

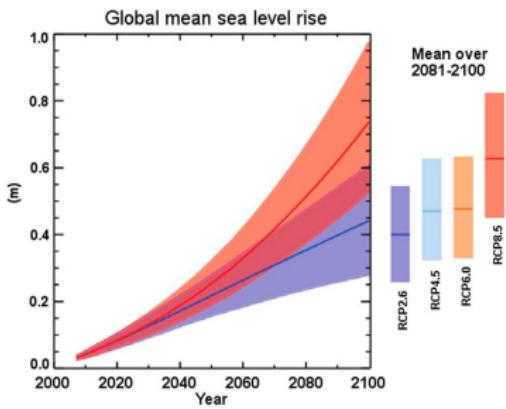
Some Bayesian methods for inverse problems

Ieva Kazlauskaitė

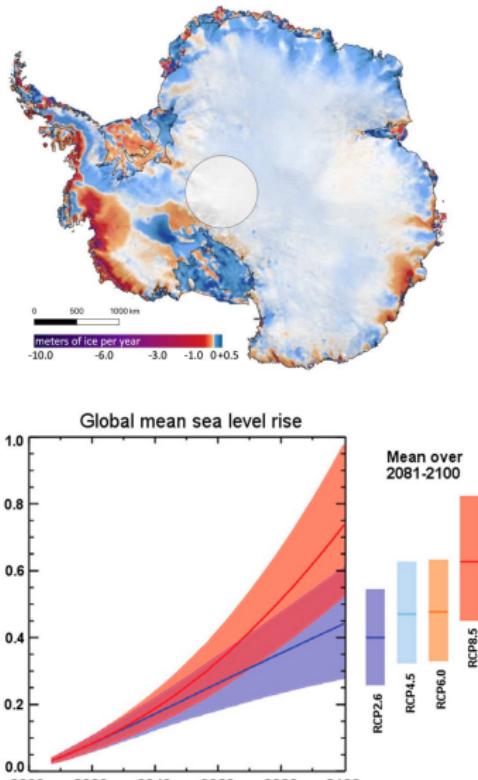
Department of Statistical Science, University College London

Motivation

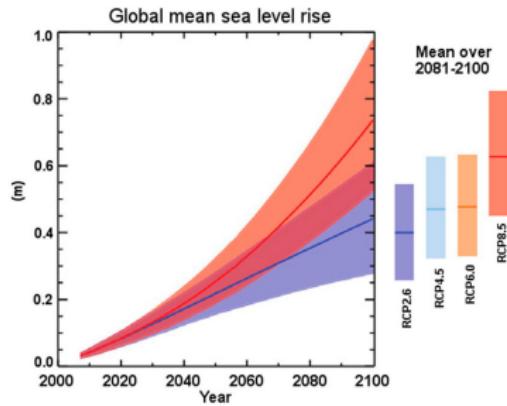
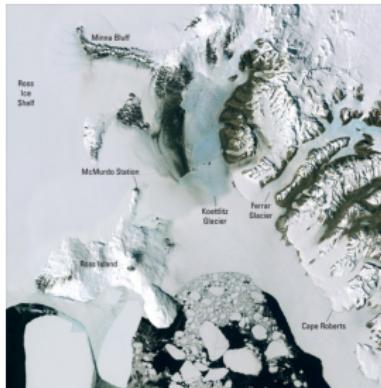
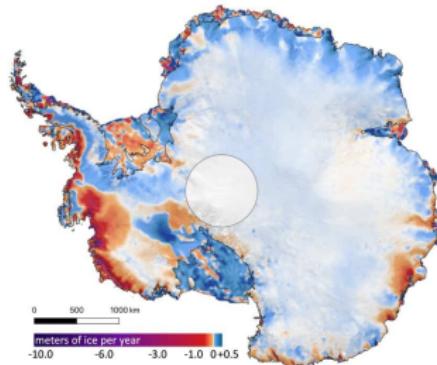
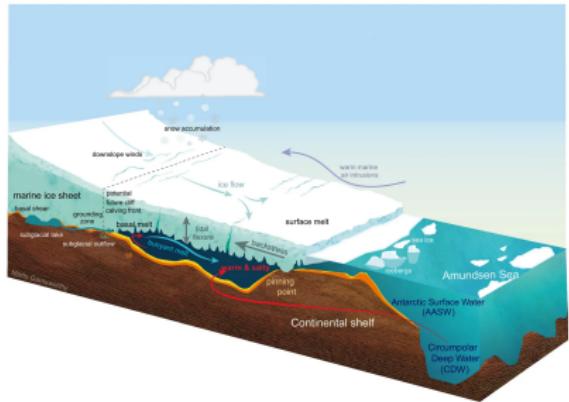
Inverse problems & UQ in complex physical models



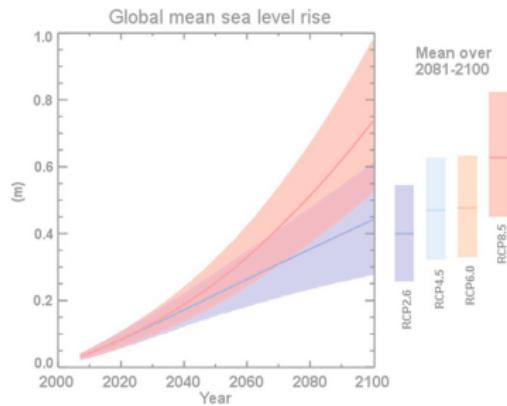
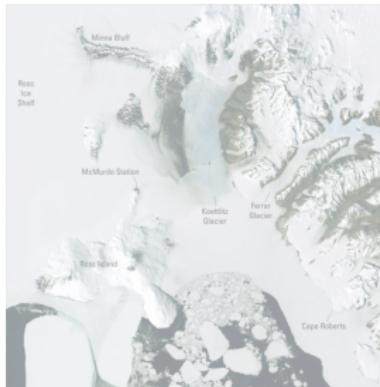
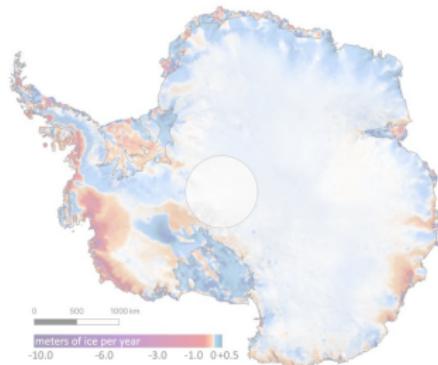
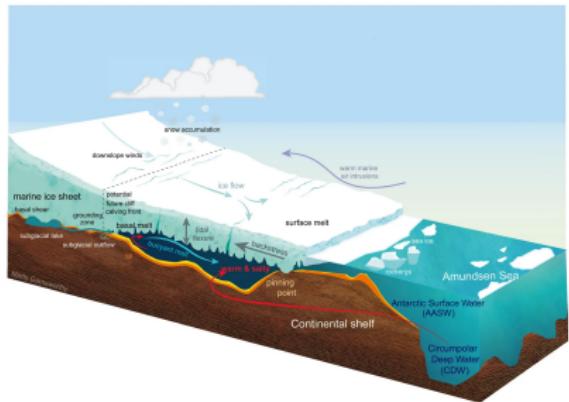
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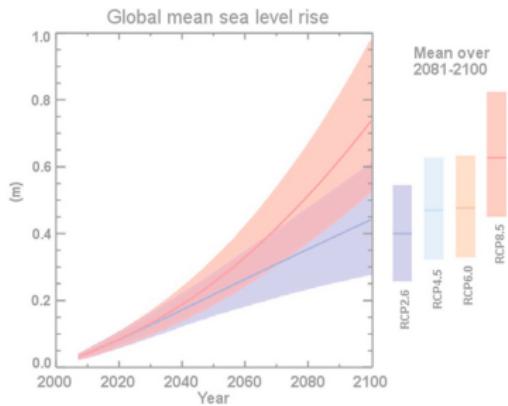
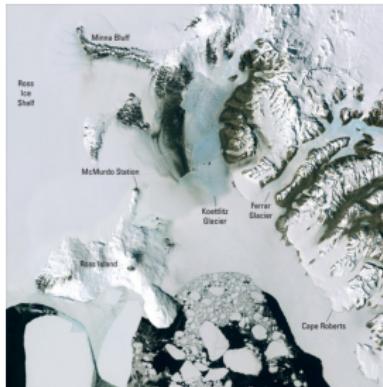
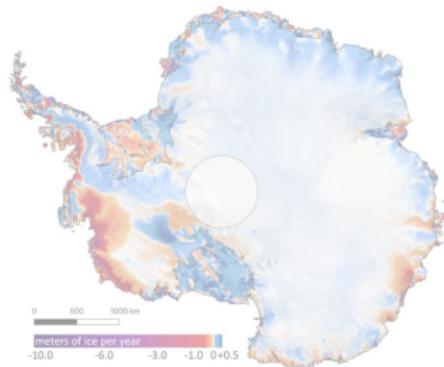
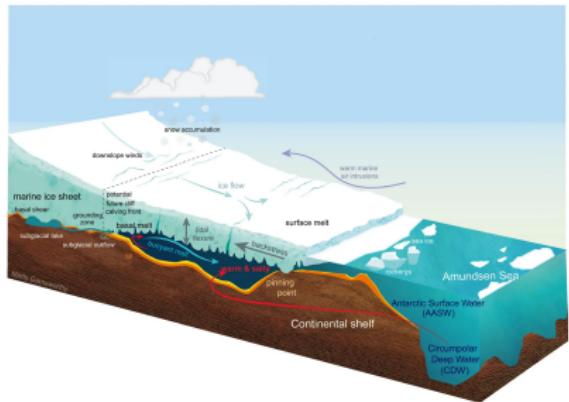
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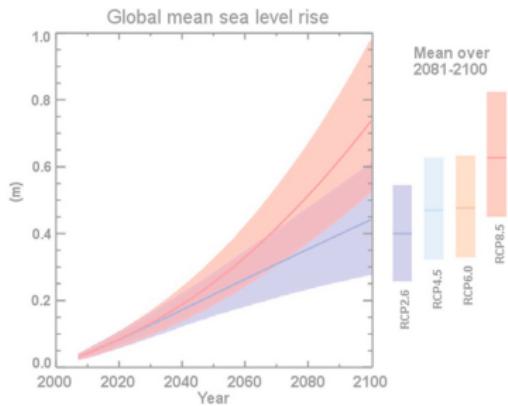
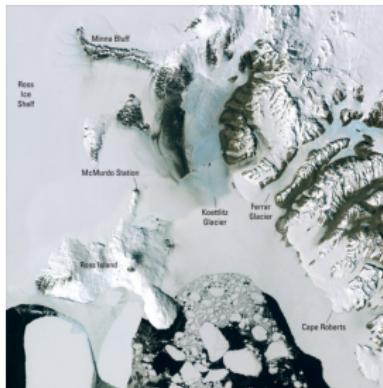
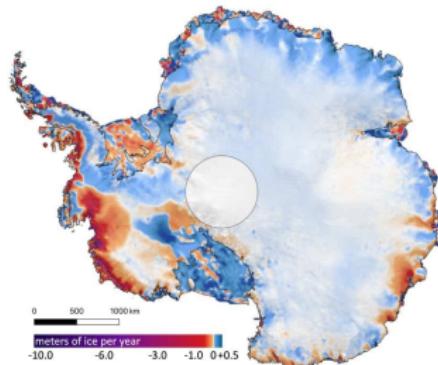
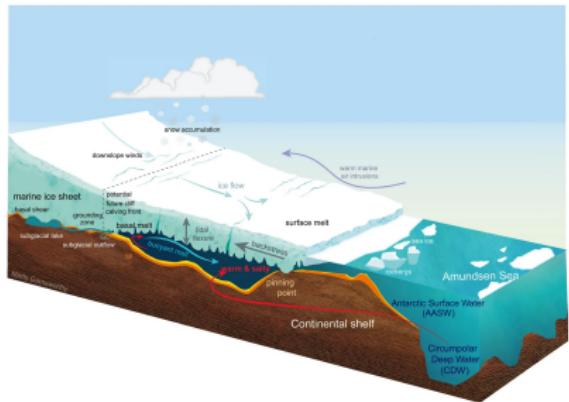
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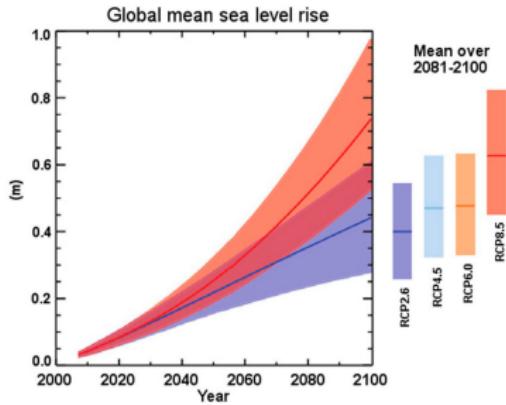
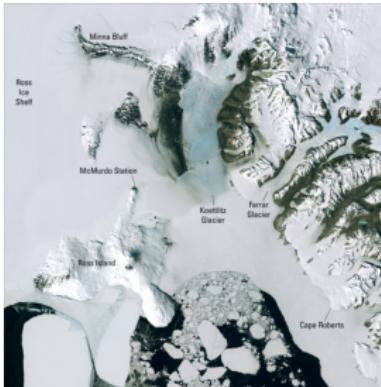
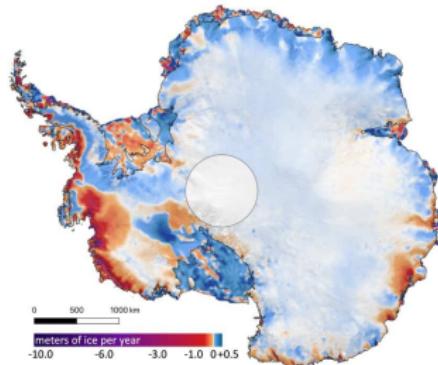
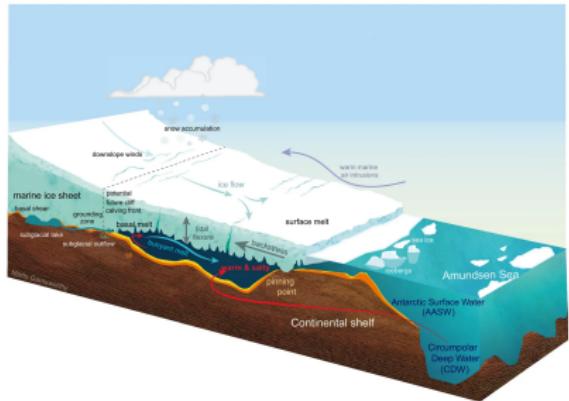
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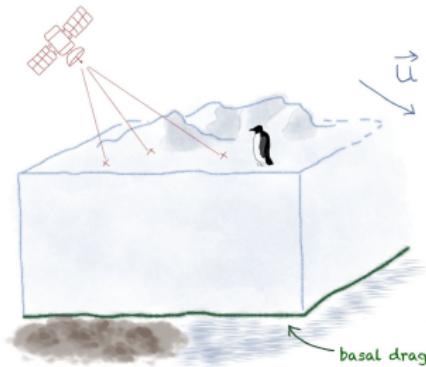
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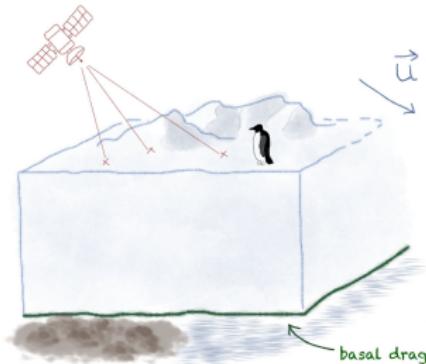
Inverse problems & UQ in complex physical models



