

Active Learning for Level Set Estimation

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Swimmers of Lake Zurich, beware!



Steffen Schmidt / EPA

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“The warming waters of one of central Europe's most popular holiday destinations, Switzerland's Lake Zurich, have created an ideal environment for a population explosion of algae including *Planktothrix rubescens*, [...]”

— *Scientific American*

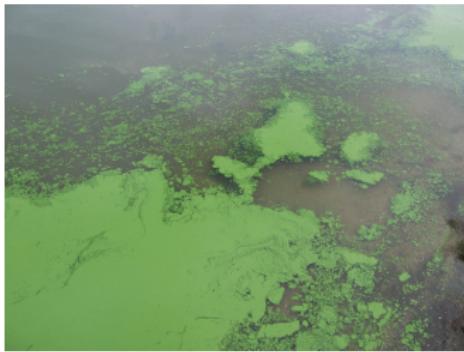
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[www.limnobiotics.ch](http://www.limnobotics.ch)

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Flickr/Dr. Jennifer L. Graham/U.S. Geological Survey

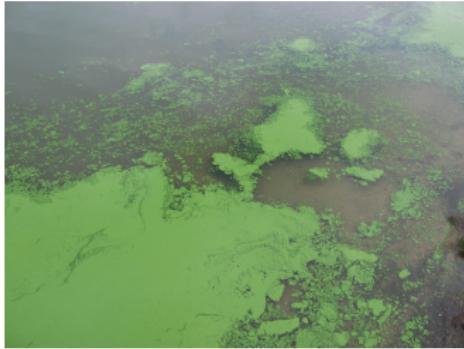
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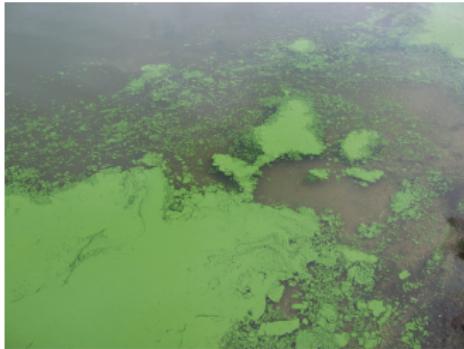
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"Microcystins [...] are cyanotoxins and can be very toxic for plants and animals including humans. Their hepatotoxicity may cause serious damage to the liver."

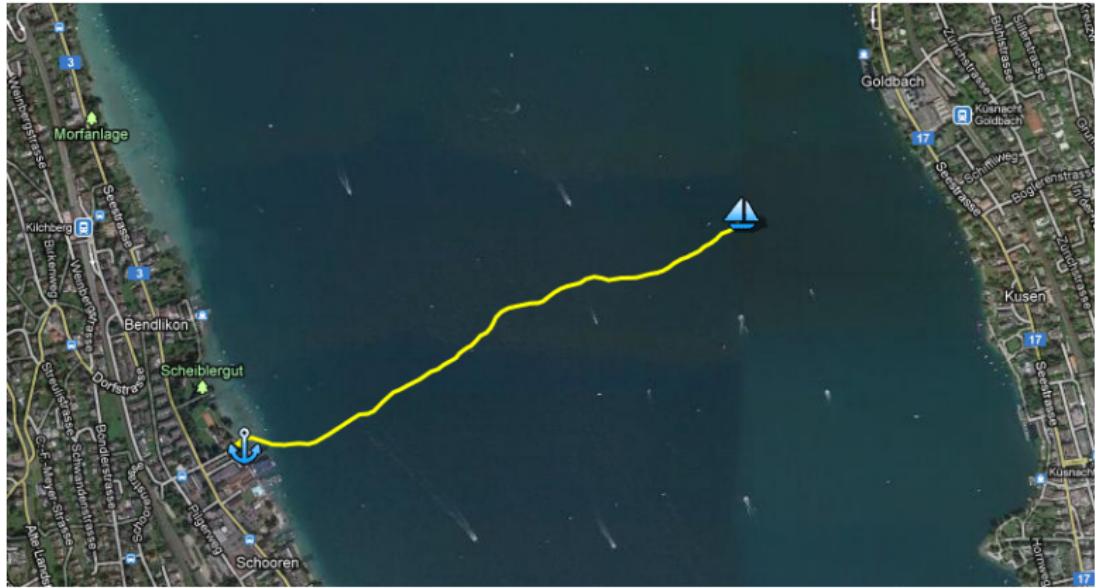
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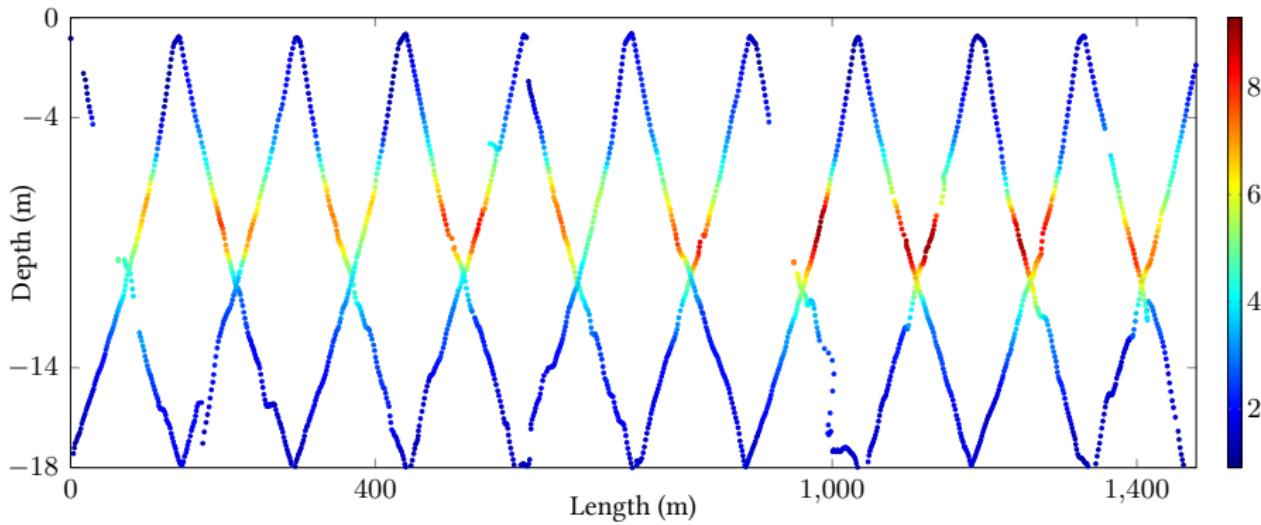


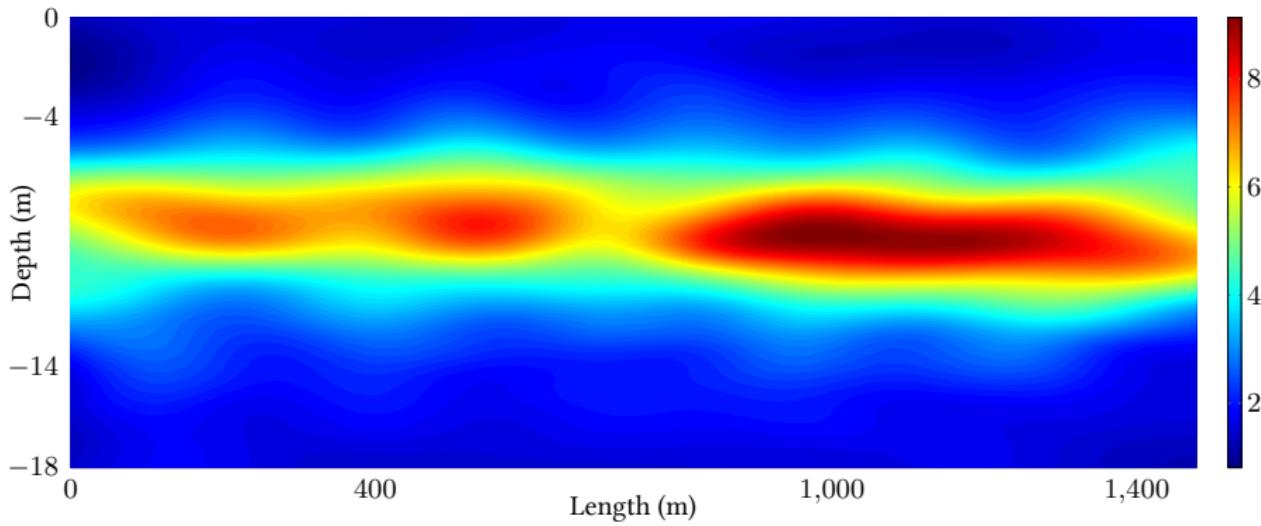
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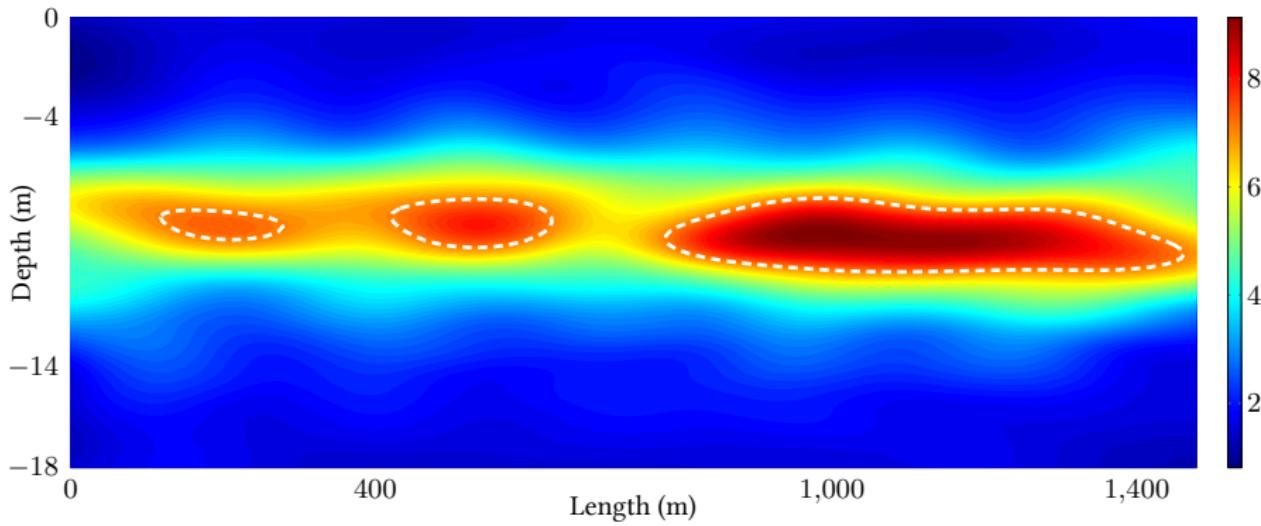


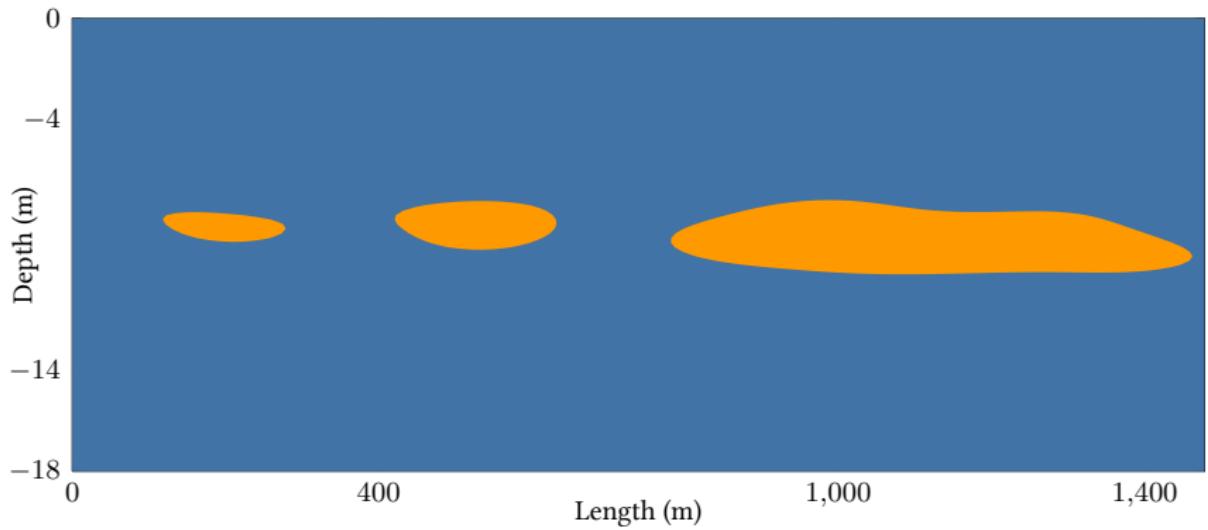
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- ▶ No measurements available in advance, just a set (pool) of possible sampling locations (D)

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- ▶ Update our estimate of f

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Gaussian processes to the rescue!

