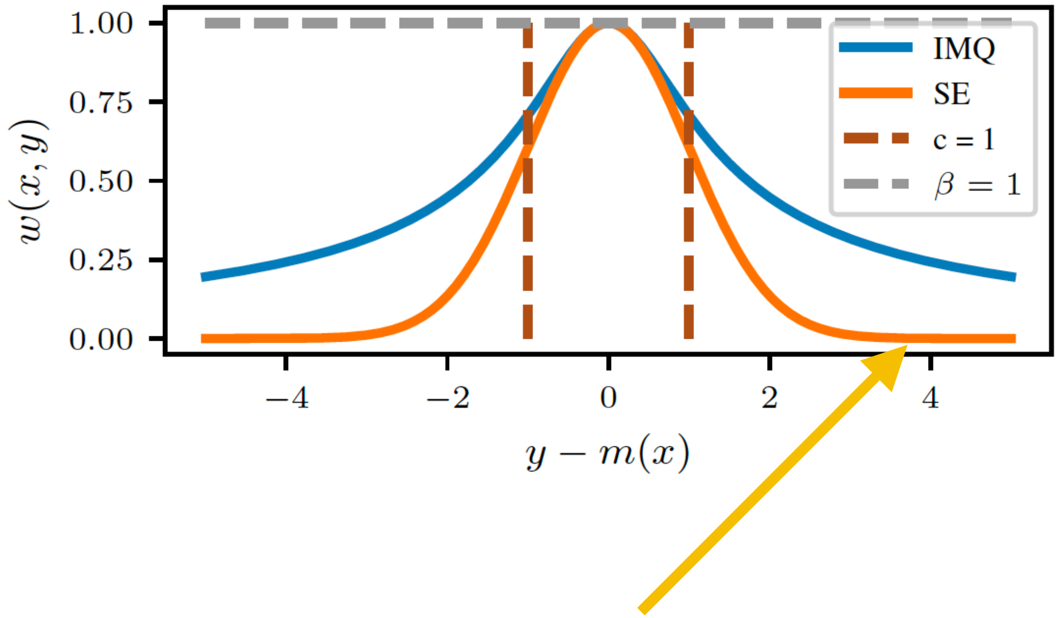

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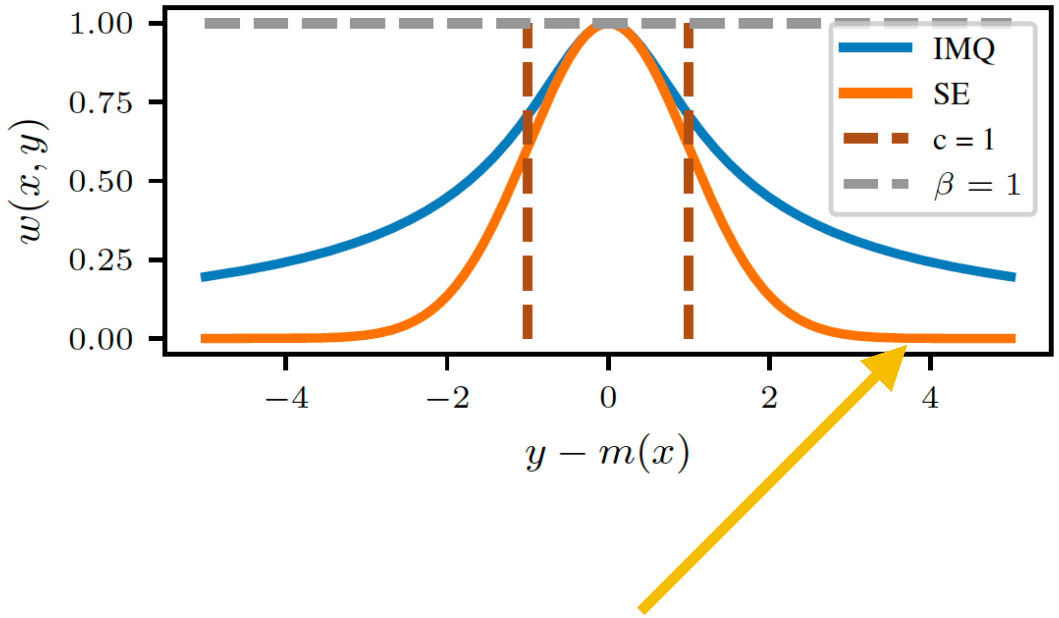

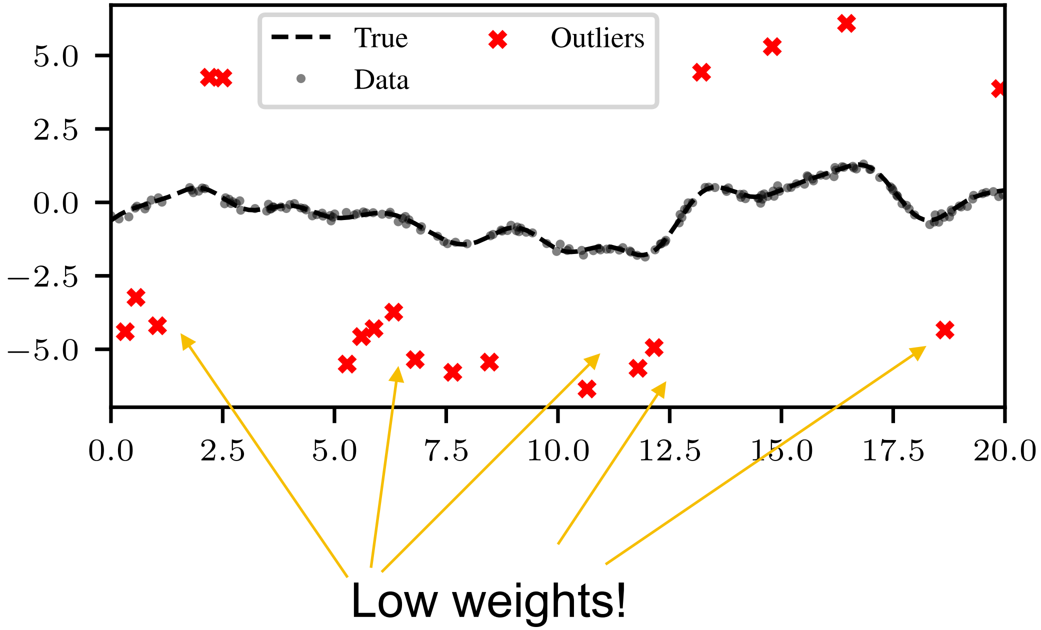

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Measuring outlier-robustness