Inverse problems in ice sheet models



Inverse problems in ice sheet models



Stokes flow with Robin BC:

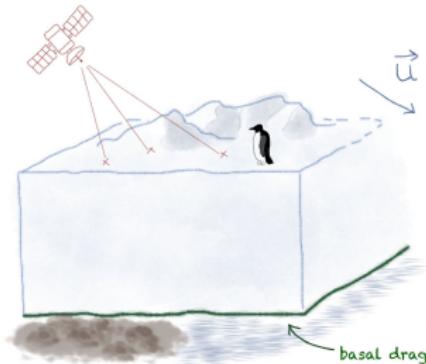
$$-\beta \Delta u + \nabla p = f \quad \text{in } \mathcal{O}$$

$$\nabla \cdot u = 0 \quad \text{in } \mathcal{O}$$

$$\partial_\nu u - \rho v + \theta u = 0 \quad \text{on } \partial\mathcal{O}$$

where f is forcing, β is viscosity, and θ is the unknown boundary parameter.

Inverse problems in ice sheet models



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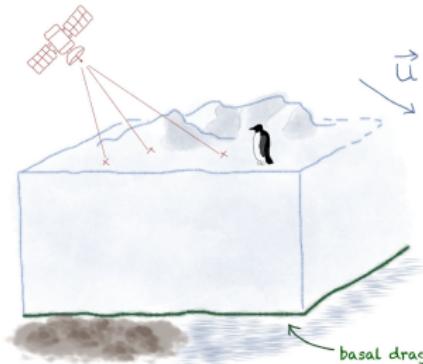
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The forward map $\mathcal{G}_\theta : \theta \mapsto u$.

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Regression problem:

$$Y_i = \mathcal{G}_\theta(X_i) + \varepsilon_i, \quad \varepsilon_i \stackrel{\text{iid}}{\sim} N(0, 1)$$

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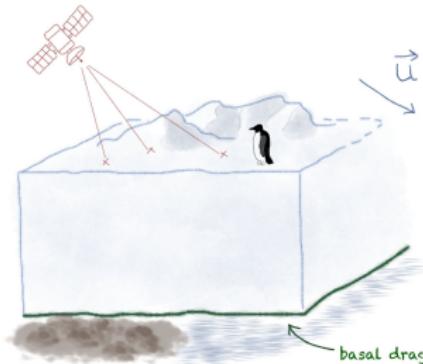
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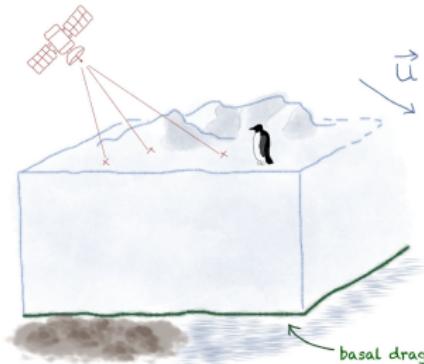
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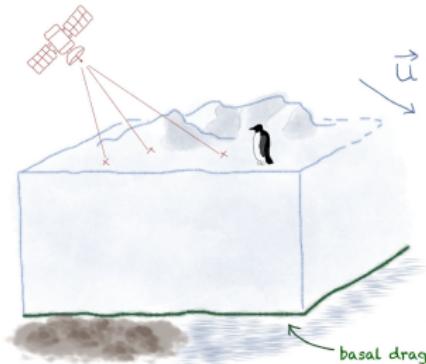
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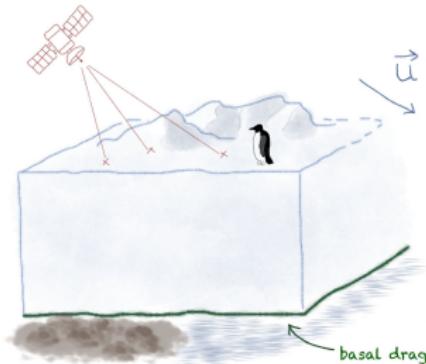
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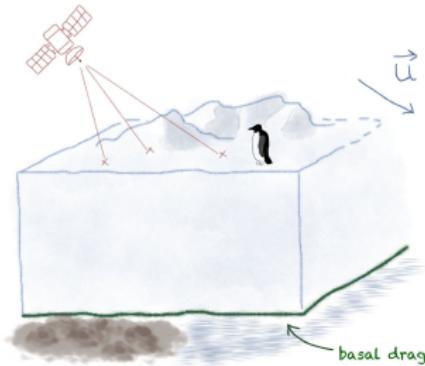
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- ▶ \mathcal{G} is 'smoothing'.

Ice sheet simulator / model /
solver $G_\theta(x_i)$

$$G_\theta(x) = u$$

\nwarrow viscosity \nearrow velocity

Observation
model : $y_i = u_i + \varepsilon_i$ $\varepsilon_i \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma)$

$$y_i = G_\theta(x_i) + \varepsilon_i$$

Regression
problem!

Three Bayesian approaches

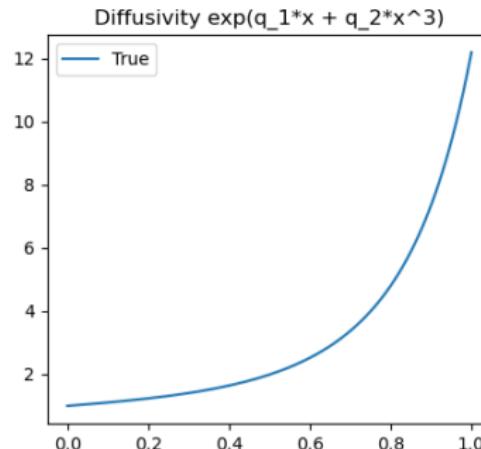
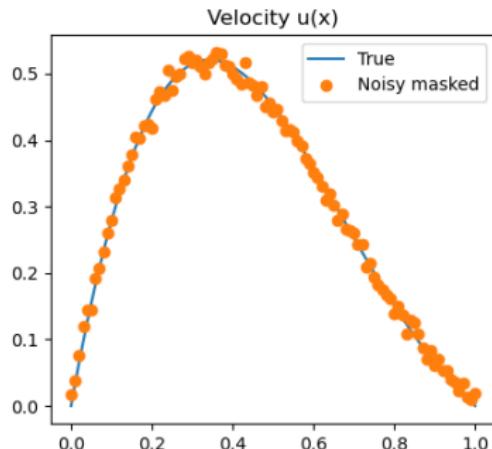
1. Bayesian approximate computation (ABC); likelihood-free inference
2. (Full) Bayesian inference
3. Bayesian optimisation (BO)

1D Poisson problem

Consider a simpler problem in 1D:

$$\begin{aligned} -\nabla \cdot \beta(x) \nabla u(x) &= f(x) && \text{in } \mathcal{O} \\ u(x) &= 0 && \text{on } \partial\mathcal{O}. \end{aligned}$$

Parameterise diffusivity as: $\beta(x) = \exp(q_1x + q_2x^3)$.