Gaussian processes

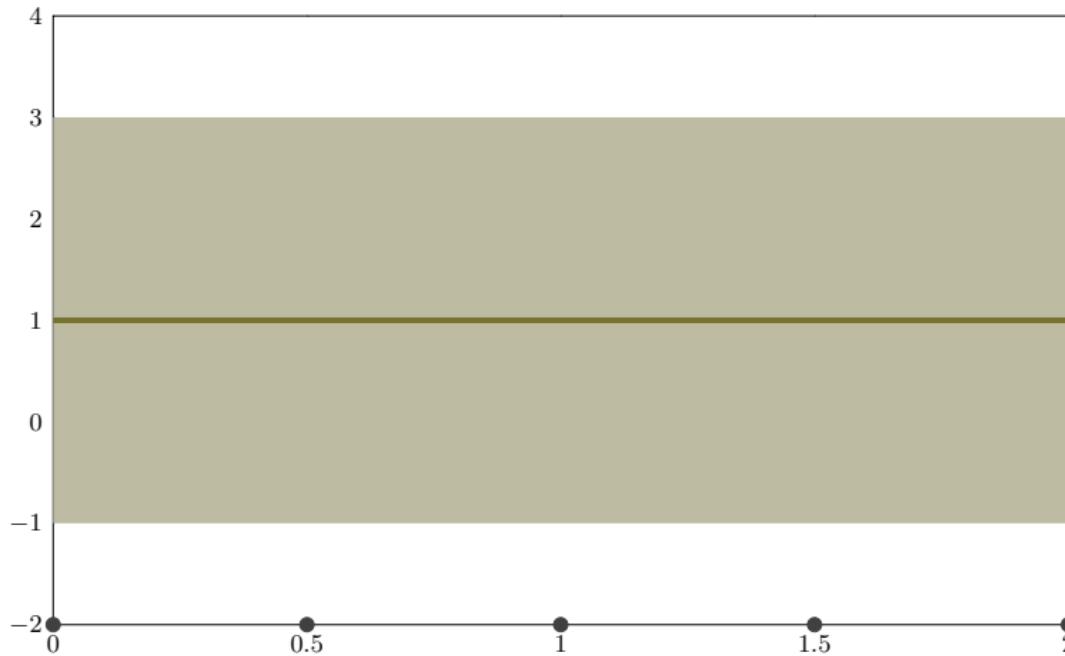
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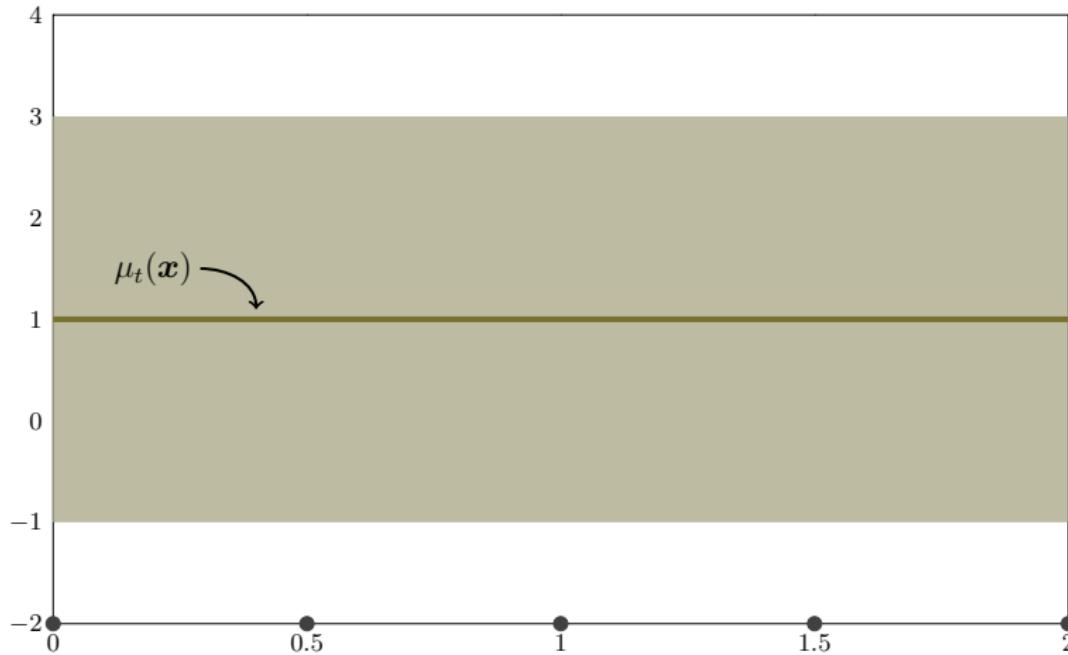
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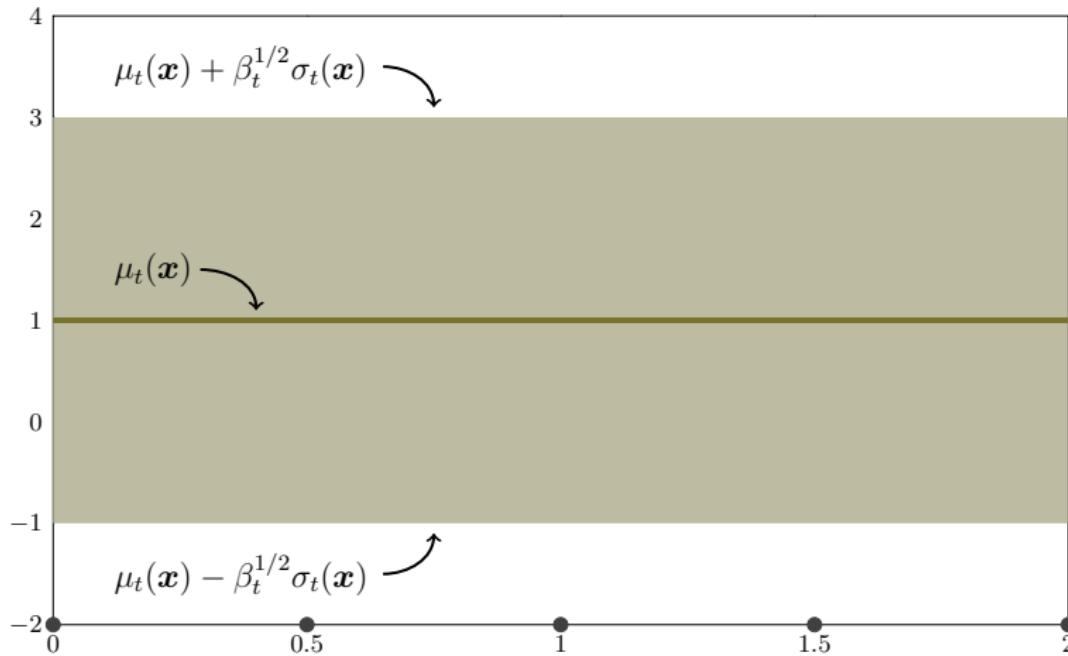
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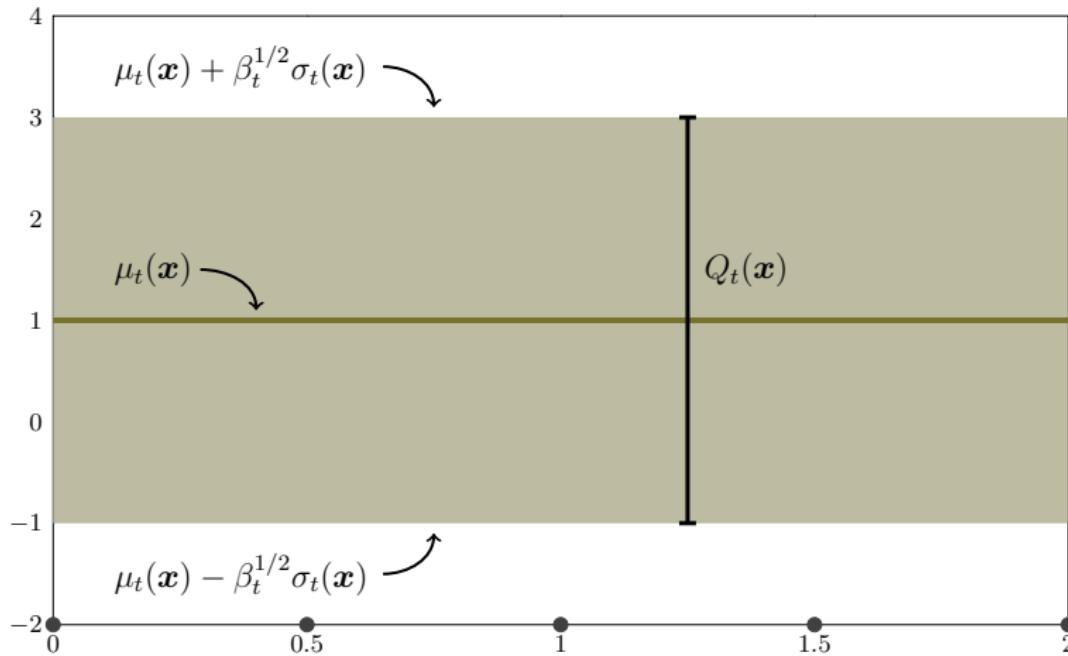
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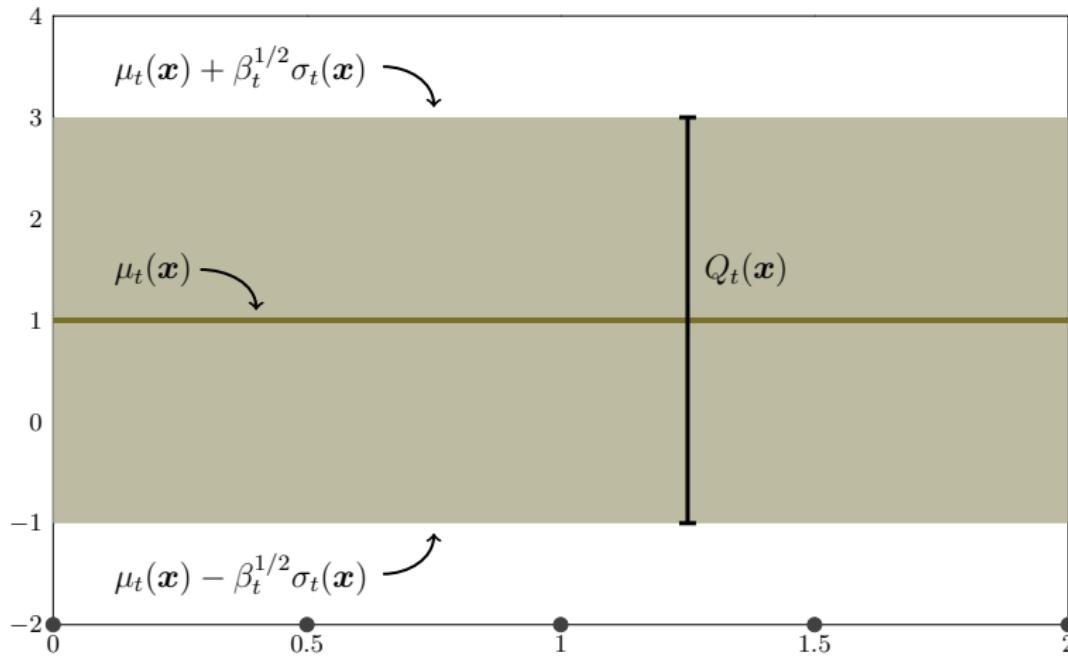
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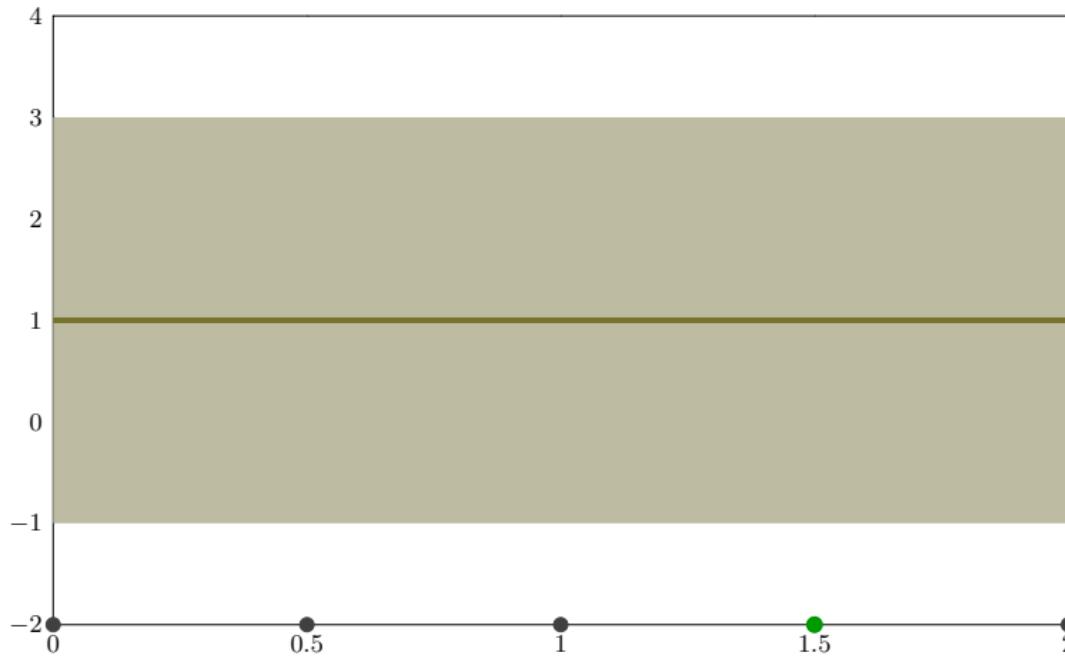
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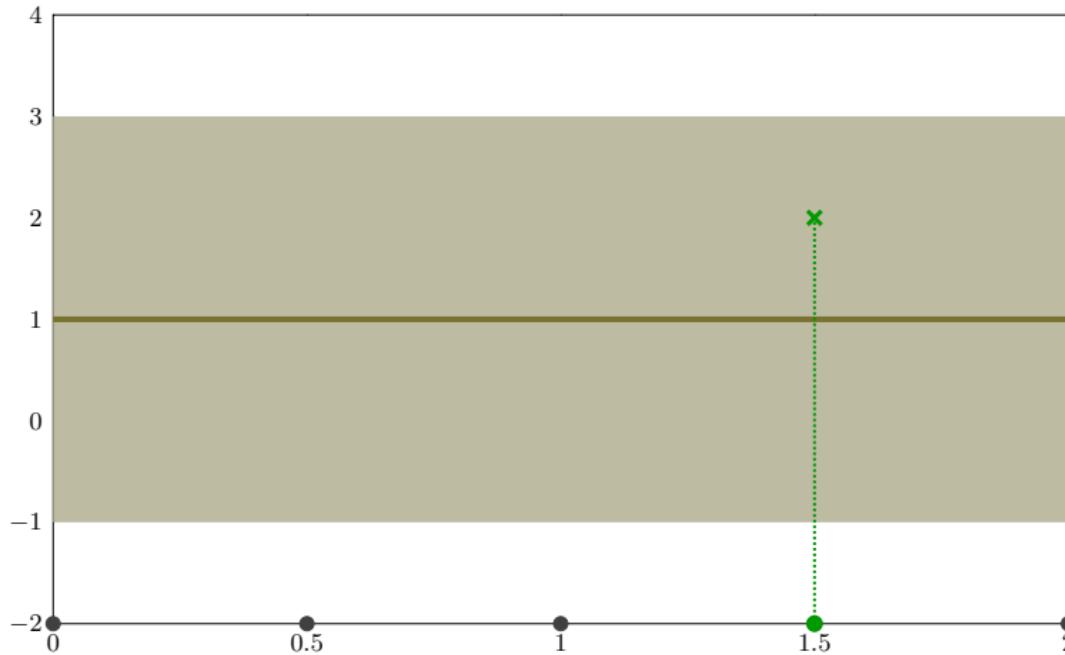
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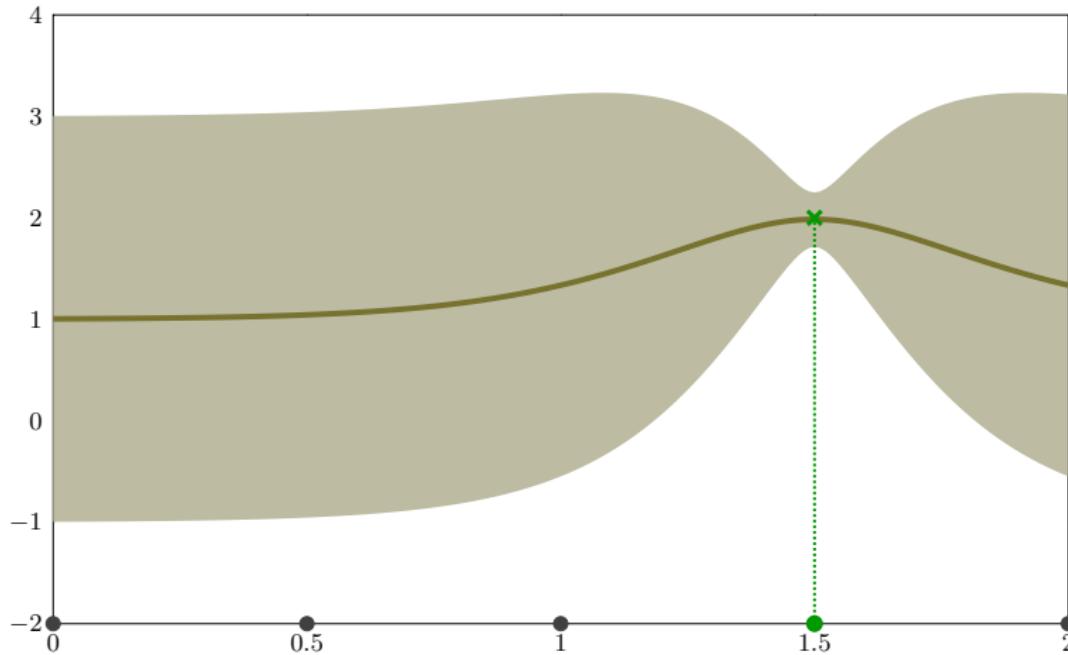