- The posterior influence function measures the impact of a single outlier on the posterior:

$$\text{PIF}(y_m^c, D) = \text{KL}\left(p(f \mid D), p(f \mid D_m^c)\right)$$

$$D = \{x_i, y_i\}_{i=1}^n \qquad D_m^c = (D \backslash \{x_m, y_m\}) \cup \{x_m, y_m^c\}$$

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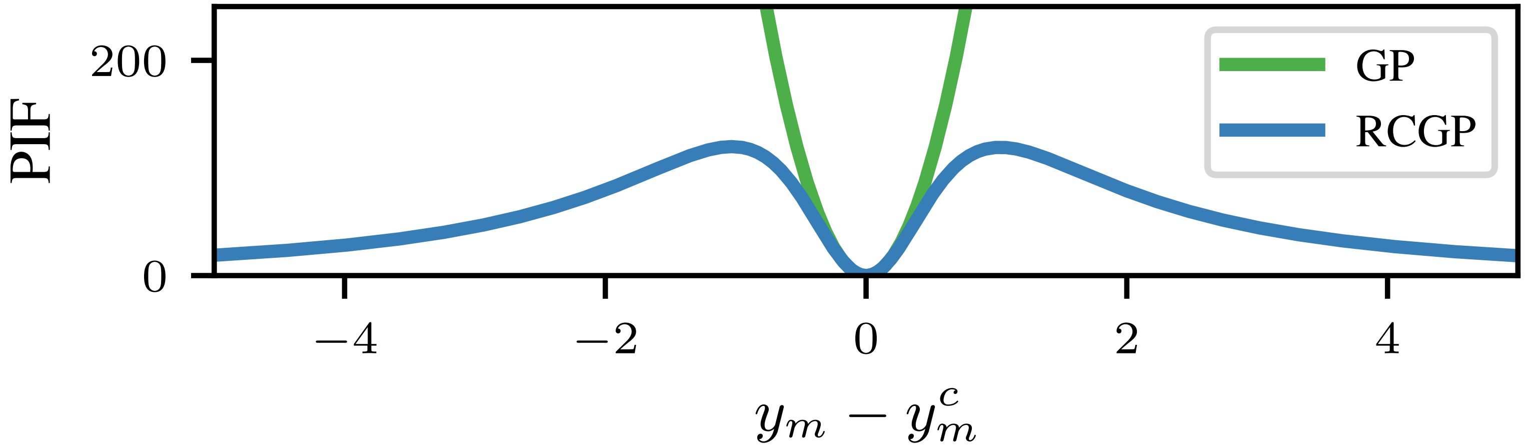
- Sadly…

$$\sup_{y_m^c} \mathrm{PIF}_{\mathrm{GP}}(y_m^c, D) = \infty$$

RCGPs are provably outlier-robust

- **Theorem (informal):** Suppose $w(x, y) = (1 + (y - m(x))^2/c^2)^{-\frac{1}{2}}$ for some $c > 0$, then RCGPs are robust since:

$$\sup_{y_m^c} \mathrm{PIF}_{\mathrm{RCGP}}(y_m^c, D) < \infty$$



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- Our alternative is to do **leave-one-out cross-validation**

$$\hat{\sigma}^2, \hat{\theta} = \arg\max_{\sigma^2, \theta} \left\{ \sum_{i=1}^{n} \log p^w(y_i \,|\, \mathbf{x}, \mathbf{y}_{-i}, \theta, \sigma^2) \right\},$$

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- This can be done efficiently through clever linear algebra tricks and gradient-based optimisation.

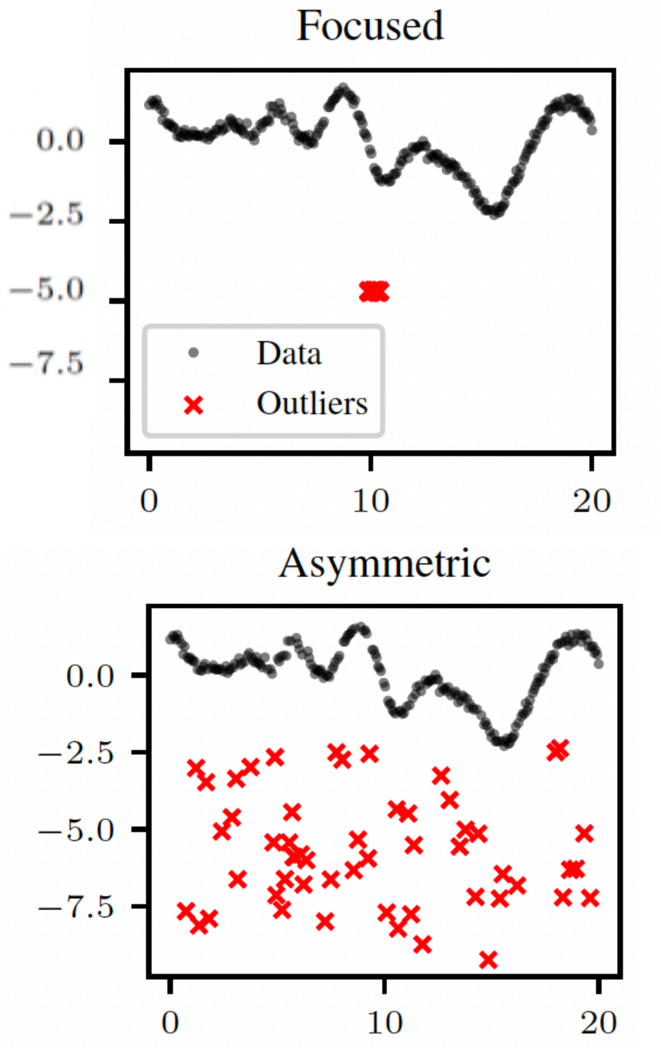
Performance when well-specified (MAE)

	GP	RCGP	t-GP	m-GP
		No Outliers		
Synthetic	**0.09 (0.00)**	**0.09 (0.00)**	**0.09 (0.00)**	0.33 (0.00)
Boston	**0.19 (0.01)**	**0.19 (0.01)**	**0.19 (0.01)**	0.28 (0.00)
Energy	0.03 (0.00)	**0.02 (0.00)**	0.03 (0.00)	0.61 (0.00)
Yacht	0.02 (0.01)	0.02 (0.01)	**0.01 (0.00)**	0.33 (0.00)

GPs and RCGPs are comparable when the model is well-specified!