I: Approximate Bayesian computation

for $i = 1$ **to** M **do**

Pick θ

Run $\mathcal{G}_\theta(X)$

Compare $u = \mathcal{G}_\theta(X_i)$ to observations y_i

Reject if error is large

end for

I: Approximate Bayesian computation

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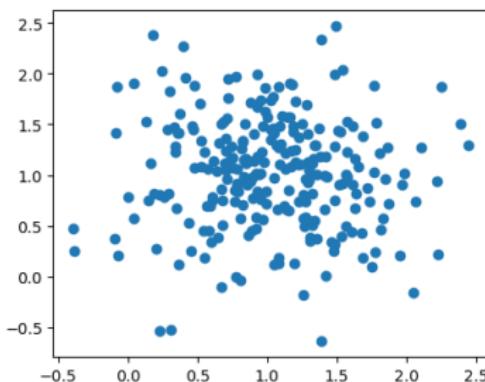
Pick $\theta \propto \text{Prior}(\theta)$

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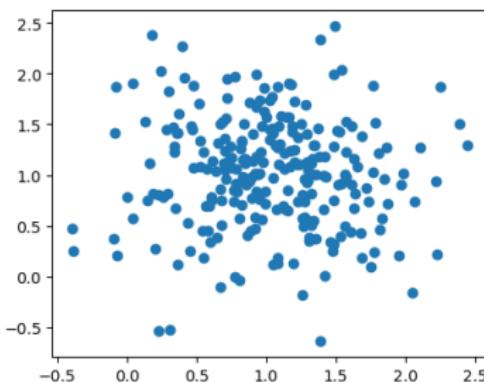
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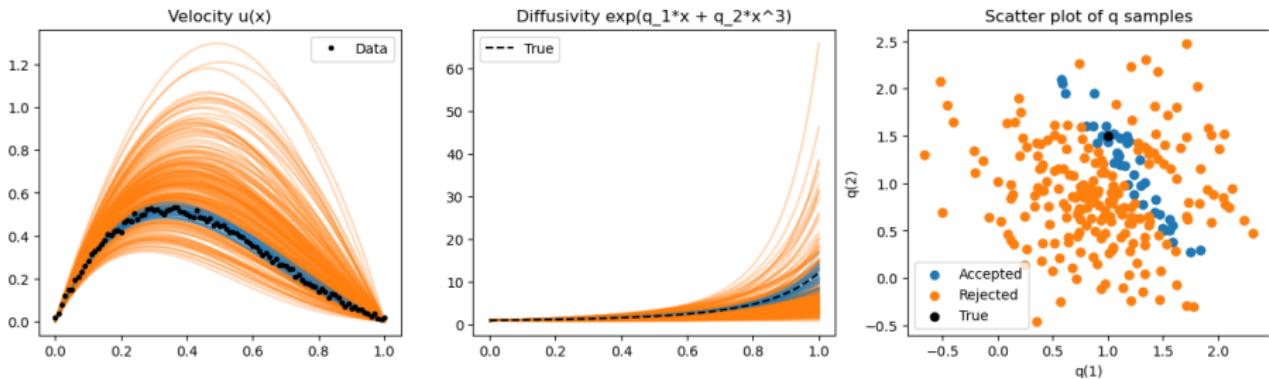
Compare $R = |\mathcal{G}_\theta(X_i) - y_i|^2$

Accept if $R < e_{\text{threshold}}$

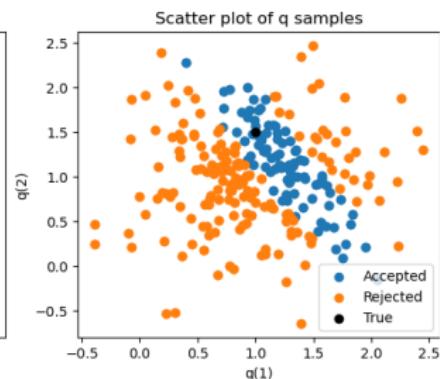
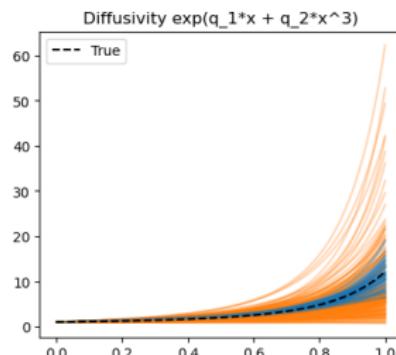
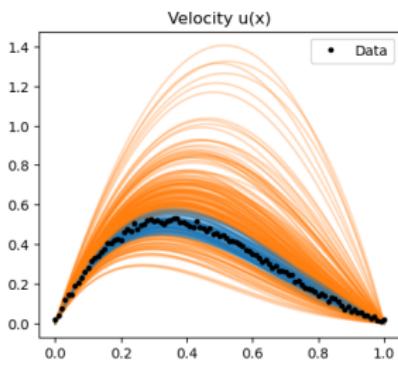
end for



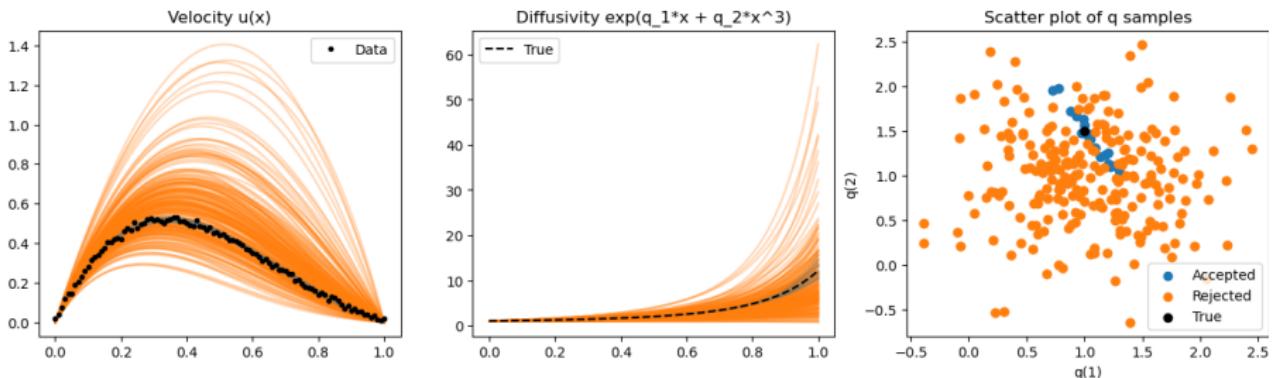
Approximate Bayesian computation



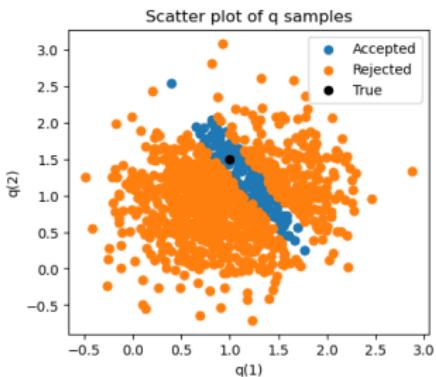
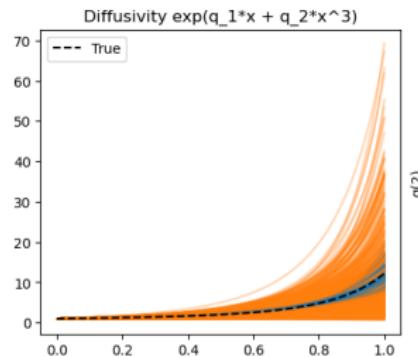
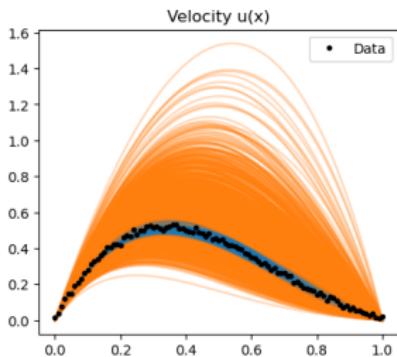
Approximate Bayesian computation: higher error threshold



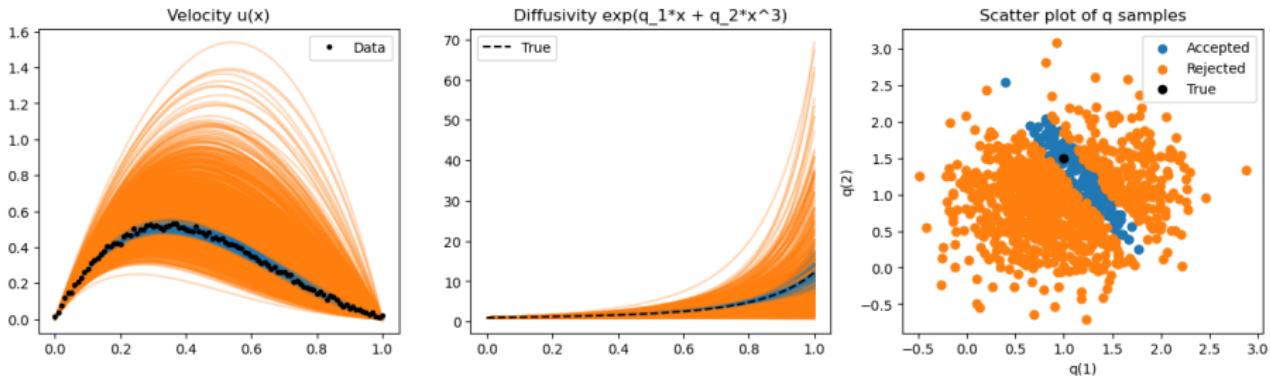
Approximate Bayesian computation: lower error threshold



Approximate Bayesian computation: More samples

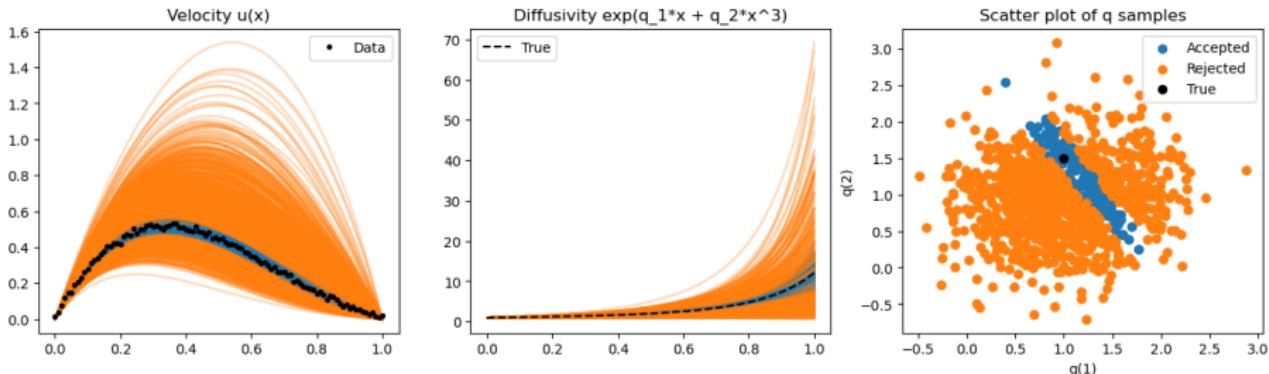


Approximate Bayesian computation: More samples



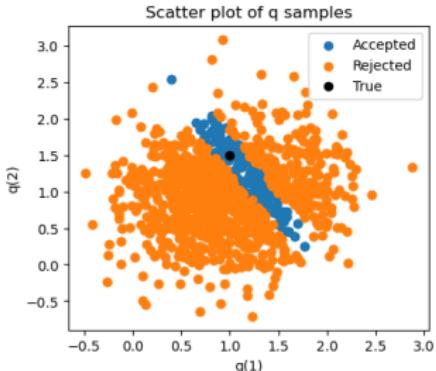
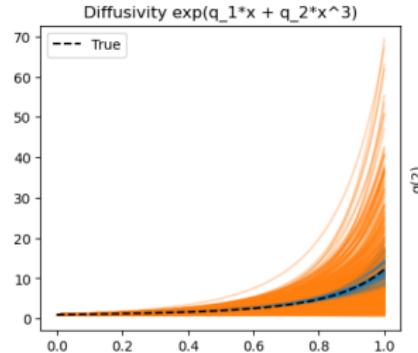
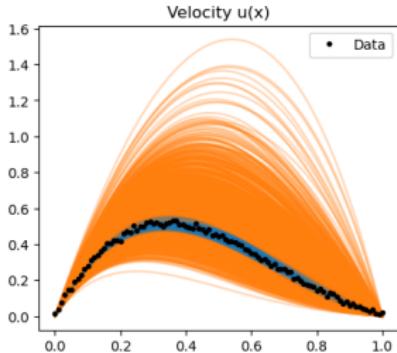
- ▶ Does not need explicit likelihood