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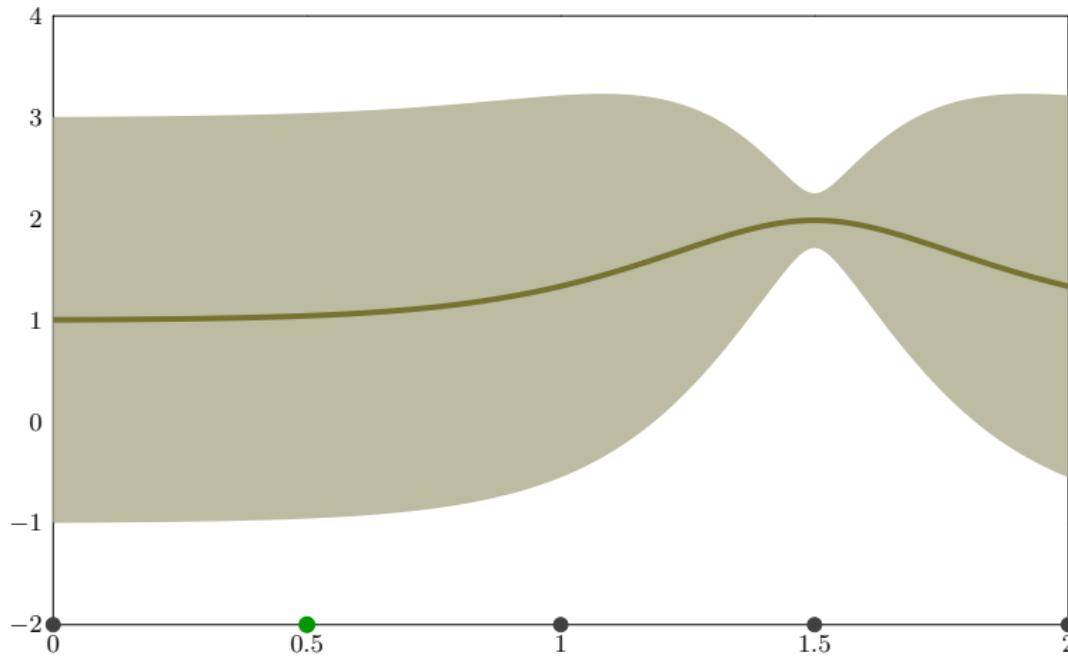
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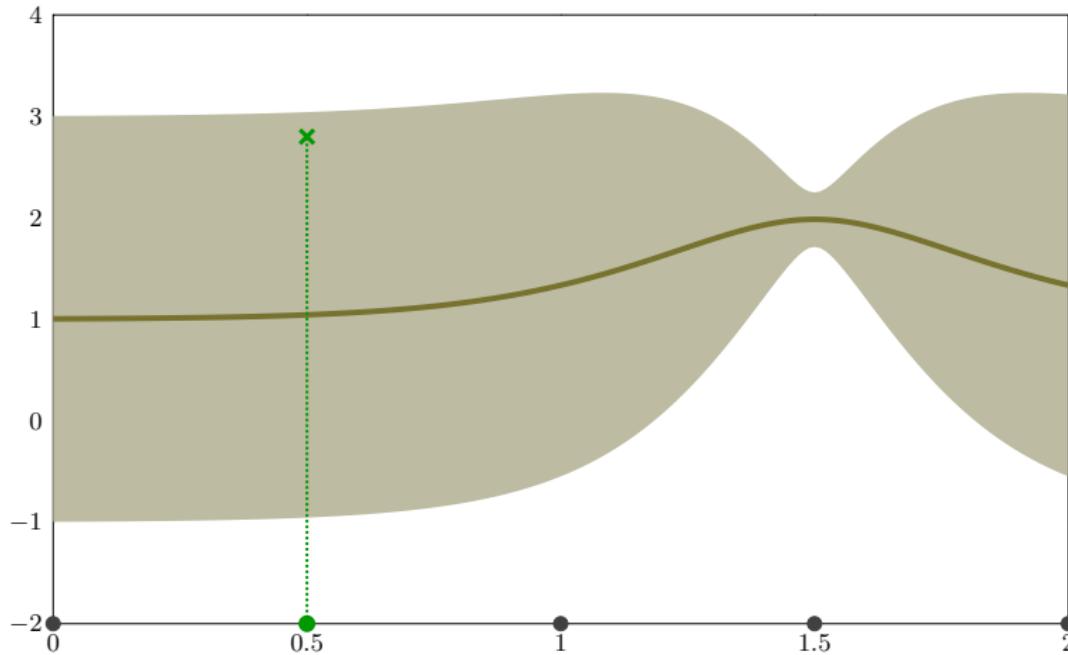
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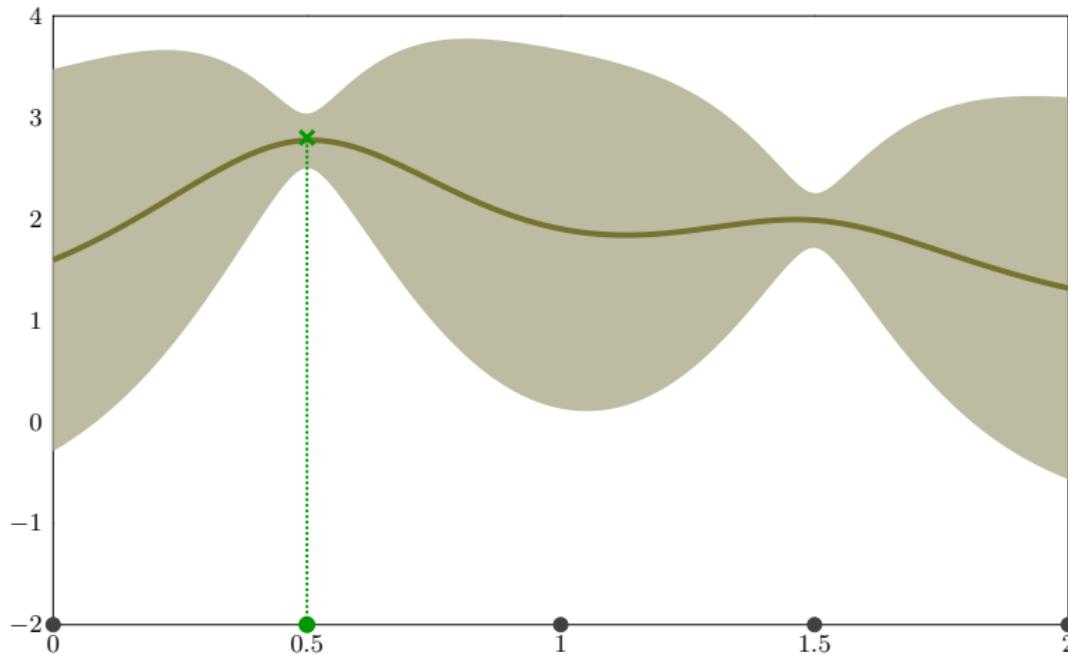
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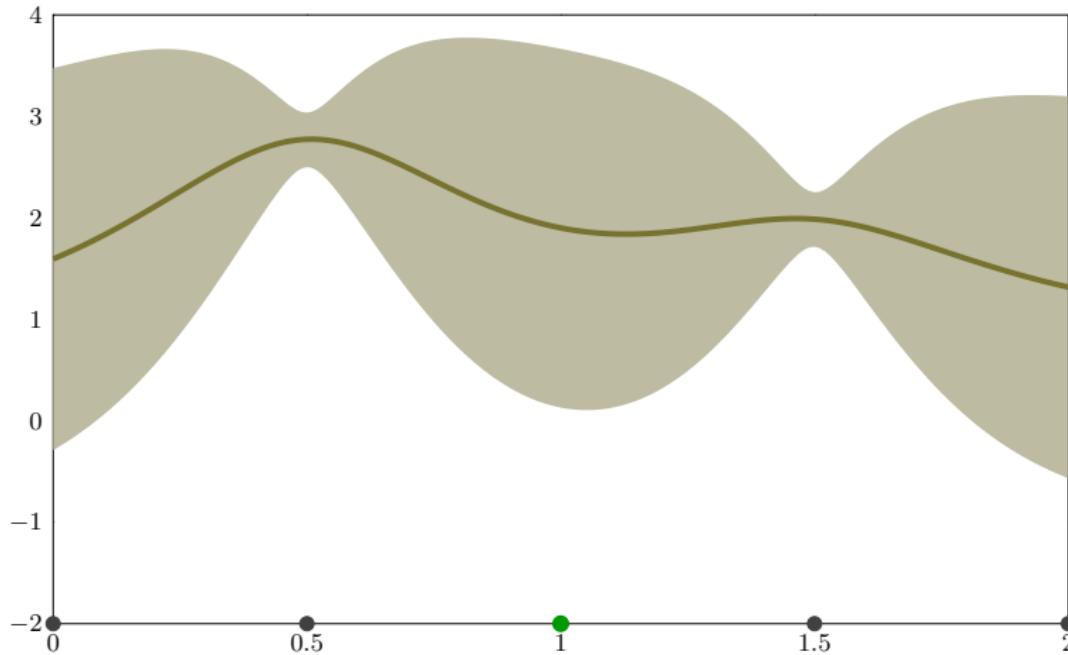
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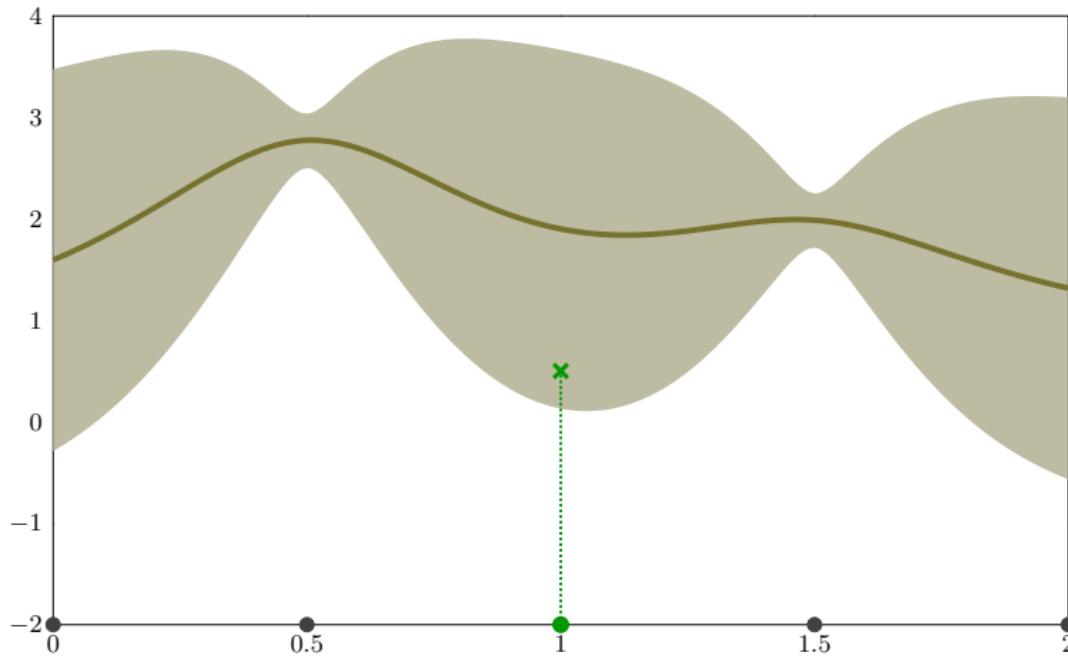
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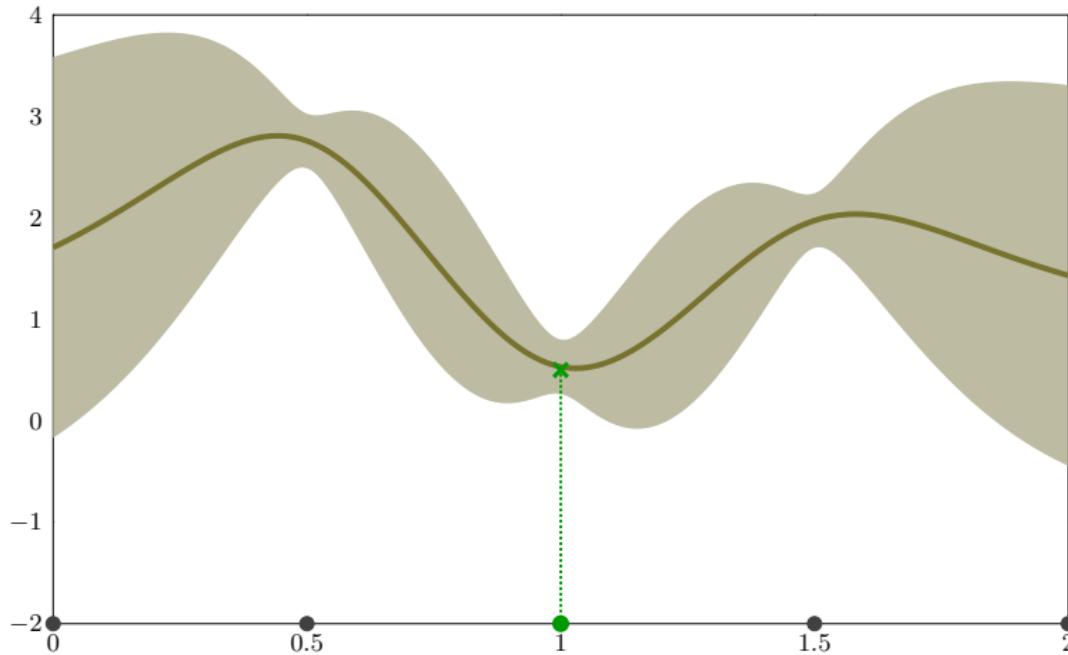
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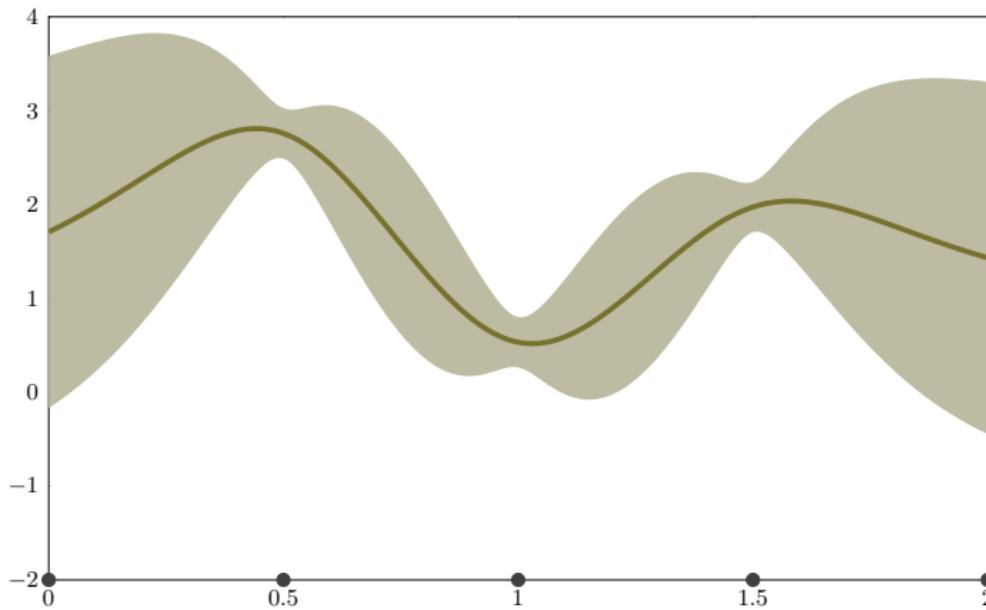
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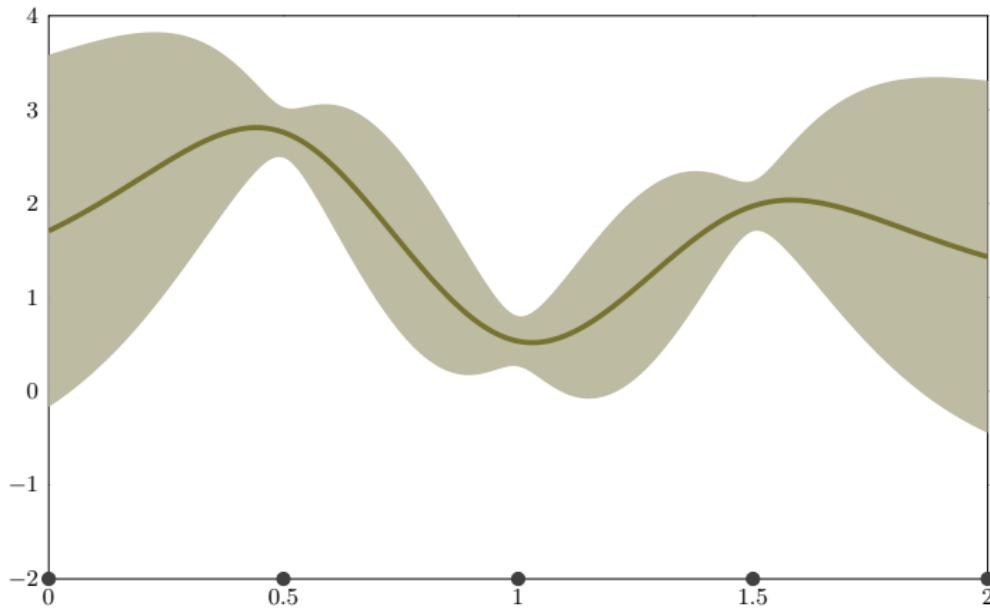