Performance when misspecified (MAE)

	GP	RCGP	t-GP	m-GP
		Focused Outliers		
Synthetic	0.19 (0.00)	**0.15 (0.00)**	0.18 (0.00)	0.23 (0.00)
Boston	0.23 (0.06)	**0.22 (0.01)**	0.27 (0.00)	0.27 (0.00)
Energy	0.03 (0.04)	**0.02 (0.00)**	0.03 (0.05)	0.24 (0.00)
Yacht	0.26 (0.15)	**0.10 (0.14)**	0.20 (0.04)	0.24 (0.00)
		Asymmetric Outliers		
Synthetic	1.14 (0.00)	0.63 (0.00)	1.06 (0.00)	**0.61 (0.00)**
Boston	0.63 (0.02)	**0.49 (0.00)**	0.52 (0.00)	0.52 (0.00)
Energy	0.54 (0.02)	0.44 (0.04)	0.42 (0.02)	**0.41 (0.00)**
Yacht	0.54 (0.06)	**0.35 (0.02)**	0.41 (0.00)	0.40 (0.00)



RCGPs are robust!

RCGPs are fast!

(Time in seconds, incl. hyper parameter optimisation)

	GP	RCGP	t-GP	m-GP
Synthetic	1.5 (0.1)	1.2 (0.0)	2.2 (0.0)	3.0 (0.0)
Boston	1.9 (0.5)	5.1 (0.9)	30.7 (6.1)	16.7 (1.7)
Energy	3.8 (0.9)	4.6 (2.0)	34.0 (11)	33.8 (0.3)
Yacht	1.6 (0.3)	2.1 (0.2)	5.6 (0.7)	4.5 (0.4)

RCGPs are much faster than other robust alternatives!

RCGPs are roughly as fast as GPs

	GP	RCGP	t-GP	m-GP
Synthetic	1.5 (0.1)	1.2 (0.0)	2.2 (0.0)	3.0 (0.0)
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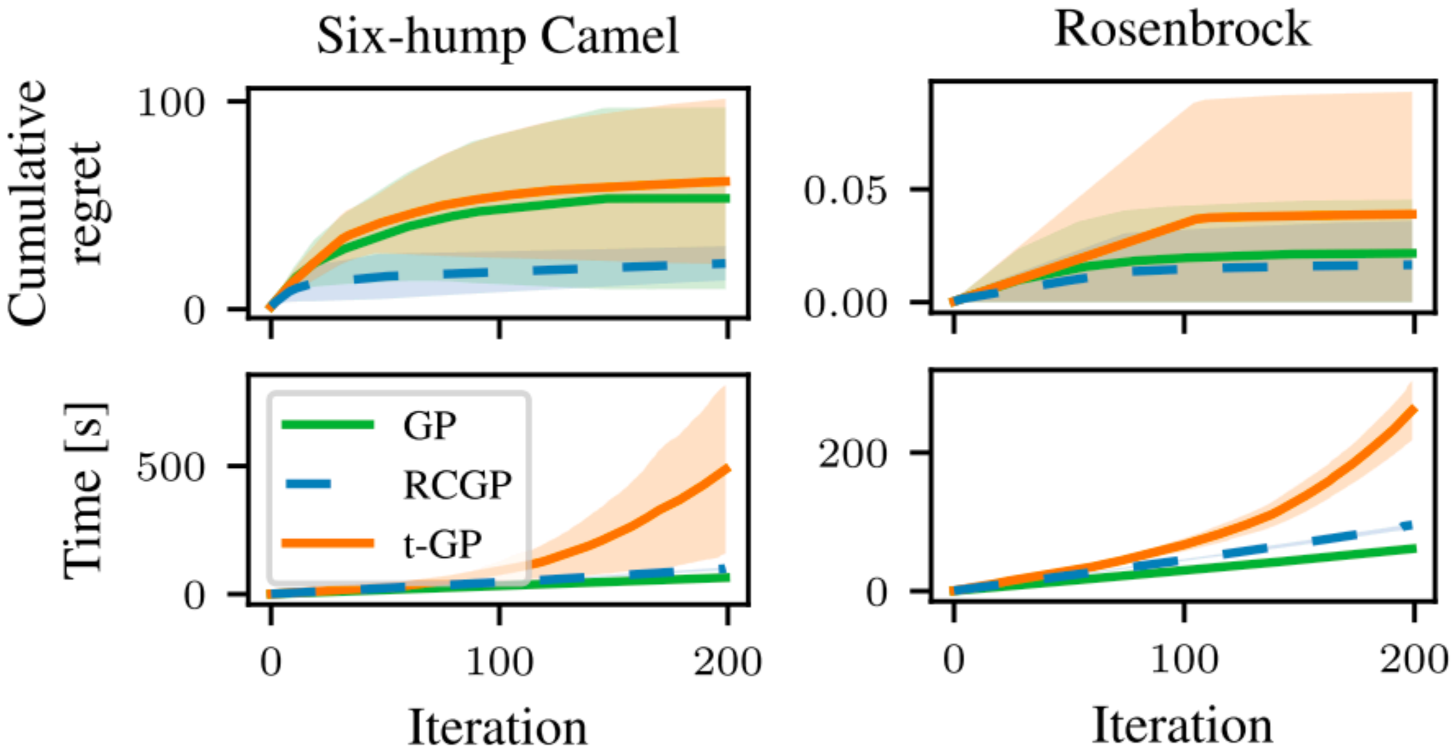
Most of the difference between GP and RCGP comes down to adaptive optimisers for hyper parameter optimisation

Robust Bayesian Optimisation

- In Bayesian optimisation, the GP posterior is used to create an acquisition function. Our RCGPs naturally lead to robust acquisition functions!