Approximate Bayesian computation: More samples



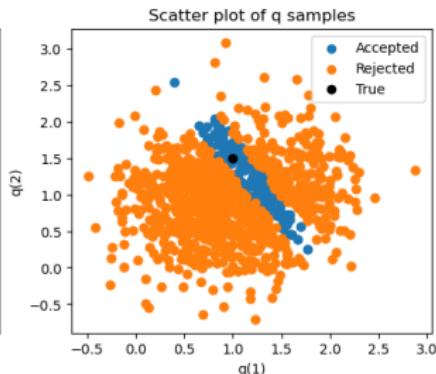
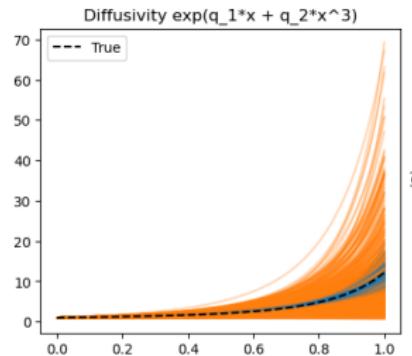
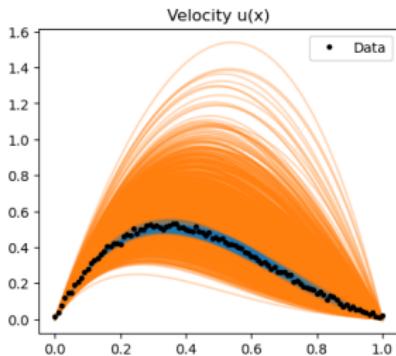
- ▶ Does not need explicit likelihood
- ▶ Easy to implement

Approximate Bayesian computation: More samples



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- ▶ Computationally expensive/wasteful

Approximate Bayesian computation: More samples



- ▶ Does not need explicit likelihood
- ▶ Easy to implement
- ▶ Computationally expensive/wasteful
- ▶ Approximately Bayesian

II: Bayesian inference

Recall Bayes' rule:

$$p(\theta \mid D) = \frac{p(D \mid \theta)p(\theta)}{p(D)}$$

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Inference in general:

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Inference in general:

- ▶ Sampling (Markov chain Monte Carlo)

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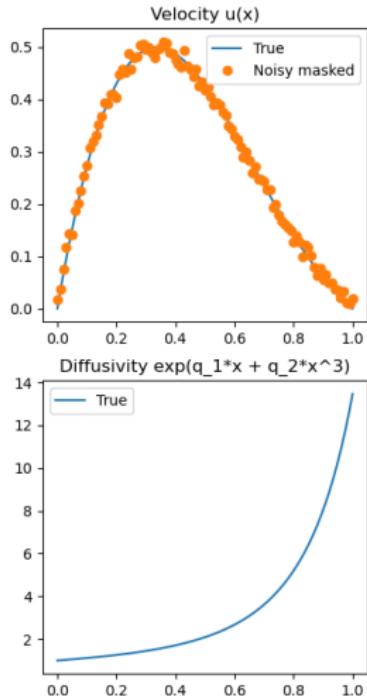
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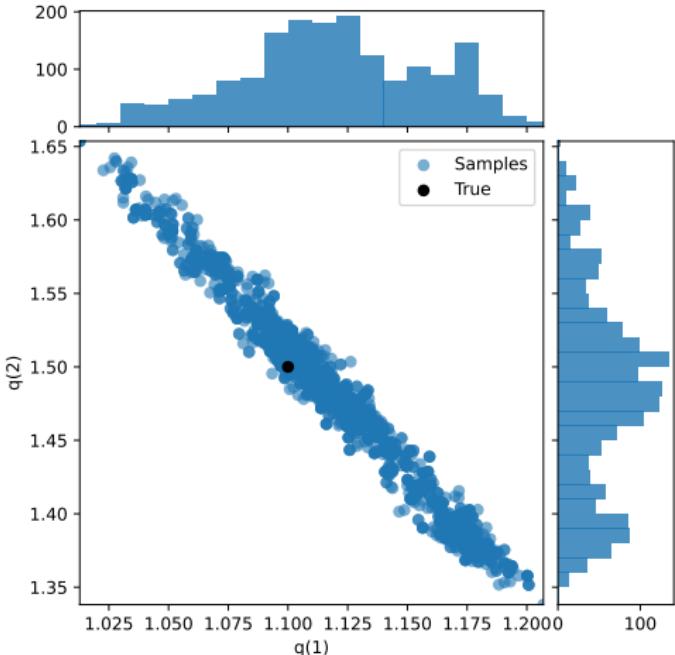
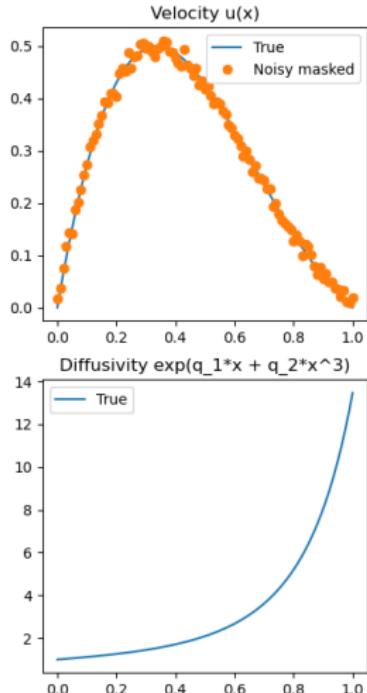
Inference in general:

- ▶ Sampling (Markov chain Monte Carlo)
- ▶ Variational inference

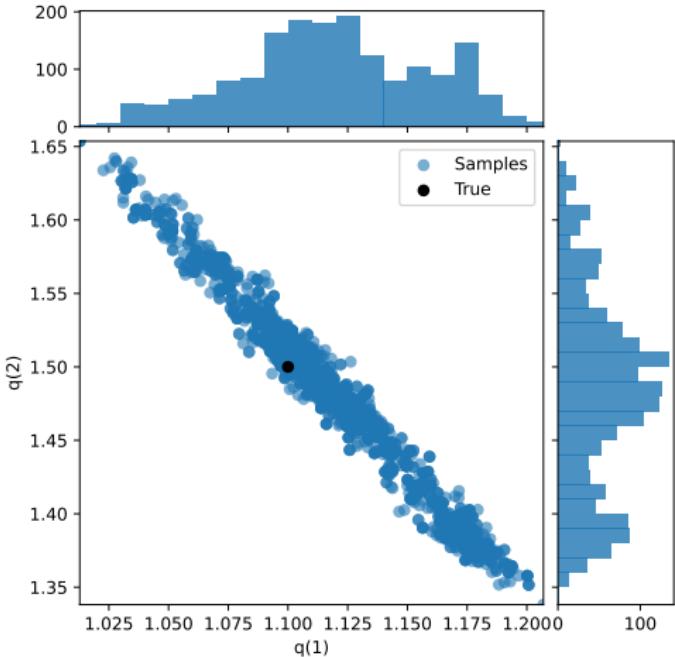
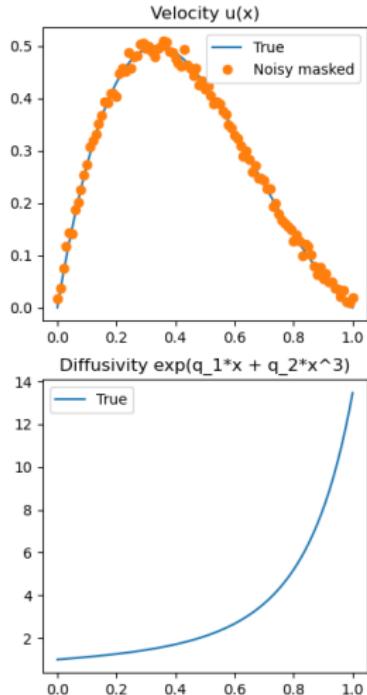
Metropolis-Hastings sampling for inference



Metropolis-Hastings sampling for inference



Metropolis-Hastings sampling for inference



Expensive!

III: Bayesian optimisation

- ▶ Global optimisation algorithm

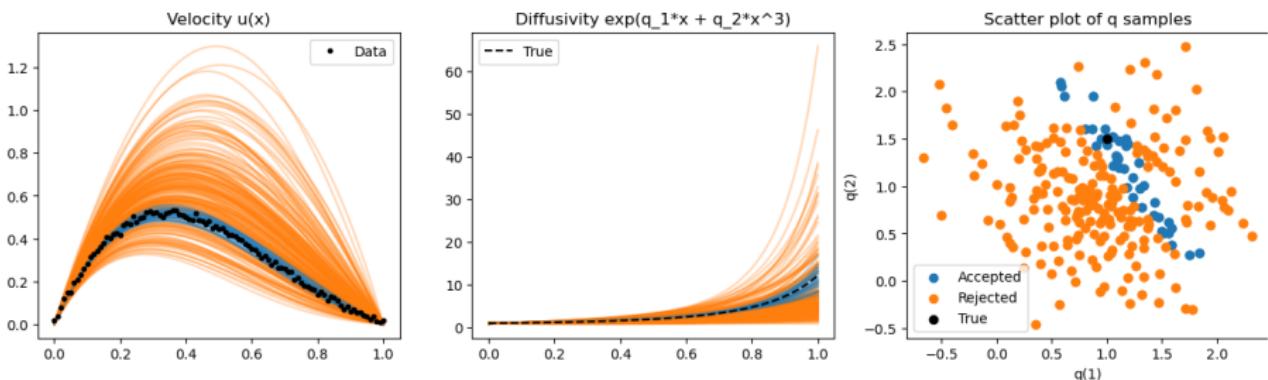
III: Bayesian optimisation

- ▶ Global optimisation algorithm
- ▶ Balances exploration and exploitation

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- ▶ Global optimisation algorithm
- ▶ Balances exploration and exploitation

Recall, for approximate Bayesian computation:



III: Bayesian optimisation

Recall, we want θ that minimises the negative log-likelihood:

$$\ell_N(\theta) = \frac{1}{2} \sum_{i=1}^N |Y_i - \mathcal{G}_\theta(X_i)|_V^2.$$

III: Bayesian optimisation

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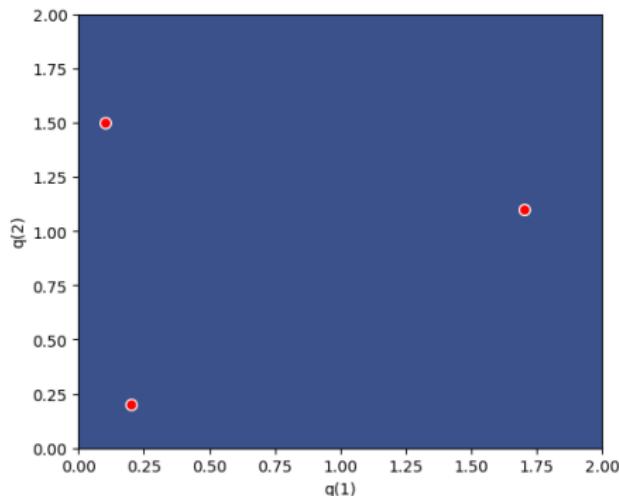
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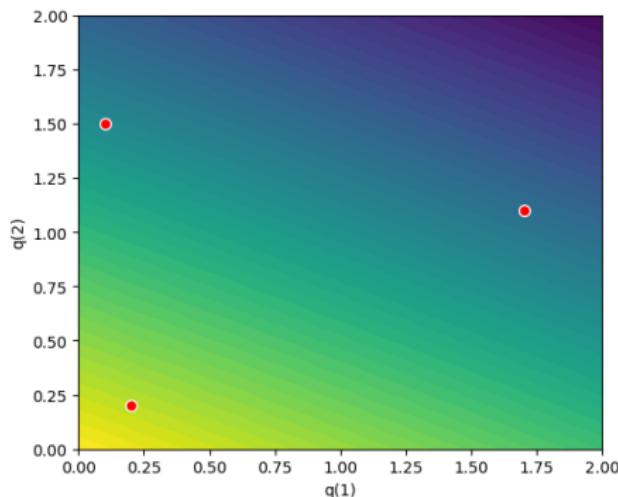