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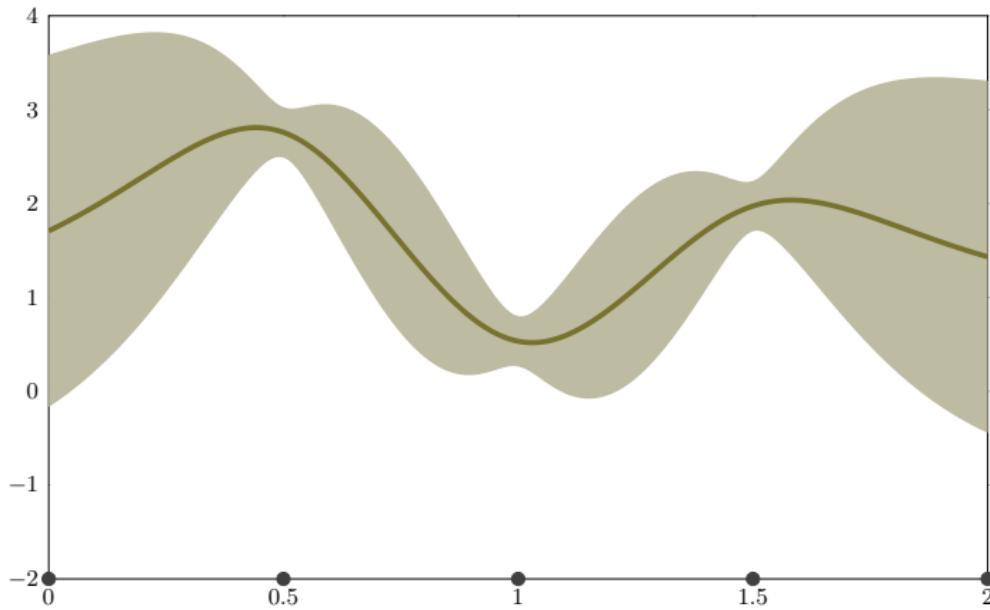