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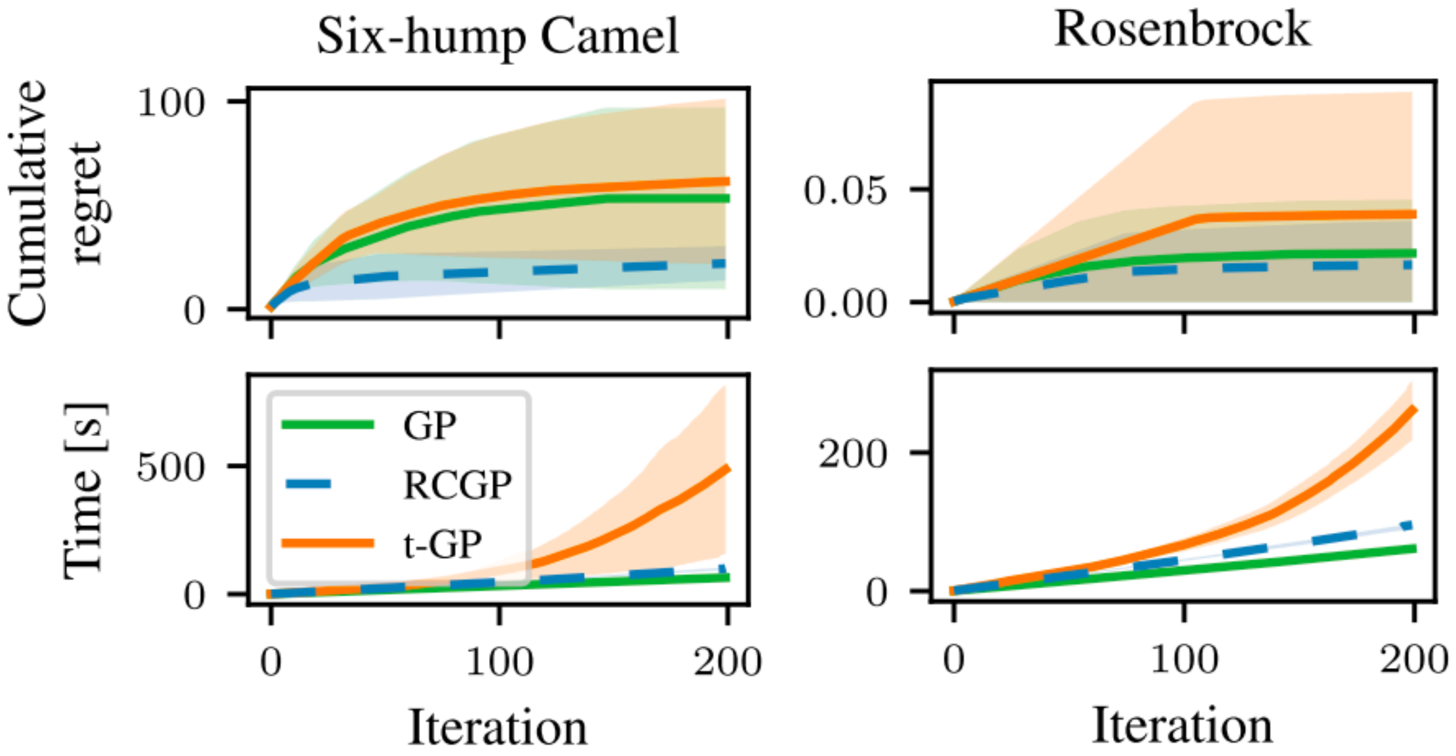
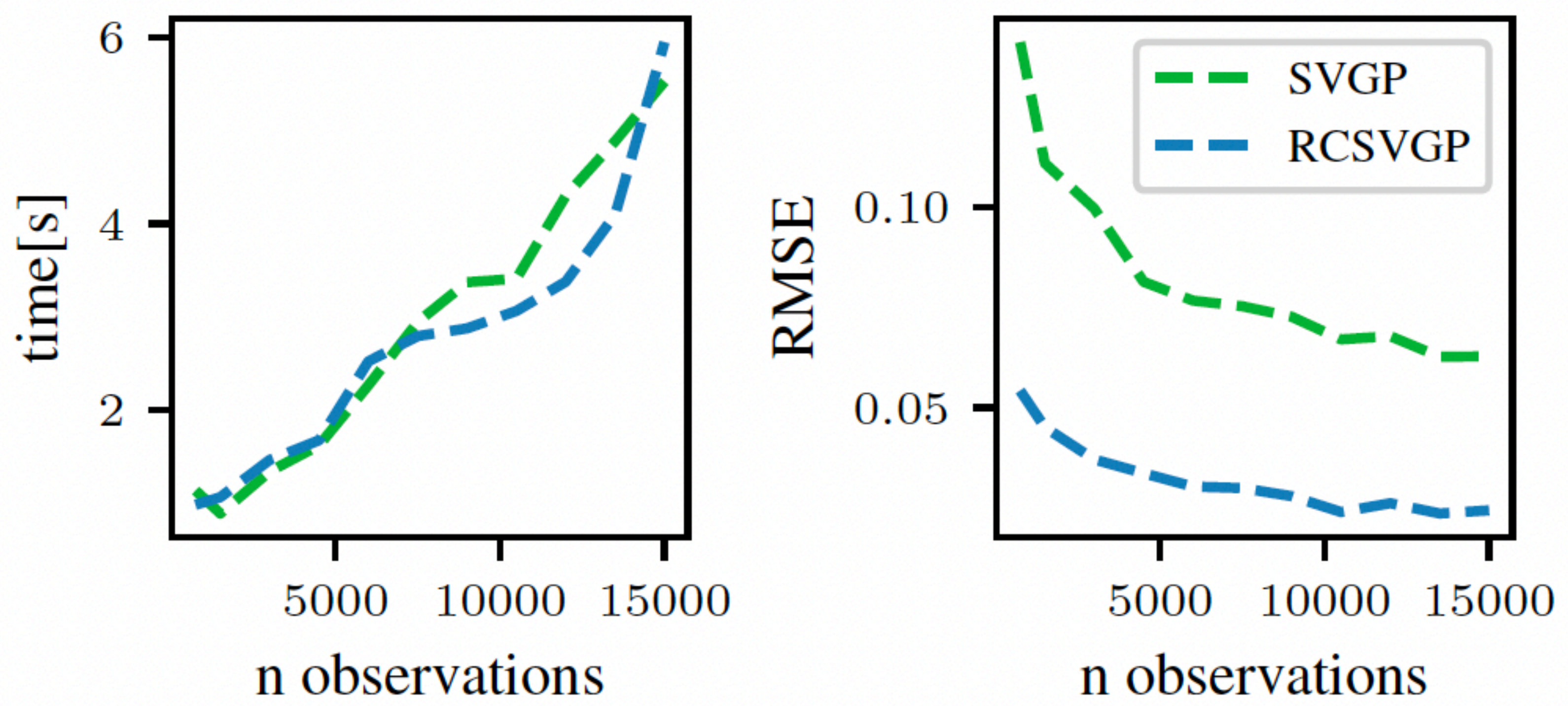


Robust!

Fast!

Robust SVGPs

- Sparse Variational GPs (SVGPs) is an approximate GP method which reduces significantly the cost of GPs from $O(n^3)$ to $O(nm^2)$ where m is small. Our approach naturally leads to a robust version!