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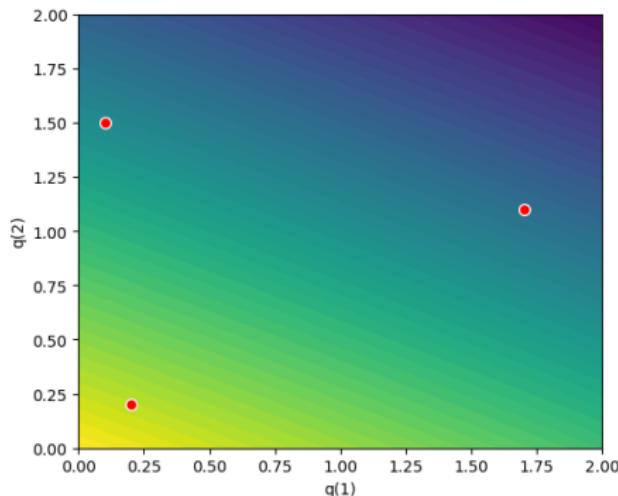
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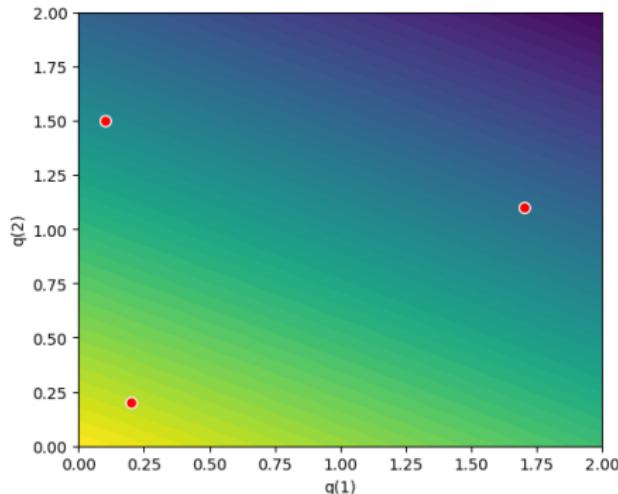
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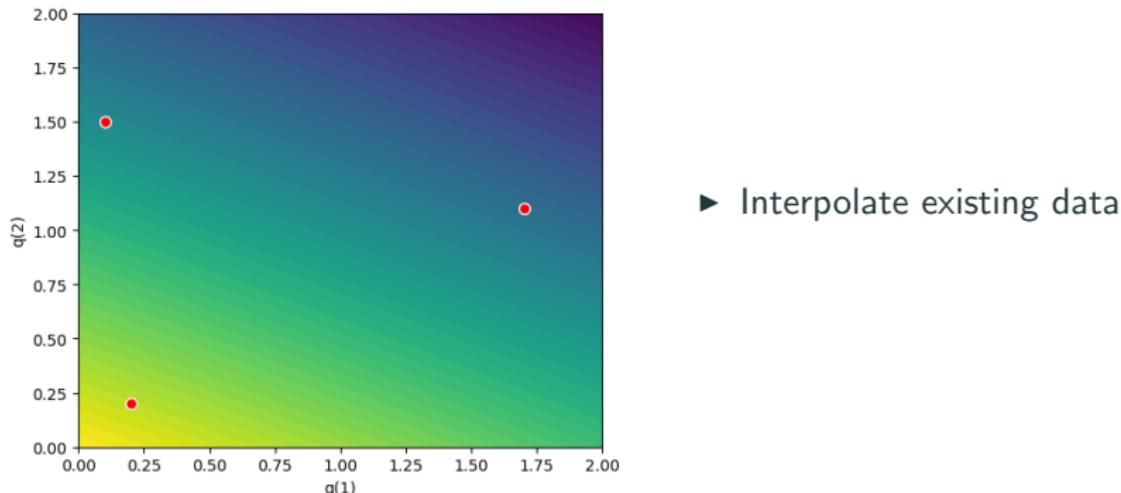
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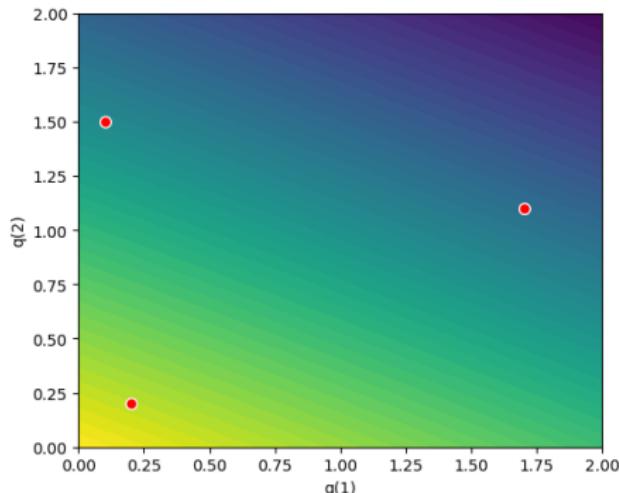
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- ▶ Quantify distance amongst data

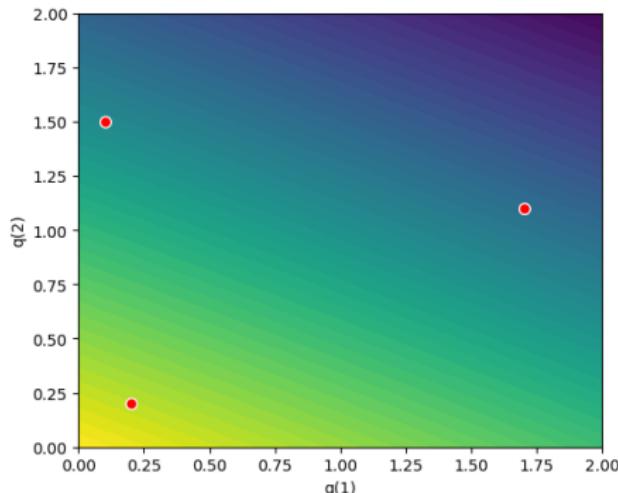
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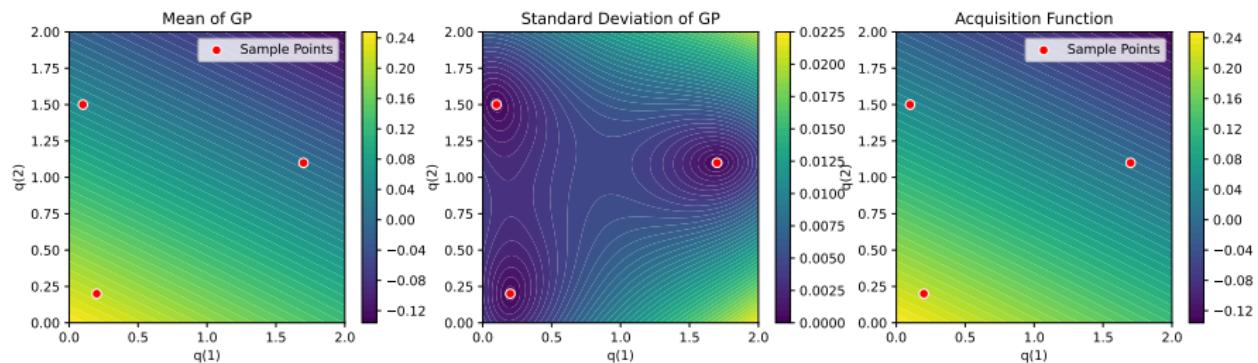
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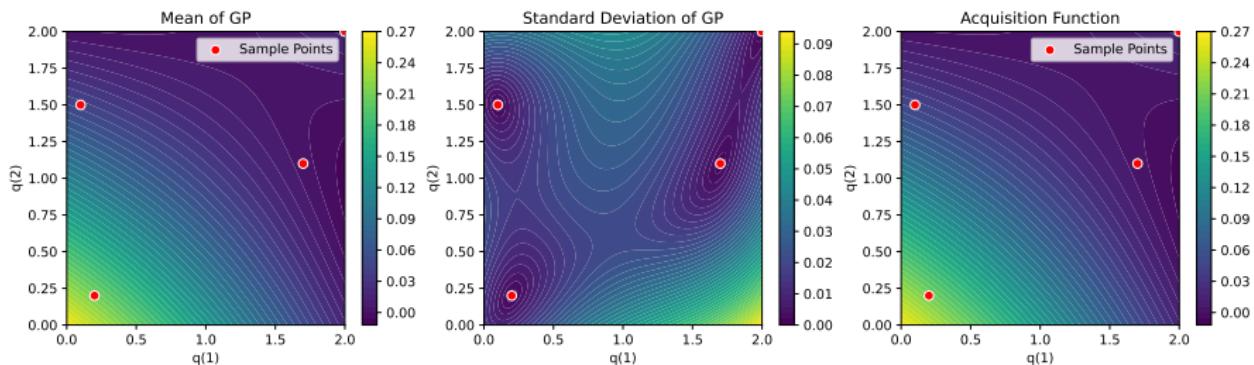
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Gaussian process!

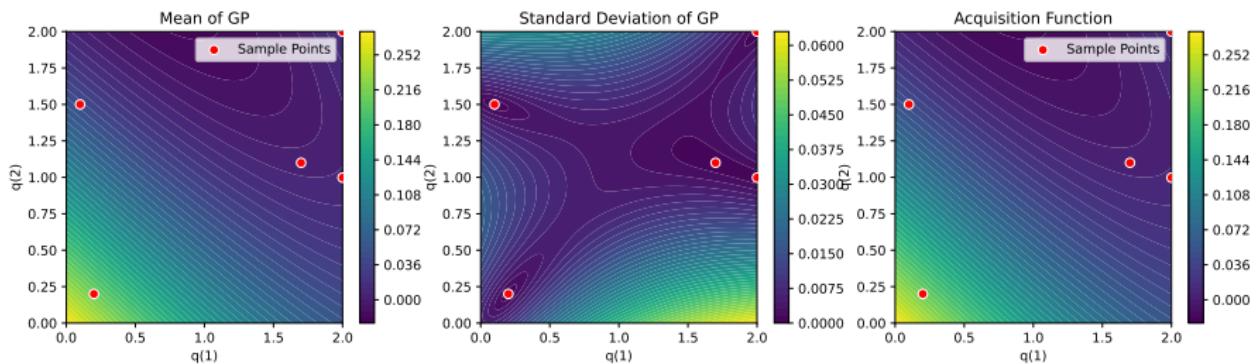
III: Bayesian optimisation: Exploitation