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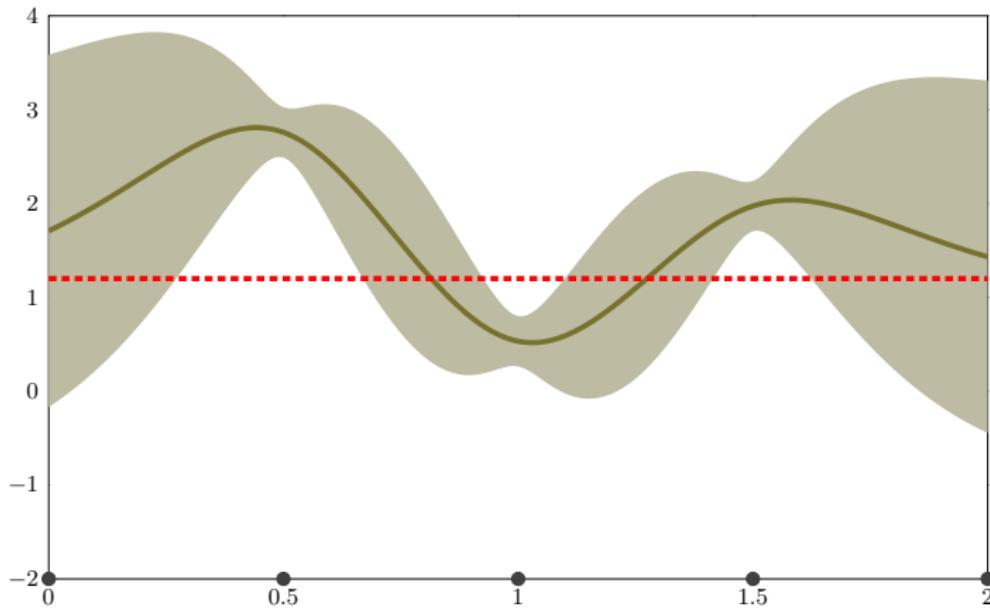
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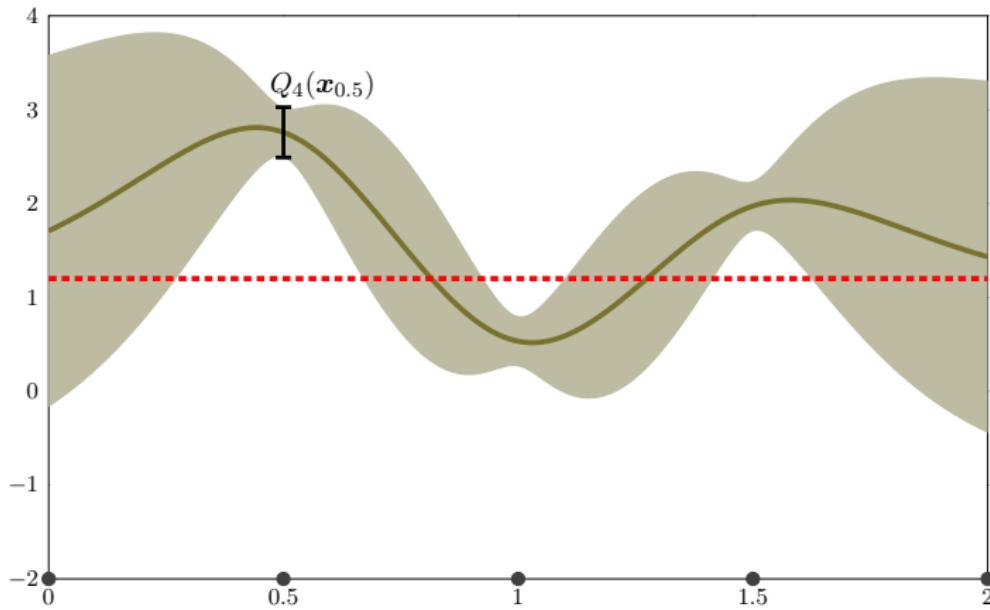
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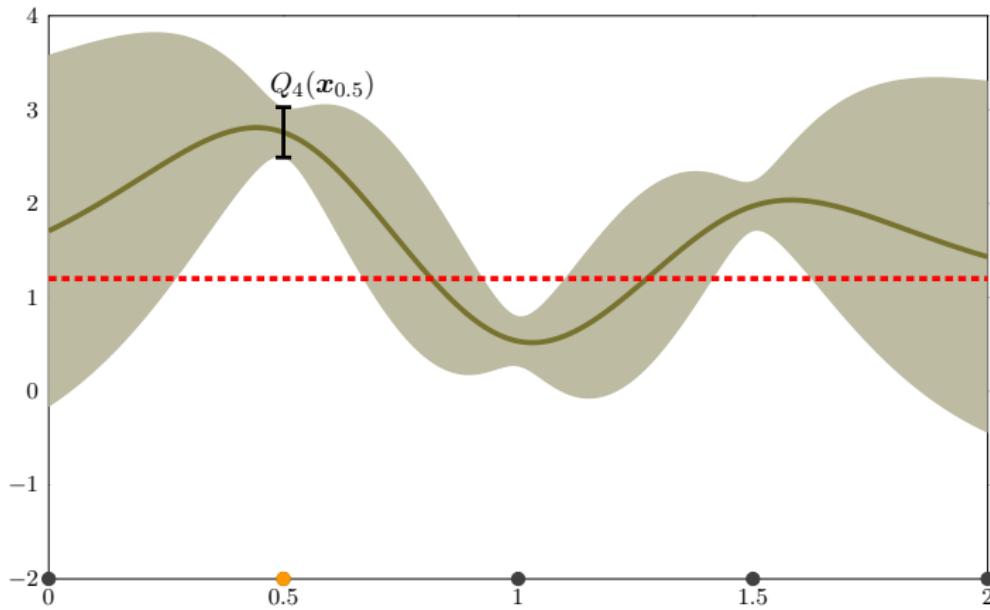
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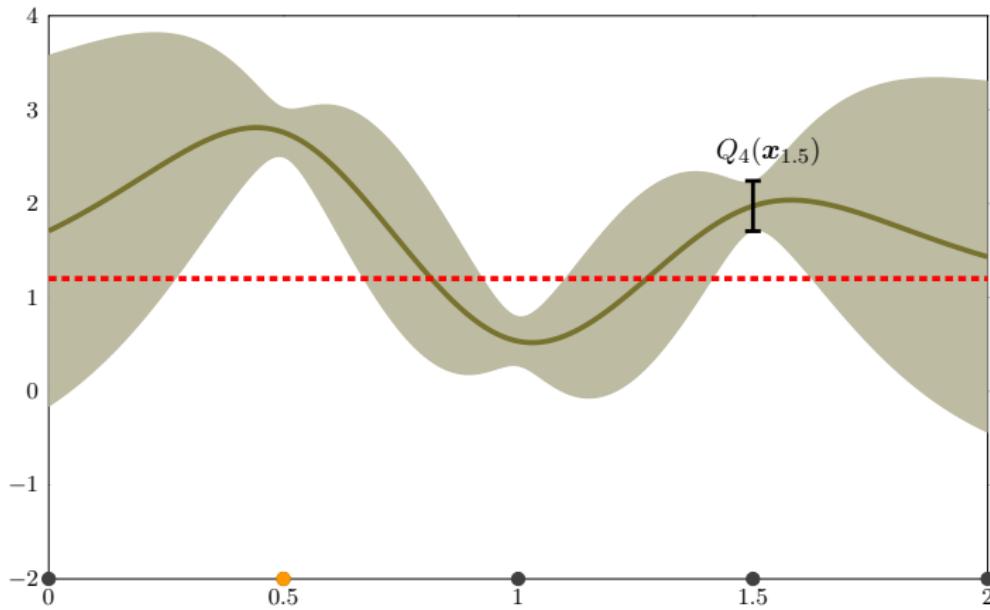
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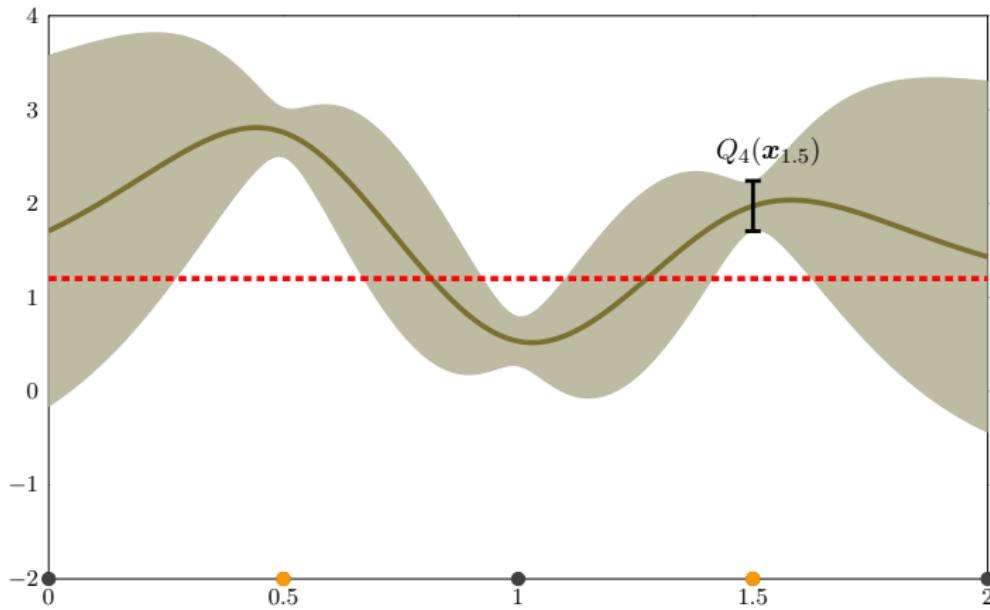
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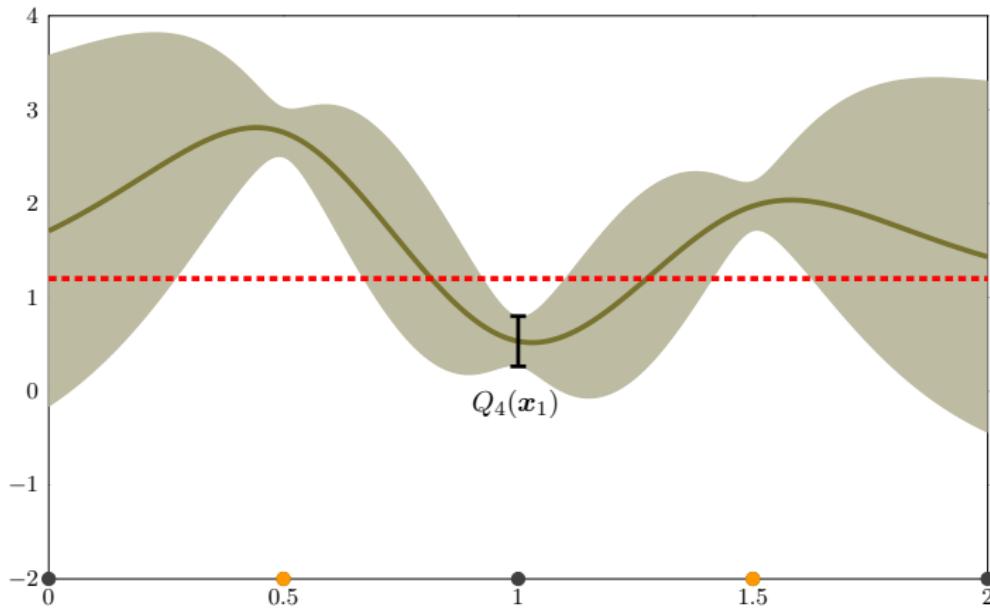
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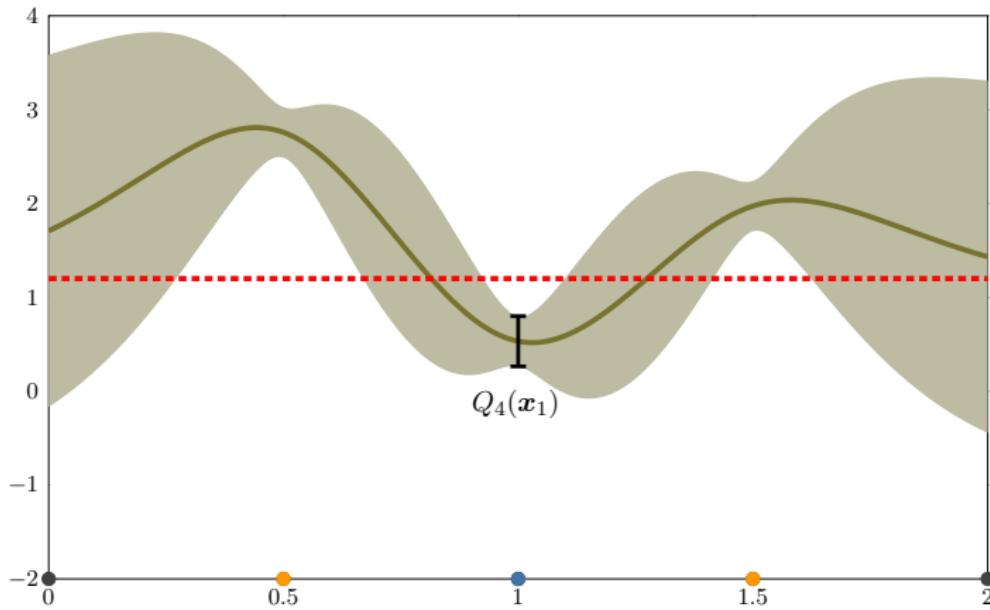
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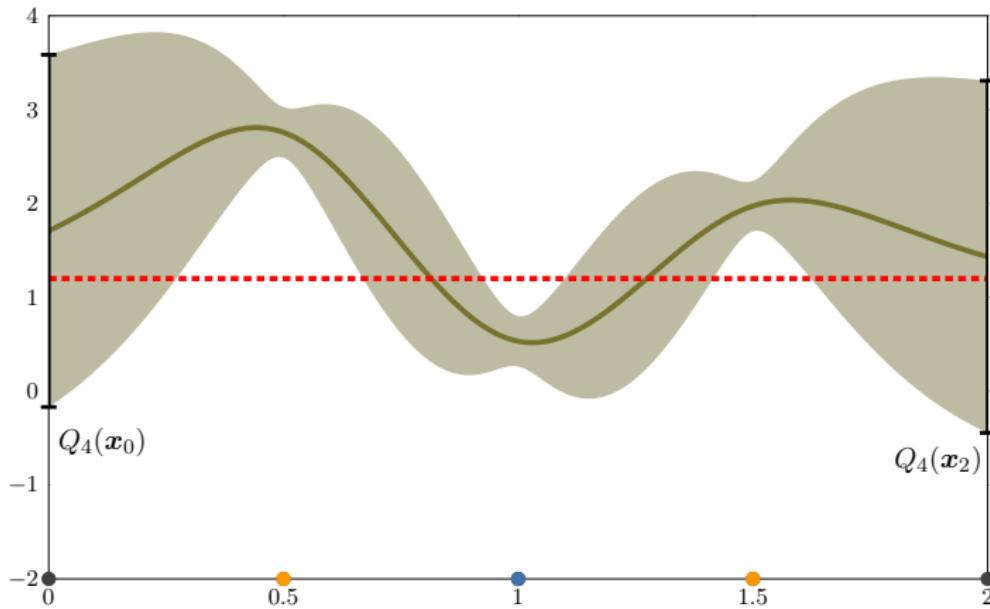
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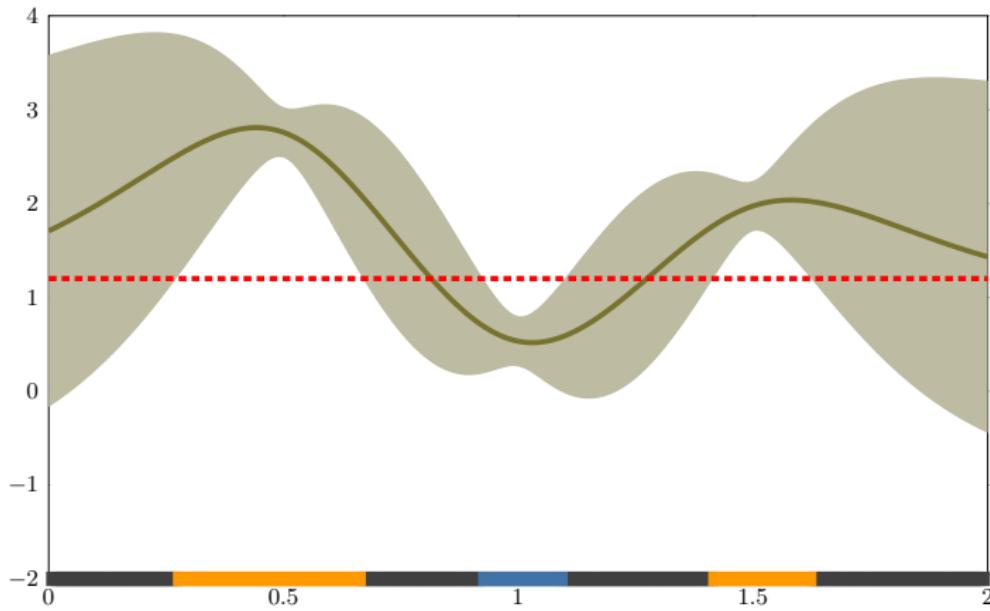
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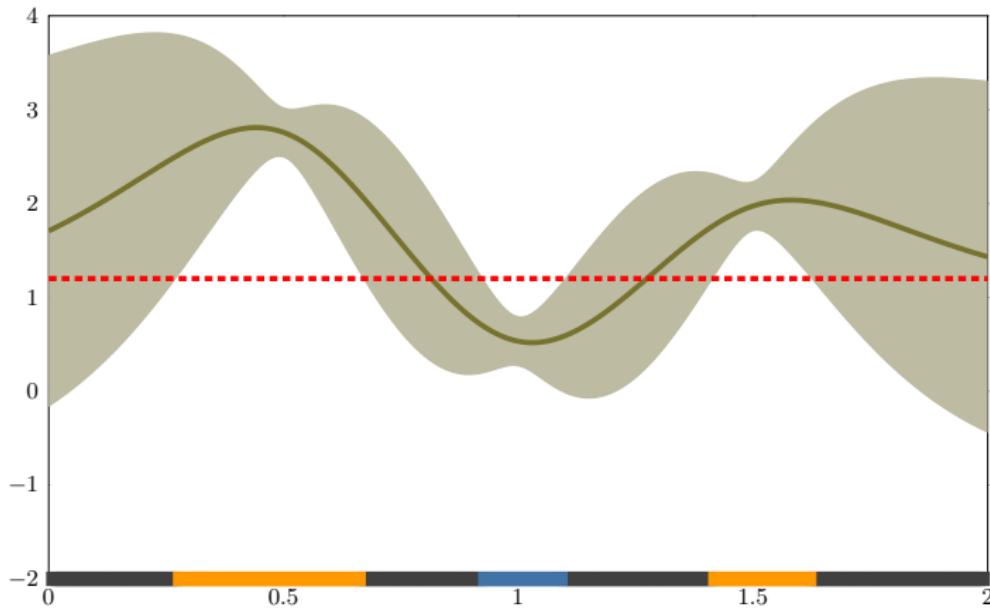
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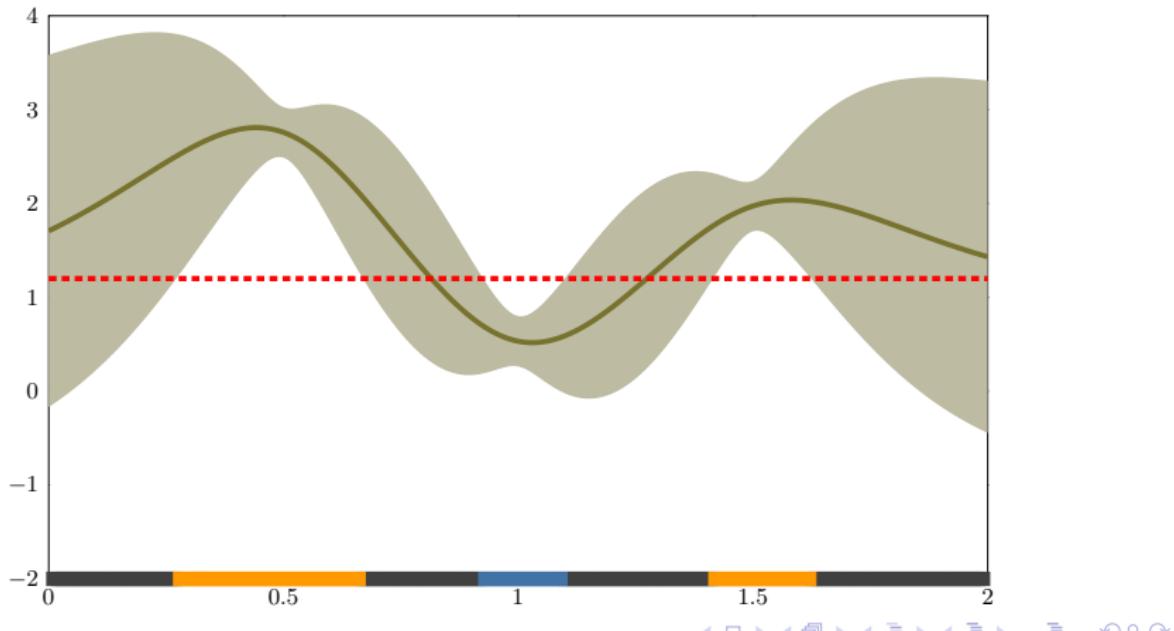