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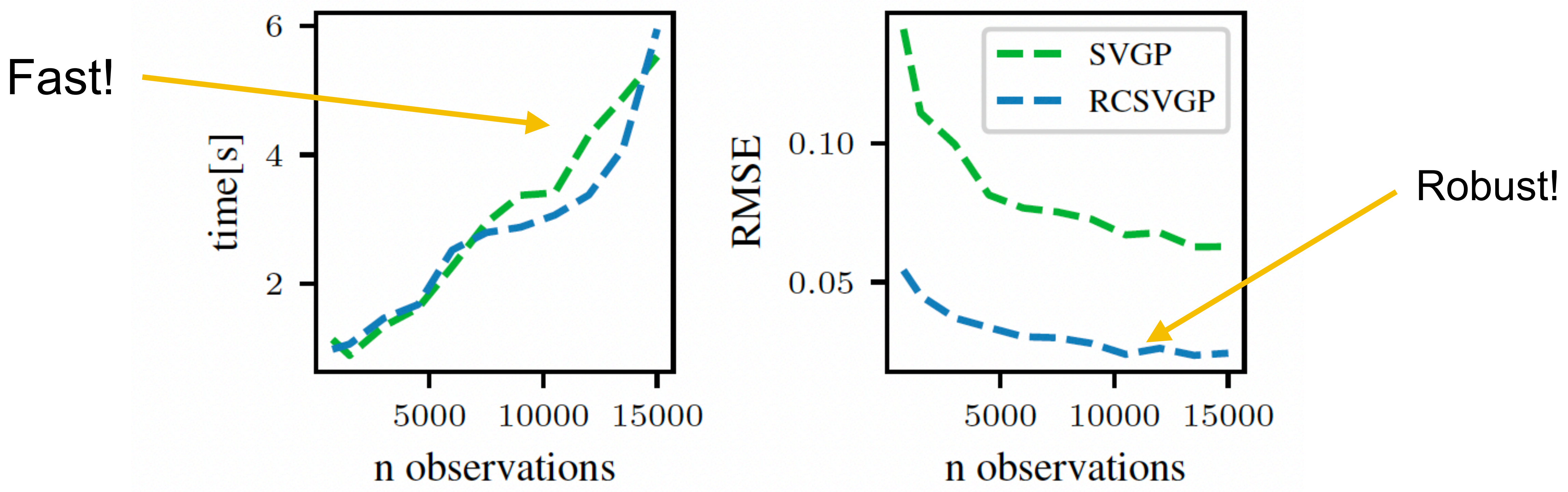
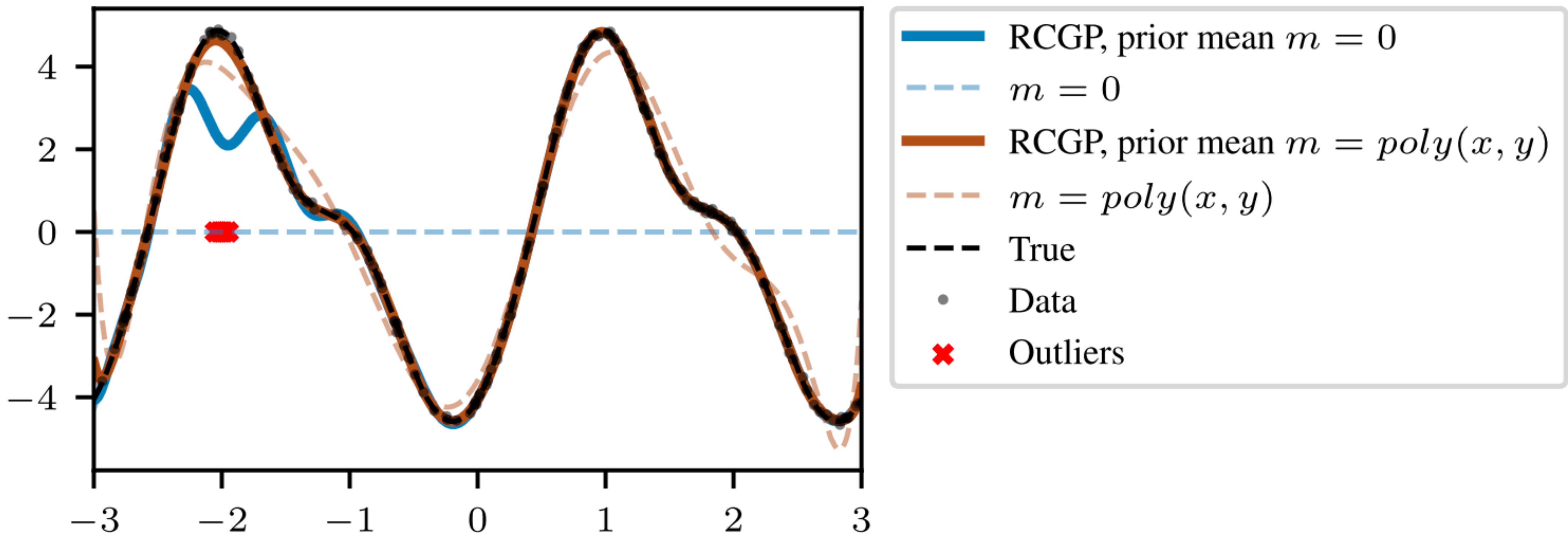


A drawback of the current approach

- It relies heavily on having a good mean function….

$$w(x, y) = \left(1 + \frac{(y - m(x))^2}{c^2}\right)^{-\frac{1}{2}}$$



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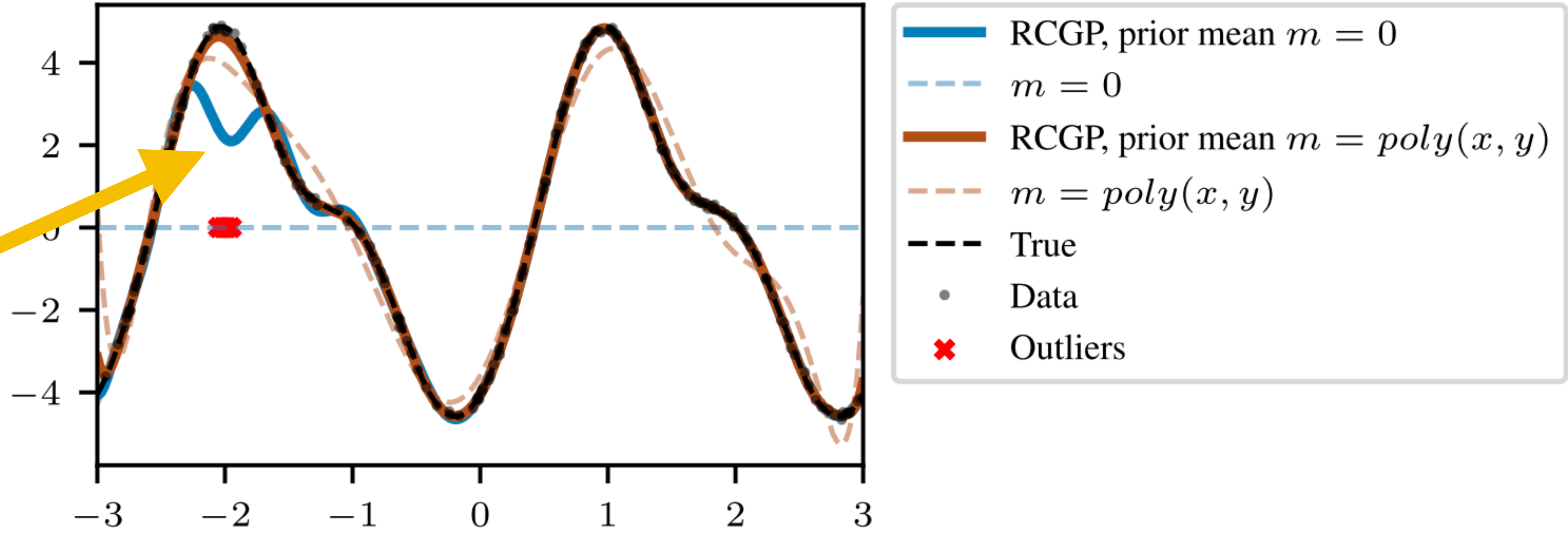