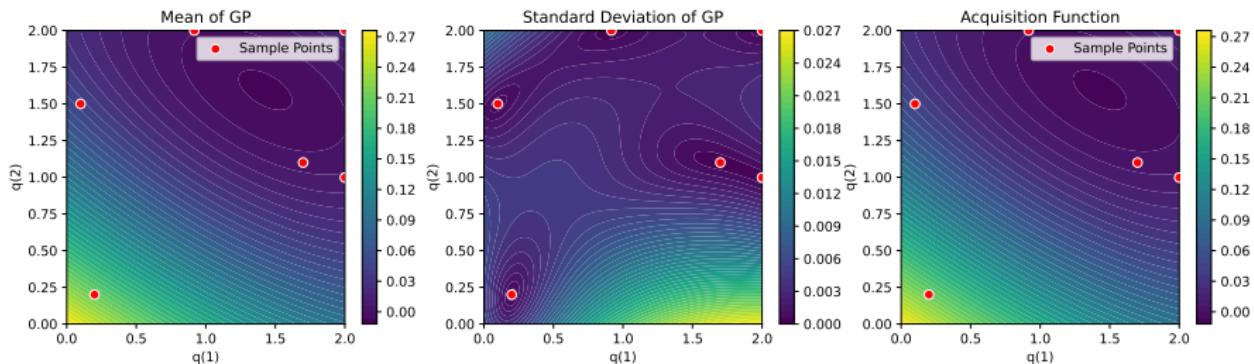
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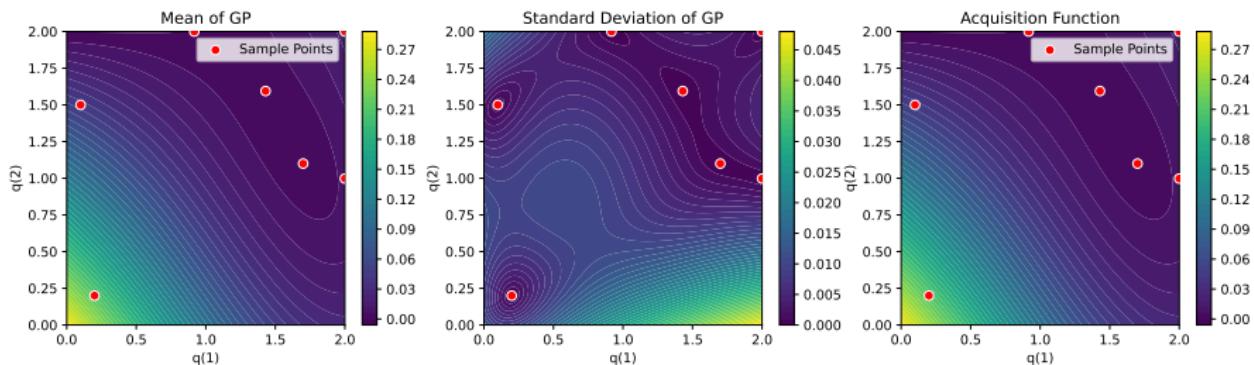
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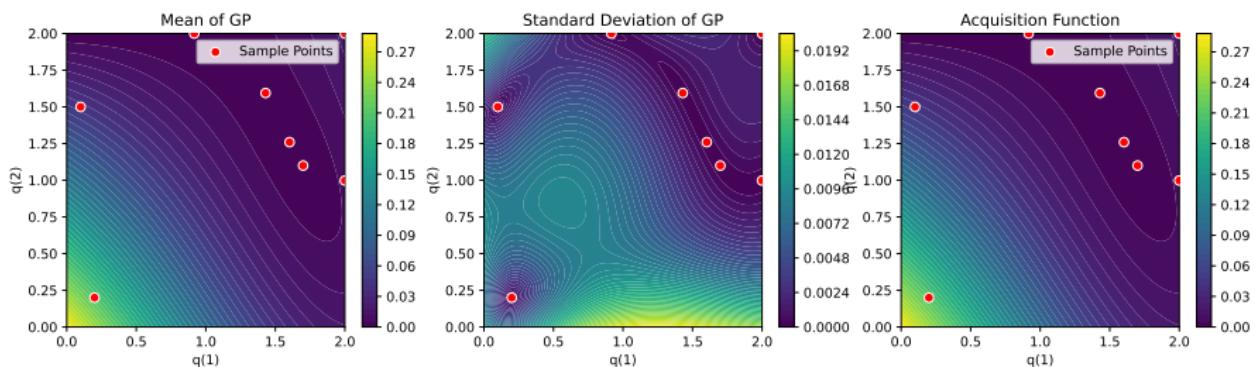
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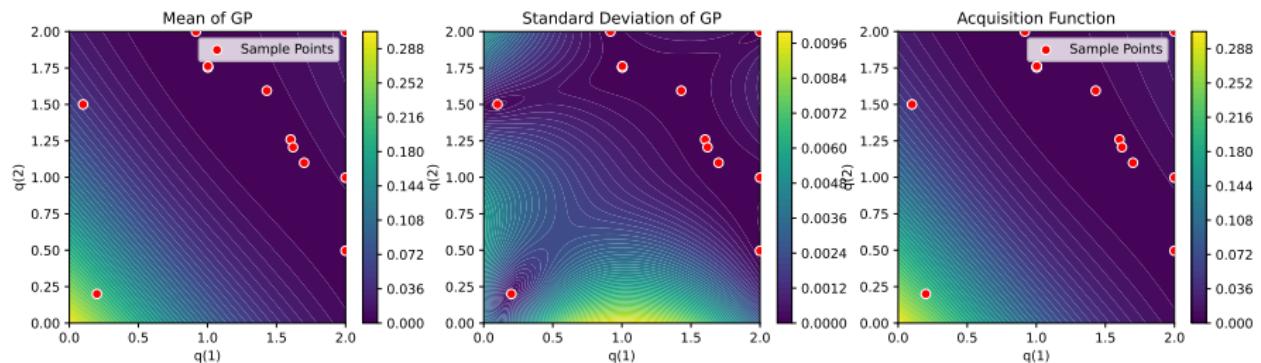
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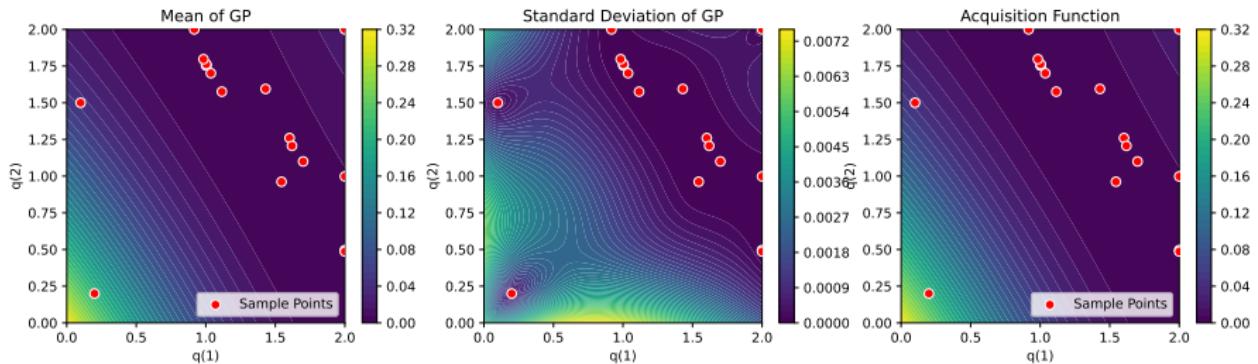
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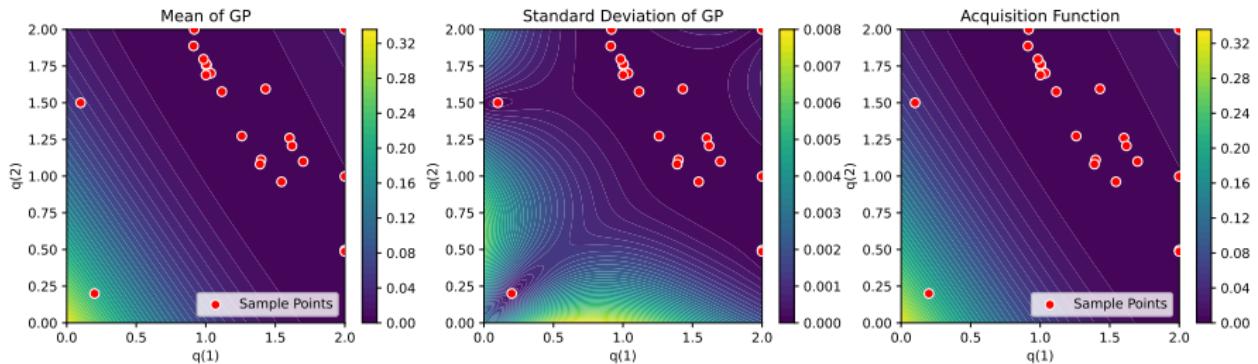
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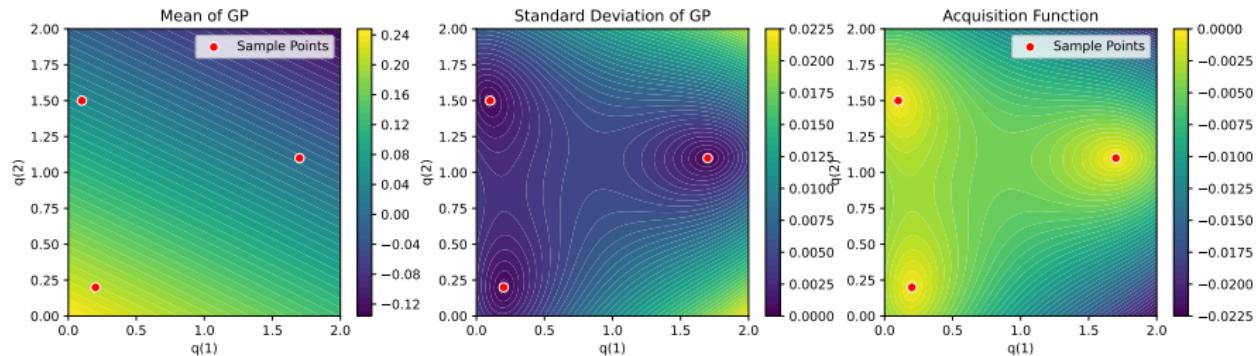


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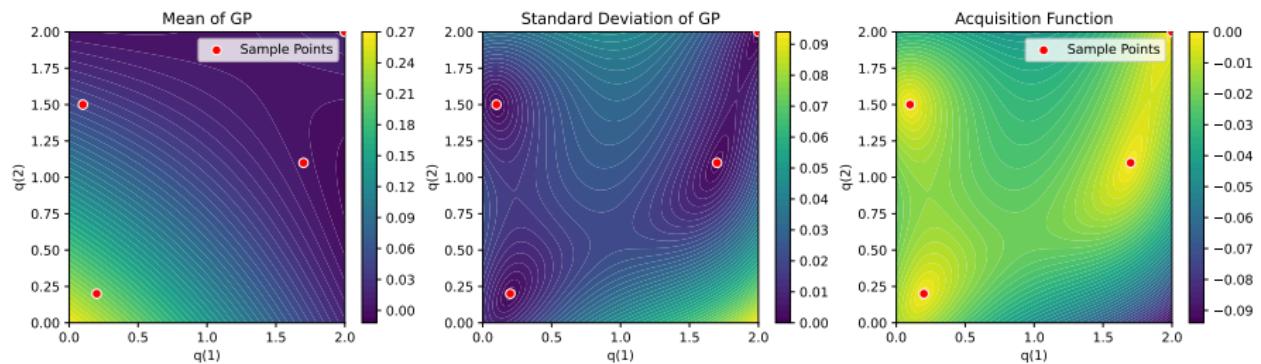


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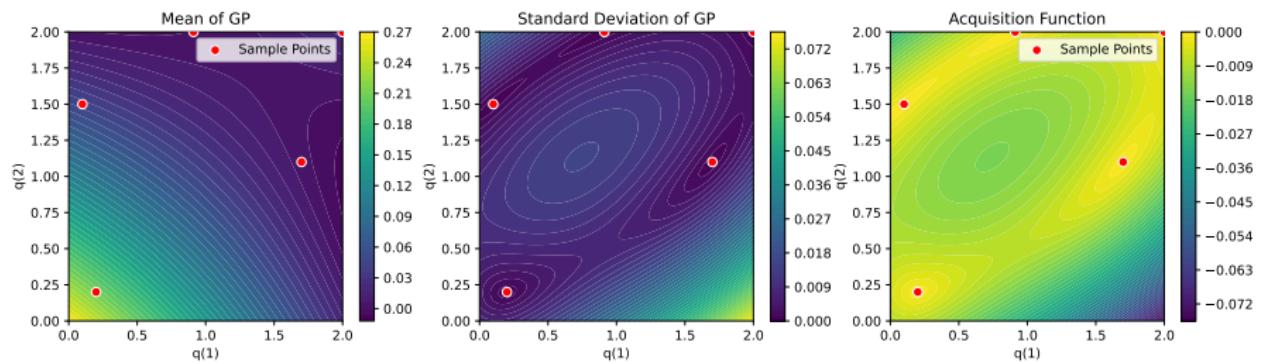
III: Bayesian optimisation: Exploration