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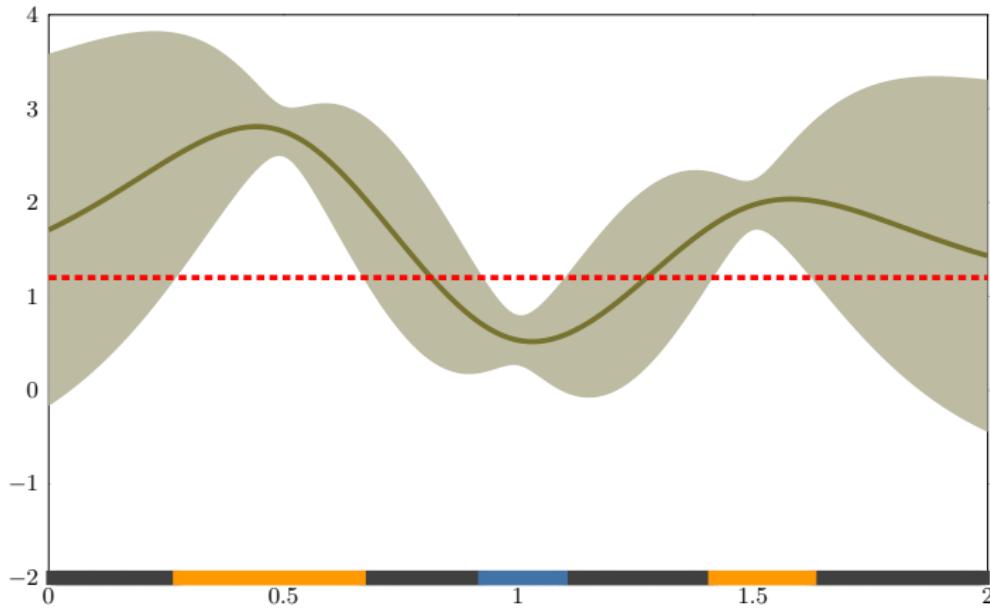
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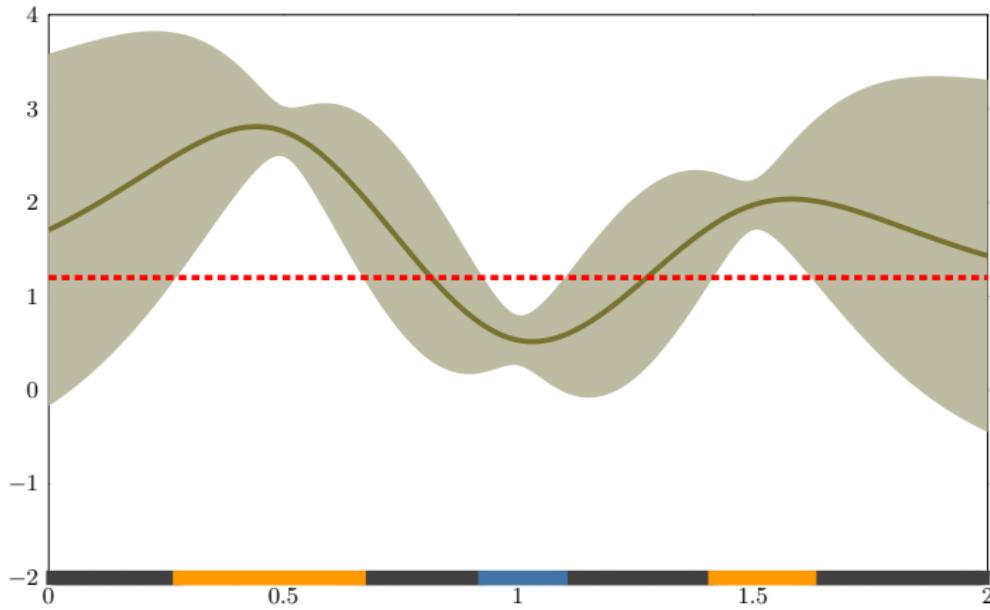
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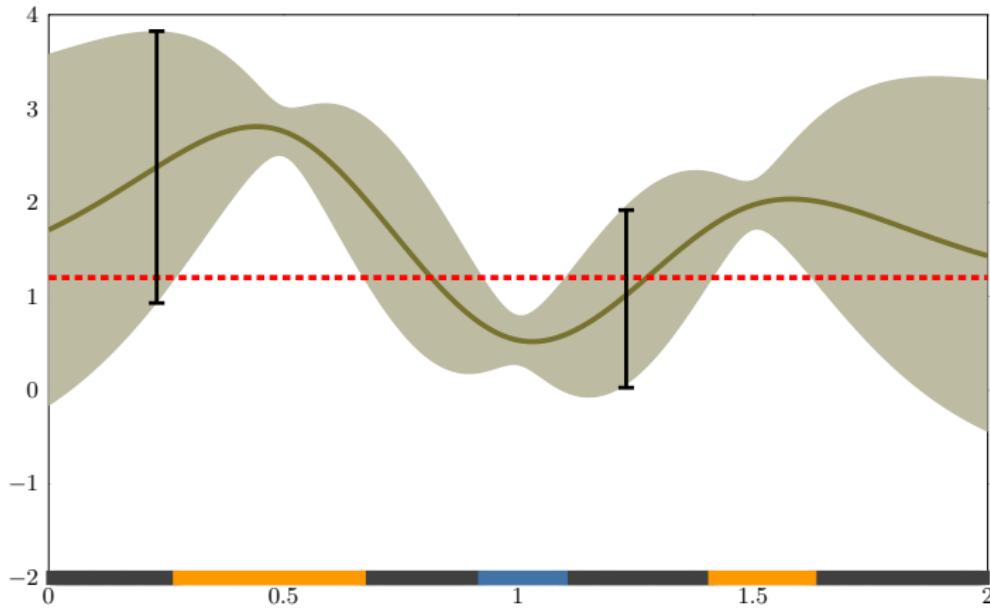
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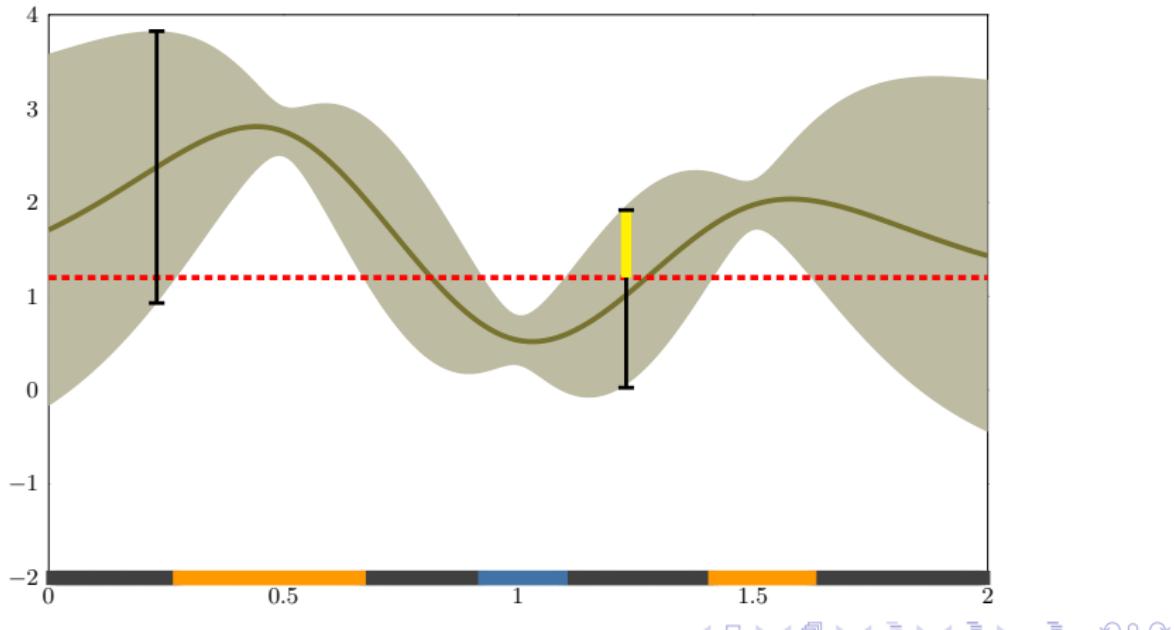
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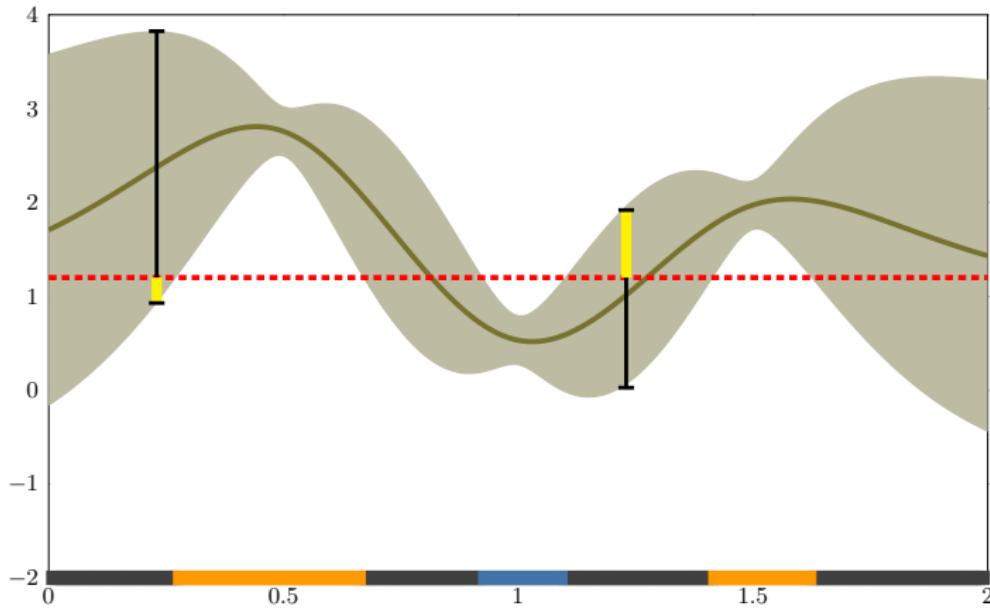
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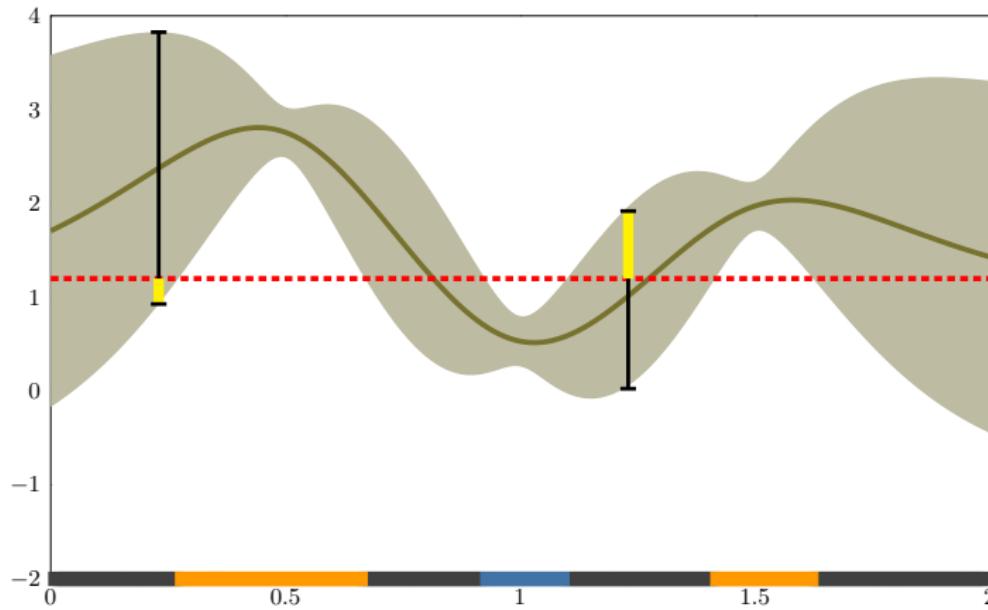