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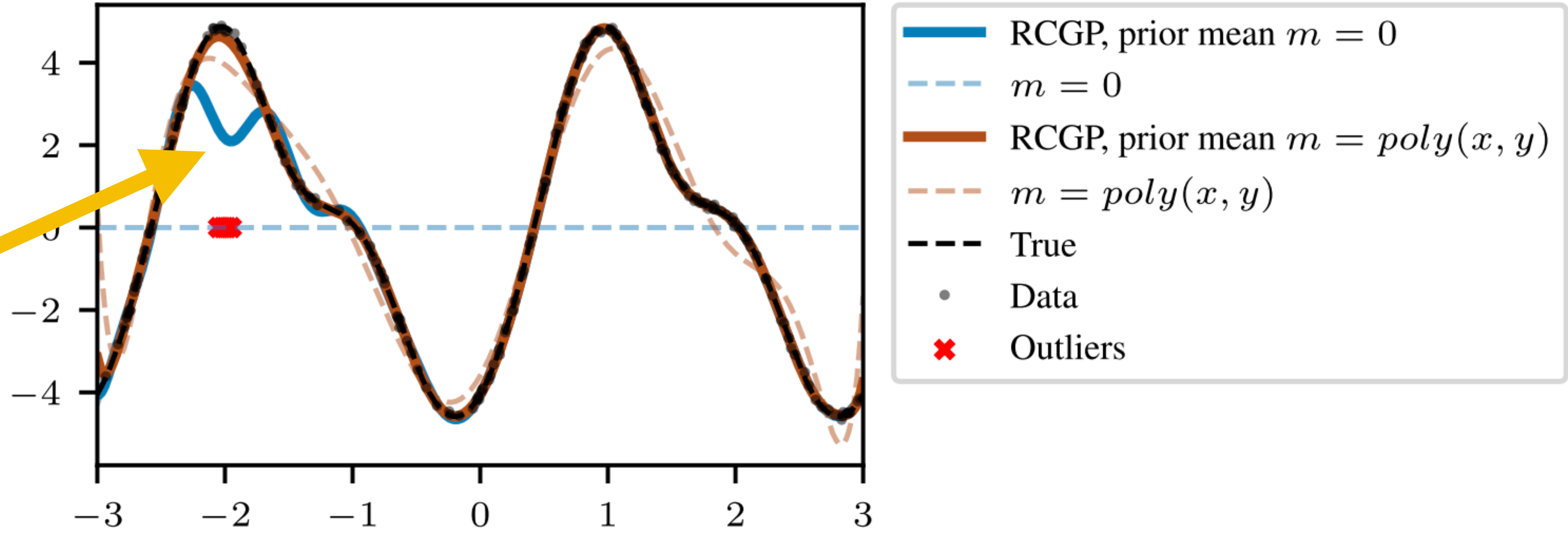
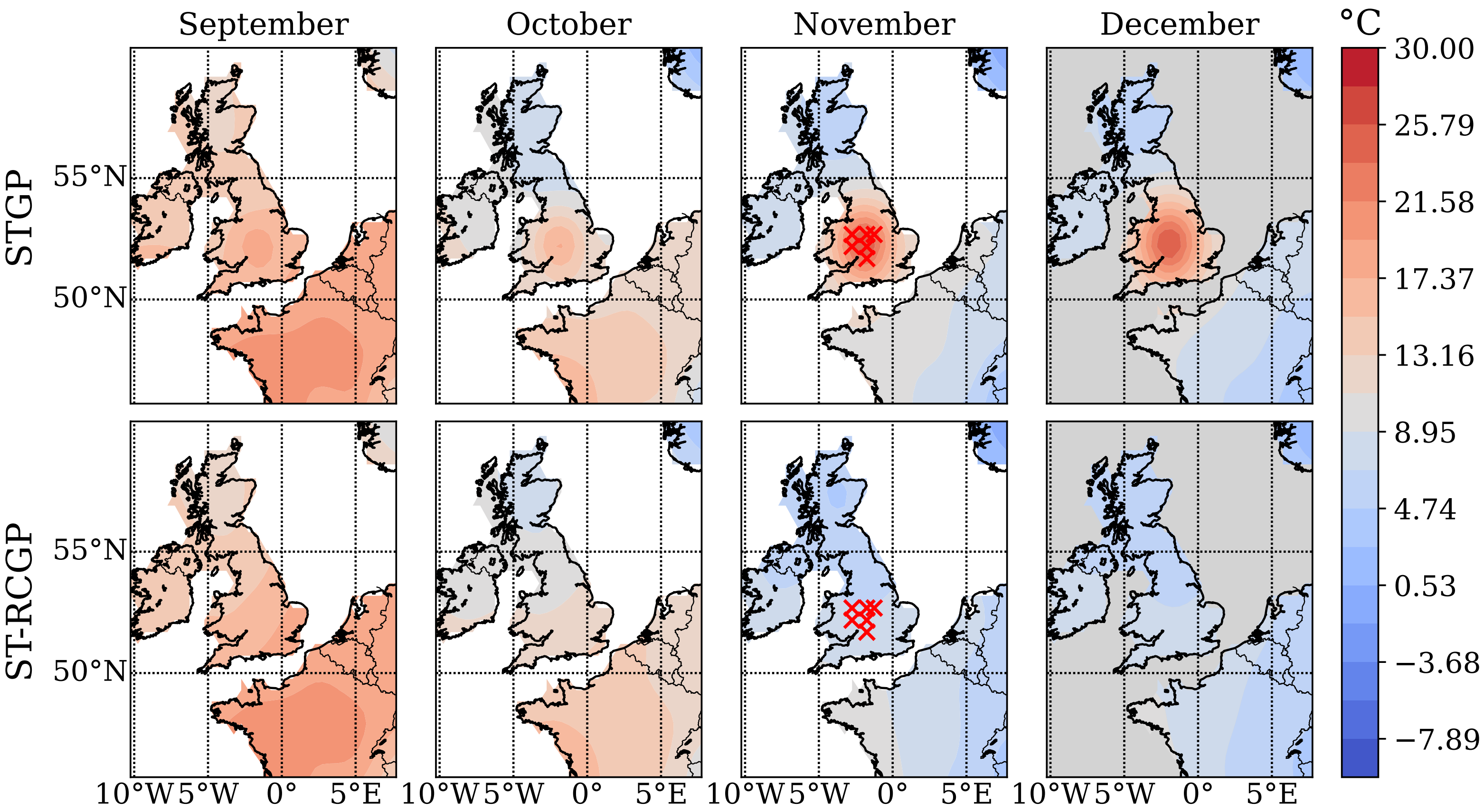


- **Potential fixes:** use a robust parametric model to fit the prior mean function first!