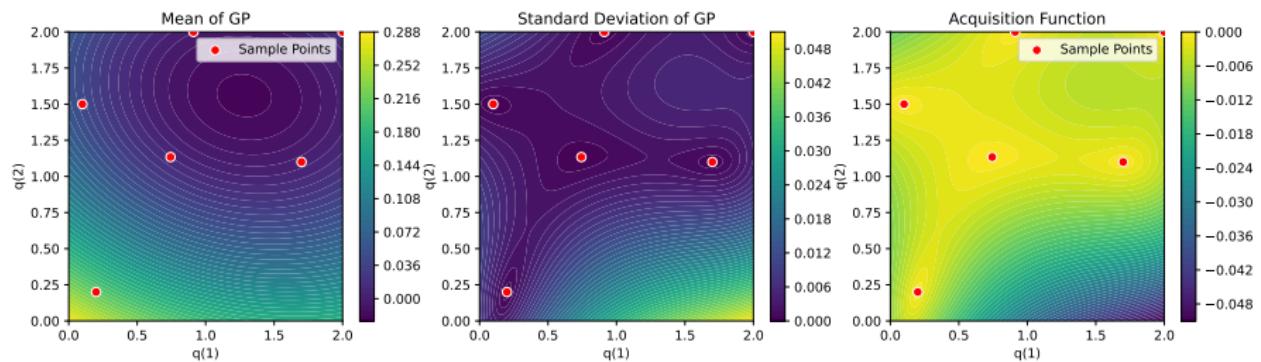
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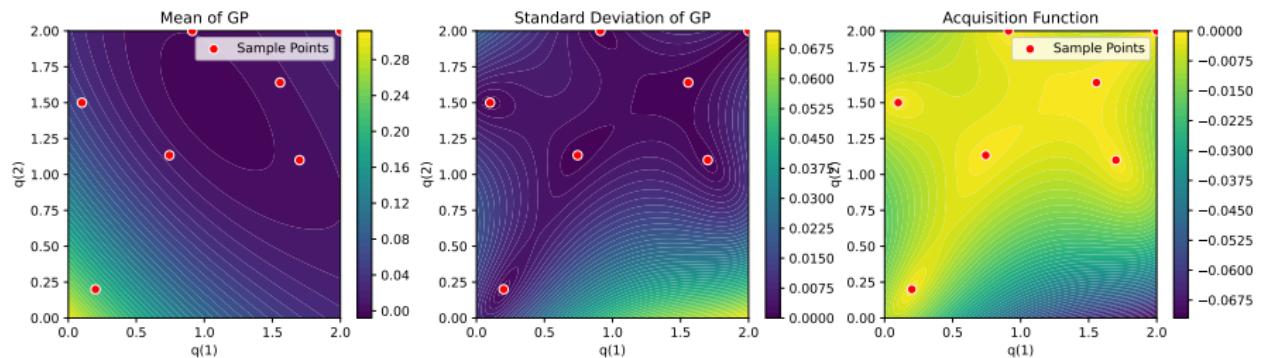
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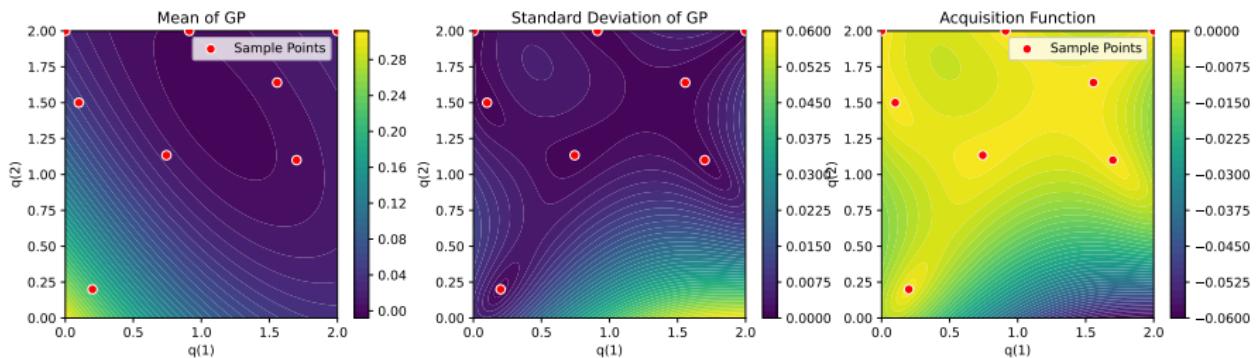
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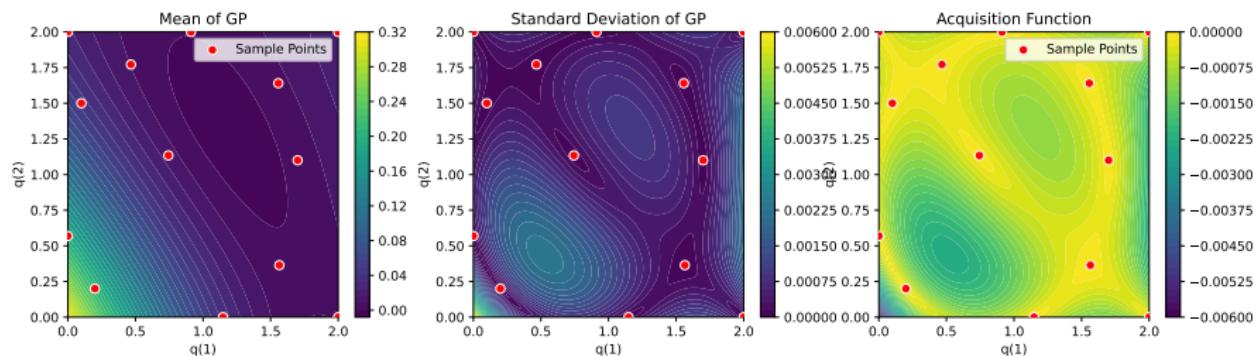
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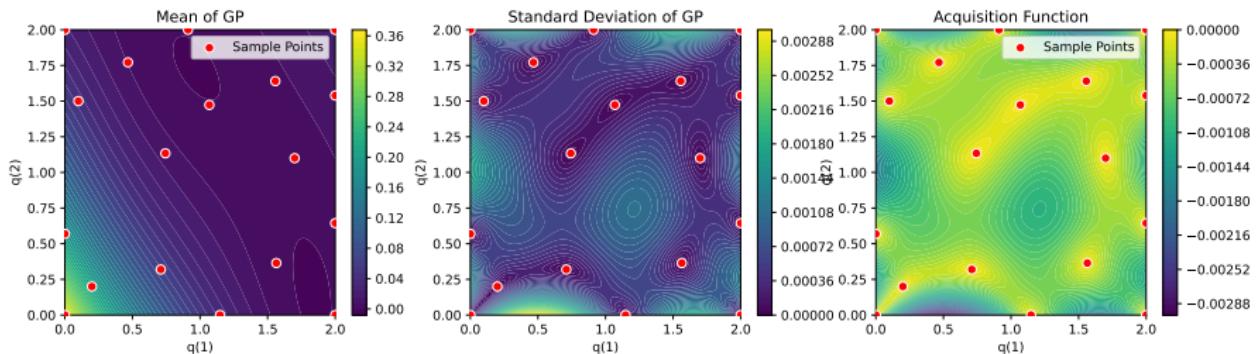
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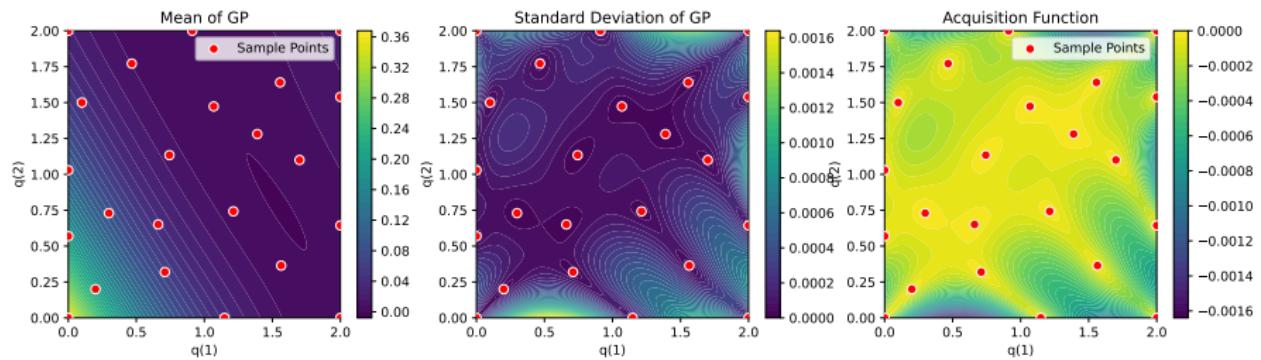
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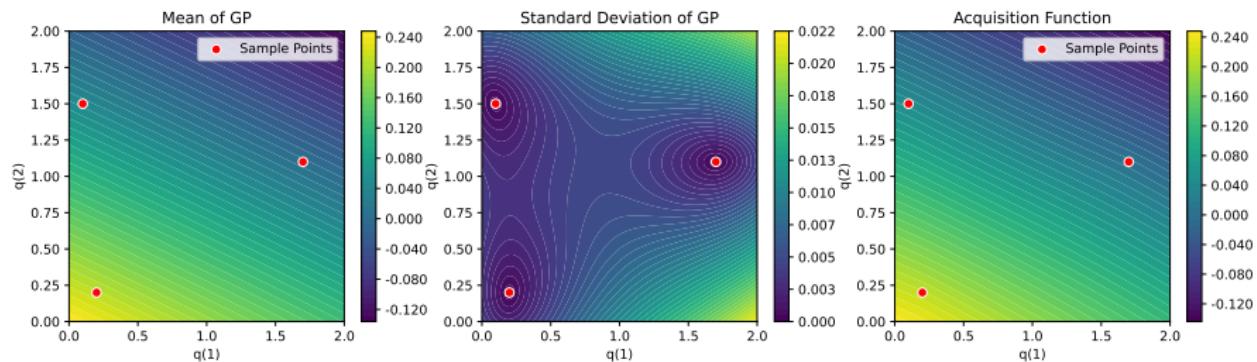


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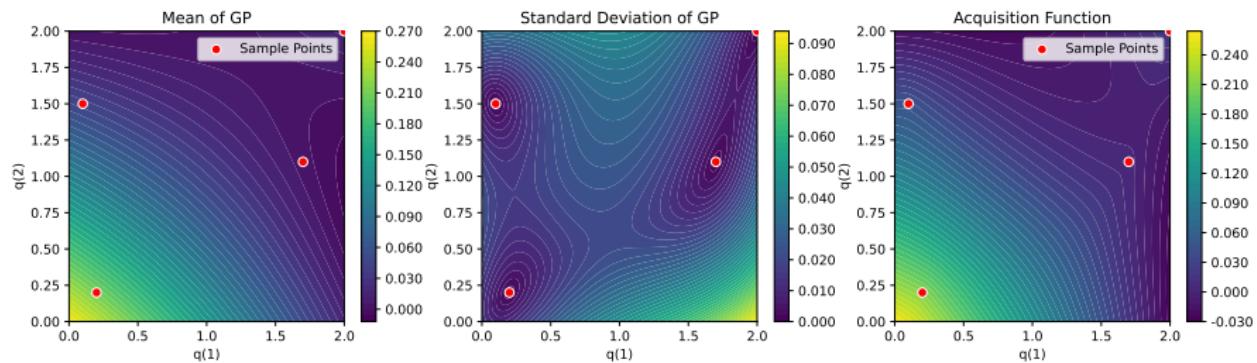