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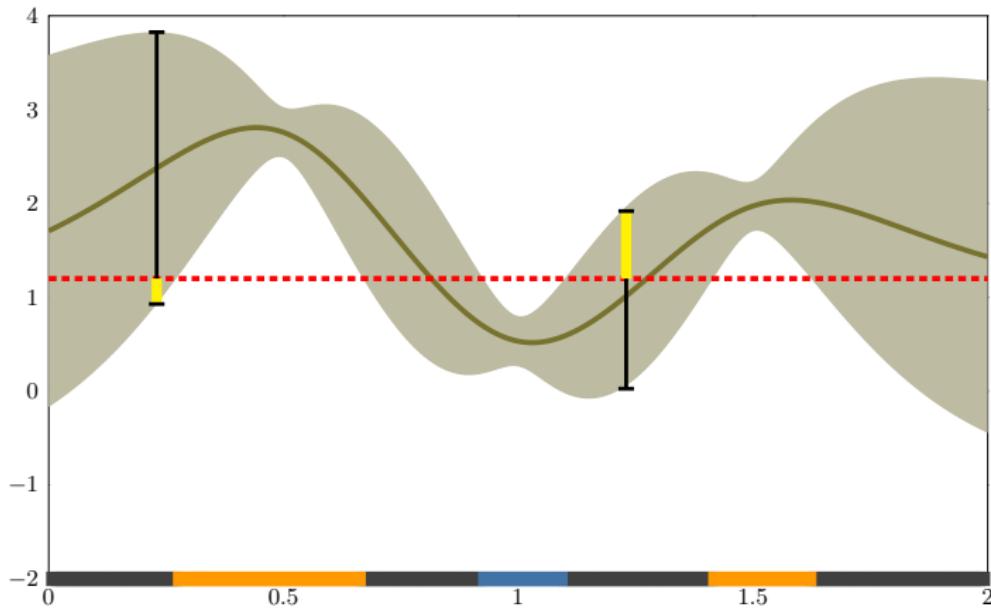
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Input: sample set D , GP prior (μ_0, k, σ_0) ,
thr. value h , accuracy parameter ϵ
Output: predicted sets \hat{H}, \hat{L}