Linear-time spatio-temporal GPs



Paper on arXiv soon….

The cost is $O(n)$ where n is the number of time points + much easier to pick weights!

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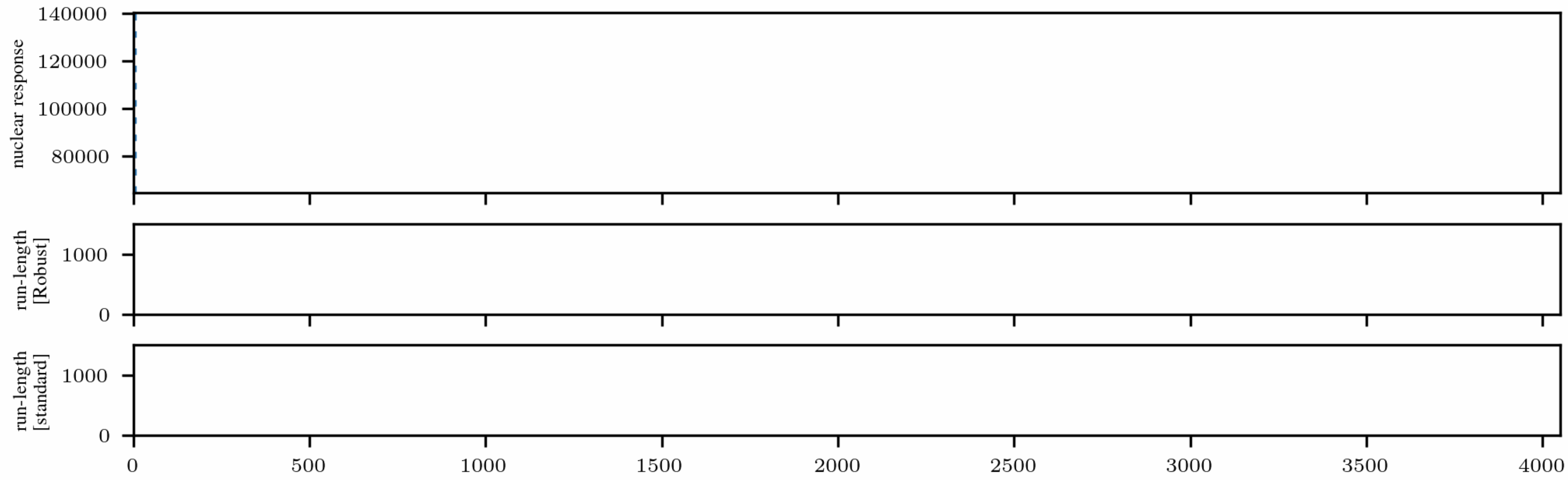
- This type of approach is also useful way beyond the GP world….!

Related work (online change point detection)



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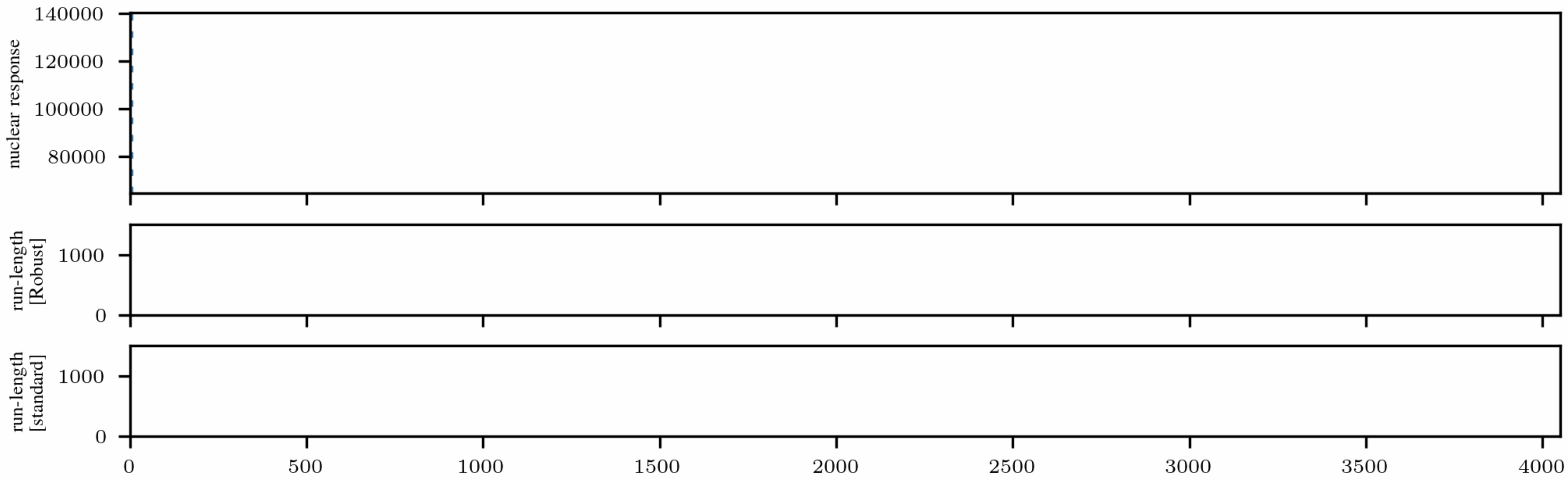