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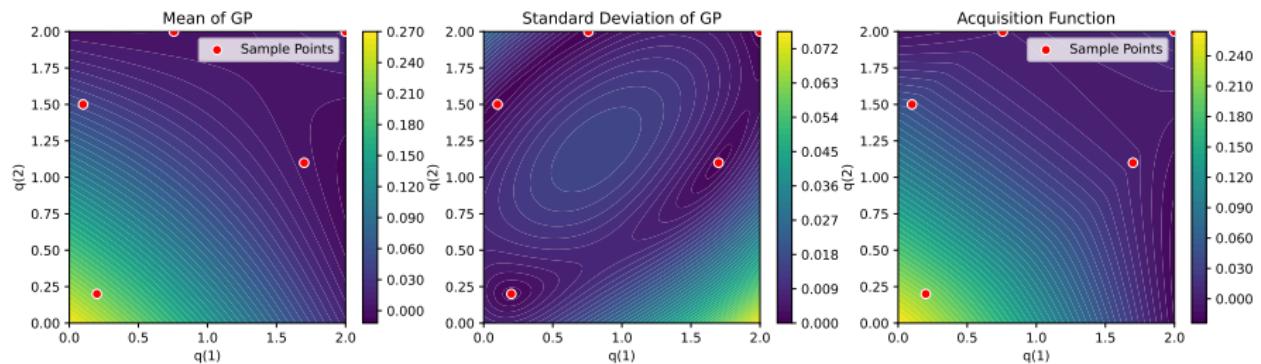
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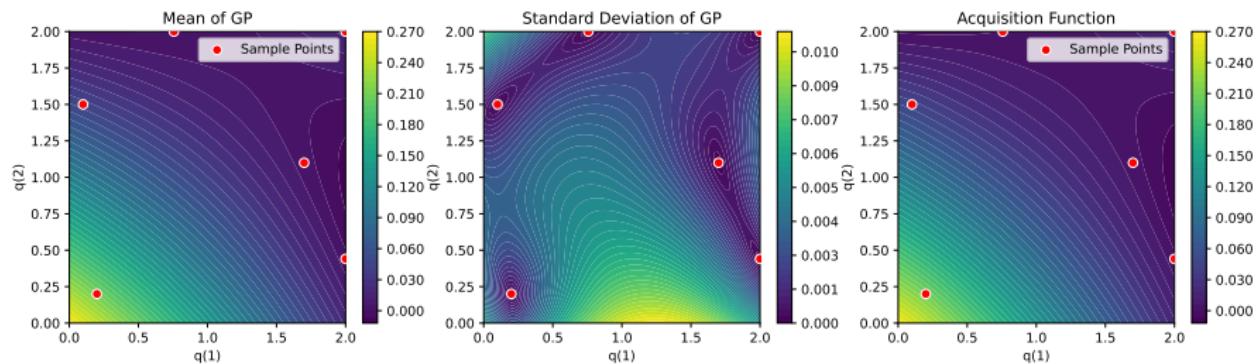
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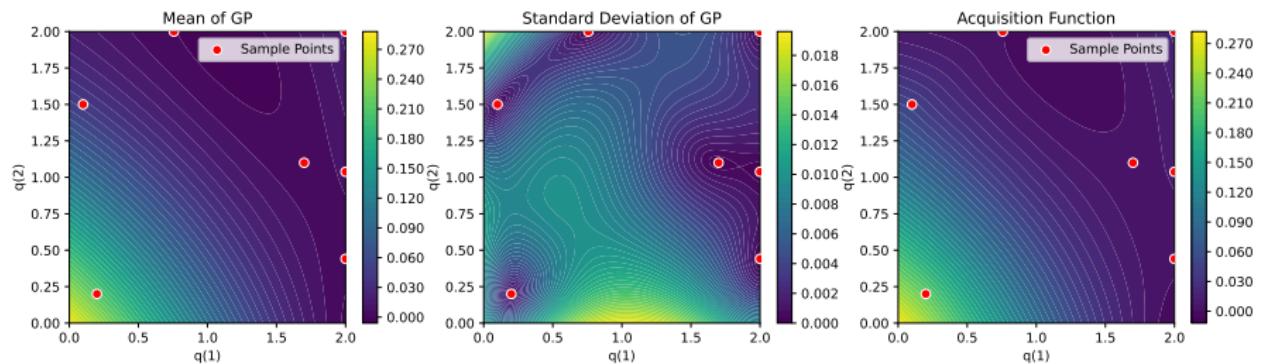
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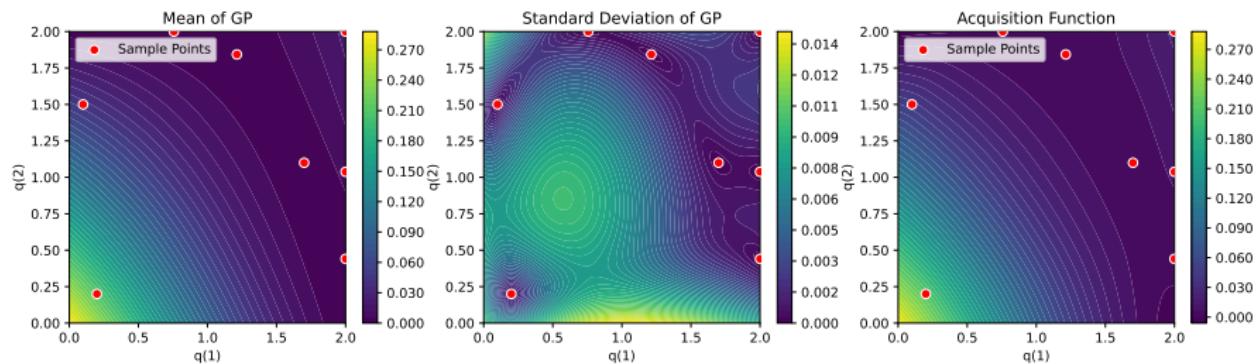
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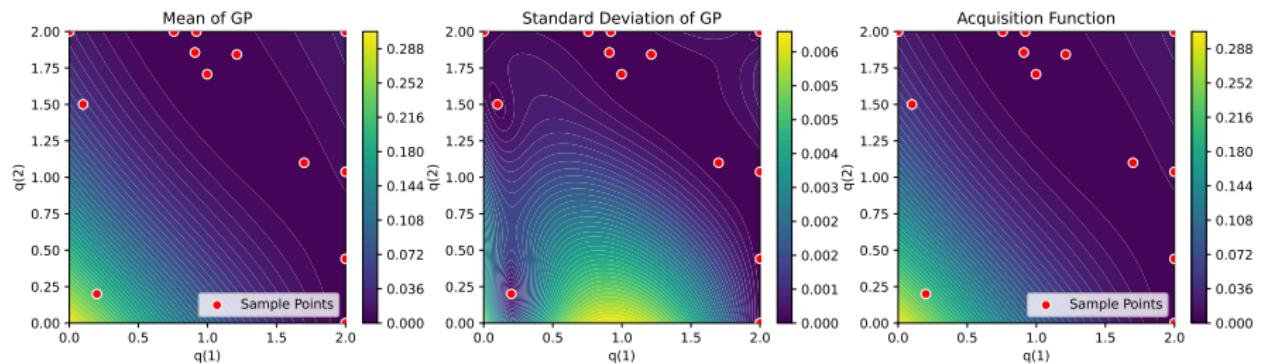
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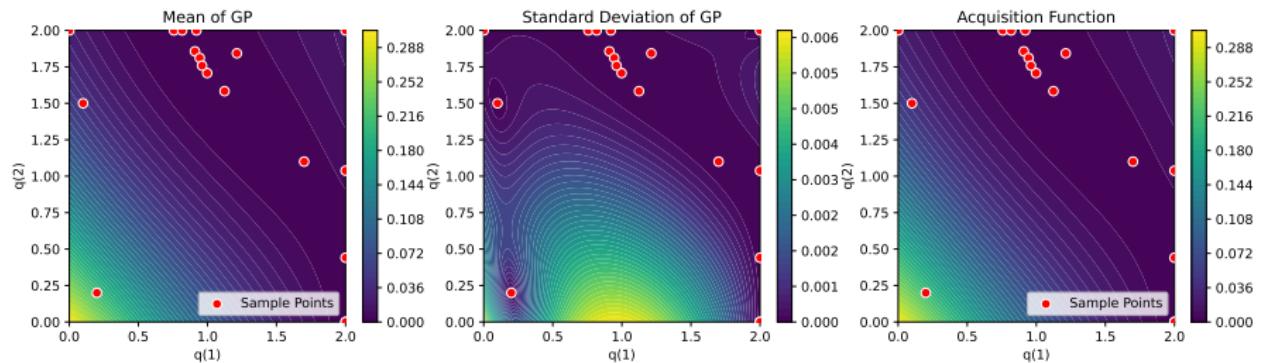
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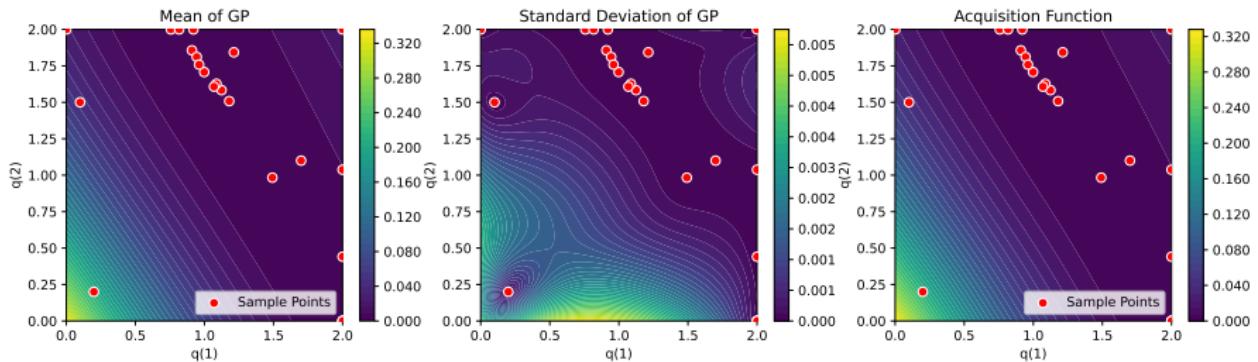
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Exploration & exploitation

Three Bayesian approaches to inverse problems

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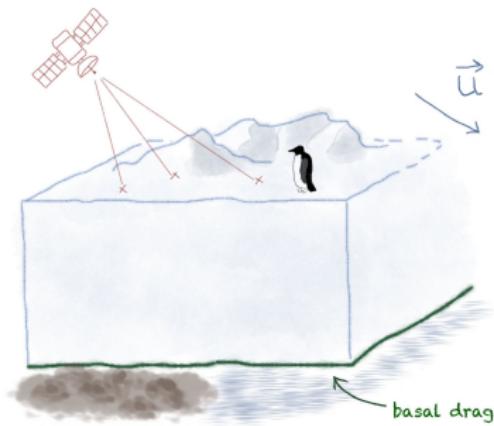
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Open questions

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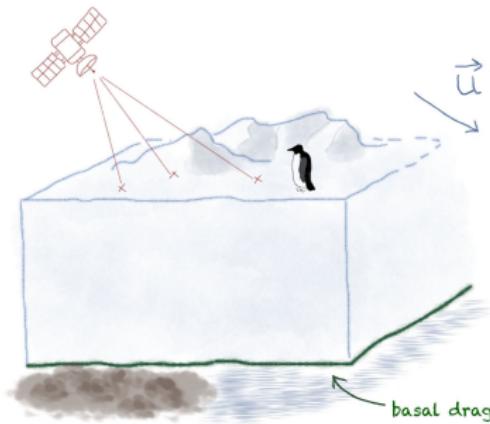
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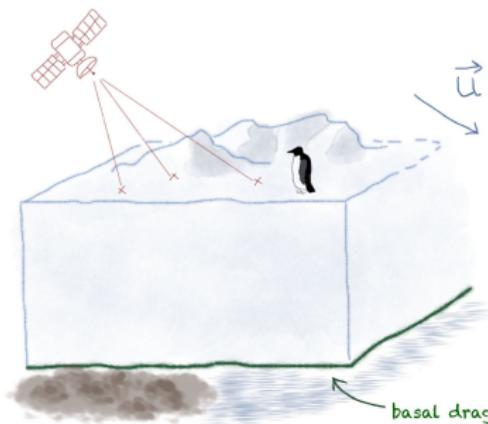
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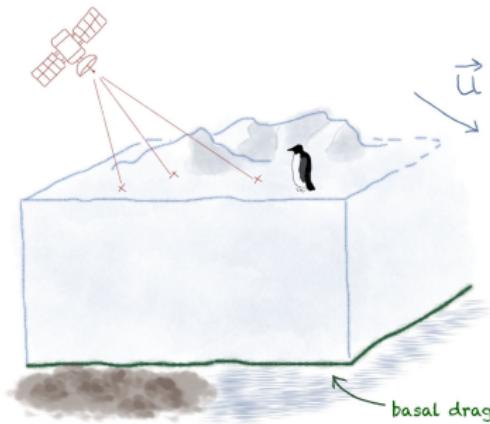
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2. What are emulators and when to use them?

- ▶ Unknown physics (parameterisations)
- ▶ Plentiful data allows to replace the physical model

Thank you