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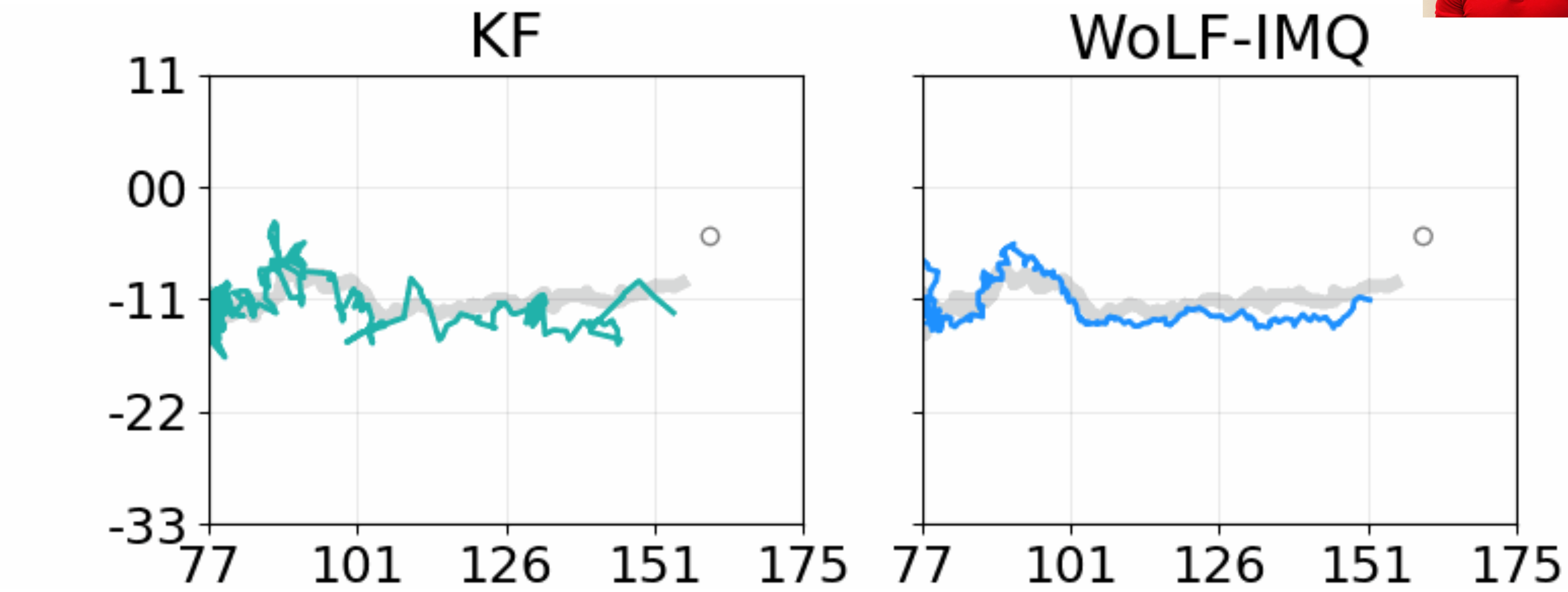



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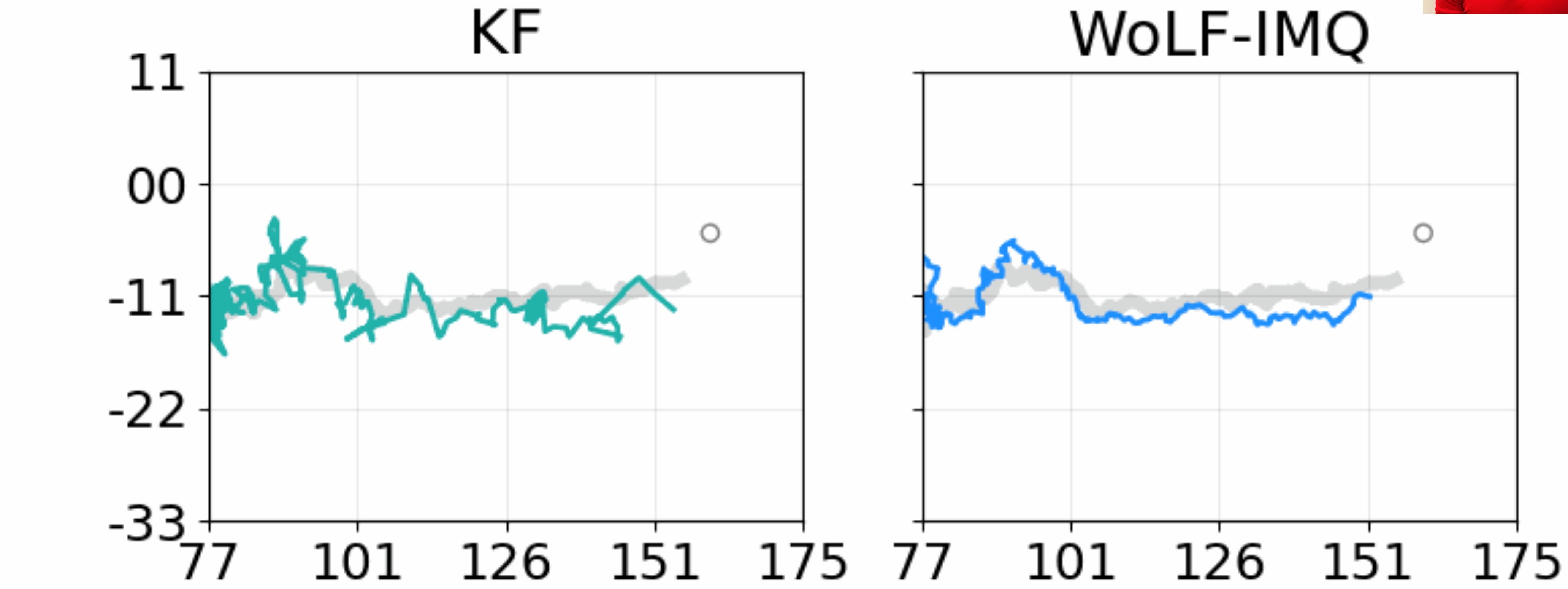

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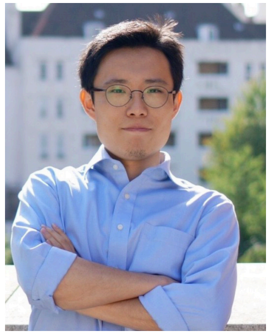
Related work (intractable likelihoods)



- Robust and conjugate generalised Bayes for **continuous doubly intractable models**!

Matsubara, T., Knoblauch, J., Briol, F.-X., & Oates, C. J. (2022). Robust generalised Bayesian inference for intractable likelihoods. JRSBB, 84(3), 997–1022.

- Robust (non-conjugate but fast!) generalised Bayes for **discrete doubly intractable models**.

Matsubara, T., Knoblauch, J., Briol, F.-X., & Oates, C. J. (2023). Generalised Bayesian inference for discrete intractable likelihood. JASA, to appear.

Any Questions?

Robust and Conjugate Gaussian Process Regression

Matias Altamirano [1] François-Xavier Briol [1] Jeremias Knoblauch [1]