The Level Set Estimation (LSE) algorithm

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Output: predicted sets \hat{H}, \hat{L}

$$H_0 \leftarrow \emptyset, L_0 \leftarrow \emptyset, U_0 \leftarrow D$$

$$C_0(x) \leftarrow \mathbb{R}, \text{ for all } x \in D$$

$$t \leftarrow 1$$

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$$\begin{aligned}\hat{H} &\leftarrow H_{t-1} \\ \hat{L} &\leftarrow L_{t-1}\end{aligned}$$

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← loop until all points have been classified

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for all $x \in U_{t-1}$ **do**

$C_t(x) \leftarrow C_{t-1}(x) \cap Q_t(x)$

if $\min(C_t(x)) + \epsilon > h$ **then**

$U_t \leftarrow U_t \setminus \{x\}$

$H_t \leftarrow H_t \cup \{x\}$

else if $\max(C_t(x)) - \epsilon \leq h$ **then**

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$x_t \leftarrow \operatorname{argmax}\{a_t(x) \mid x \in U_t\}$

$y_t \leftarrow f(x_t) + n_t$

The Level Set Estimation (LSE) algorithm

← loop until all points have been classified

← classify

← select max. ambiguity point

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$H_t \leftarrow H_{t-1}, L_t \leftarrow L_{t-1}, U_t \leftarrow U_{t-1}$

for all $x \in U_{t-1}$ **do**

$C_t(x) \leftarrow C_{t-1}(x) \cap Q_t(x)$

if $\min(C_t(x)) + \epsilon > h$ **then**

$U_t \leftarrow U_t \setminus \{x\}$

$H_t \leftarrow H_t \cup \{x\}$

else if $\max(C_t(x)) - \epsilon \leq h$ **then**

$U_t \leftarrow U_t \setminus \{x\}$

$L_t \leftarrow L_t \cup \{x\}$

end if

end for

$x_t \leftarrow \operatorname{argmax}\{a_t(x) \mid x \in U_t\}$

$y_t \leftarrow f(x_t) + n_t$

 Compute $\mu_t(x)$ and $\sigma_t(x), \forall x \in U_t$

$t \leftarrow t + 1$

end while

$\hat{H} \leftarrow H_{t-1}$

$\hat{L} \leftarrow L_{t-1}$

The Level Set Estimation (lse) algorithm

← loop until all points have been classified

← classify

← select max. ambiguity point

← update GP estimate

Input: sample set D , GP prior (μ_0, k, σ_0) ,
thr. value h , accuracy parameter ϵ

Output: predicted sets \hat{H}, \hat{L}

$$H_0 \leftarrow \emptyset, L_0 \leftarrow \emptyset, U_0 \leftarrow D$$

$$C_0(x) \leftarrow \mathbb{R}, \text{ for all } x \in D$$

$$t \leftarrow 1$$

while $U_{t-1} \neq \emptyset$ **do**

$$H_t \leftarrow H_{t-1}, L_t \leftarrow L_{t-1}, U_t \leftarrow U_{t-1}$$

for all $x \in U_{t-1}$ **do**

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if $\min(C_t(x)) + \epsilon > h$ **then**

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end if

end for

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Compute $\mu_t(x)$ and $\sigma_t(x)$, $\forall x \in U_t$

$$t \leftarrow t + 1$$

end while

$$\hat{H} \leftarrow H_{t-1}$$

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The Level Set Estimation (LSE) algorithm

► Monotonicity of

1. confidence intervals
2. classification

Input: sample set D , GP prior (μ_0, k, σ_0) ,
thr. value h , accuracy parameter ϵ

Output: predicted sets \hat{H}, \hat{L}

$$H_0 \leftarrow \emptyset, L_0 \leftarrow \emptyset, U_0 \leftarrow D$$

$$C_0(x) \leftarrow \mathbb{R}, \text{ for all } x \in D$$

$$t \leftarrow 1$$

while $U_{t-1} \neq \emptyset$ **do**

$$H_t \leftarrow H_{t-1}, L_t \leftarrow L_{t-1}, U_t \leftarrow U_{t-1}$$

for all $x \in U_{t-1}$ **do**

$$C_t(x) \leftarrow C_{t-1}(x) \cap Q_t(x)$$

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end for

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Compute $\mu_t(x)$ and $\sigma_t(x), \forall x \in U_t$

$$t \leftarrow t + 1$$

end while

$$\hat{H} \leftarrow H_{t-1}$$

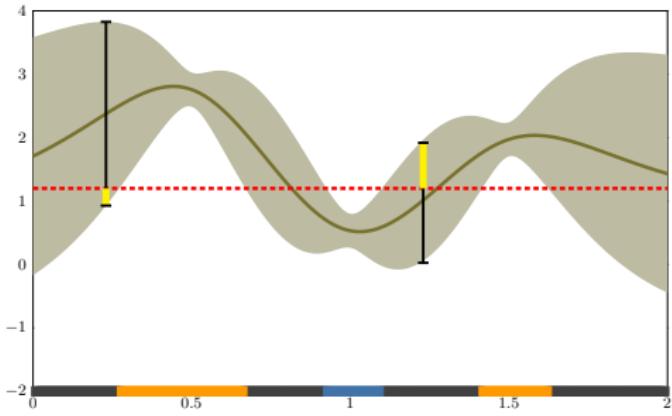
$$\hat{L} \leftarrow L_{t-1}$$

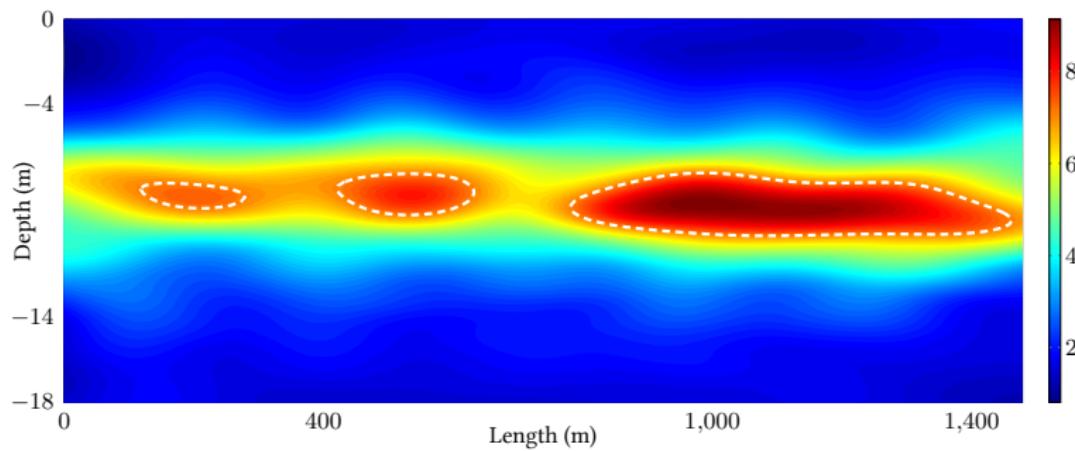
The Level Set Estimation (LSE) algorithm

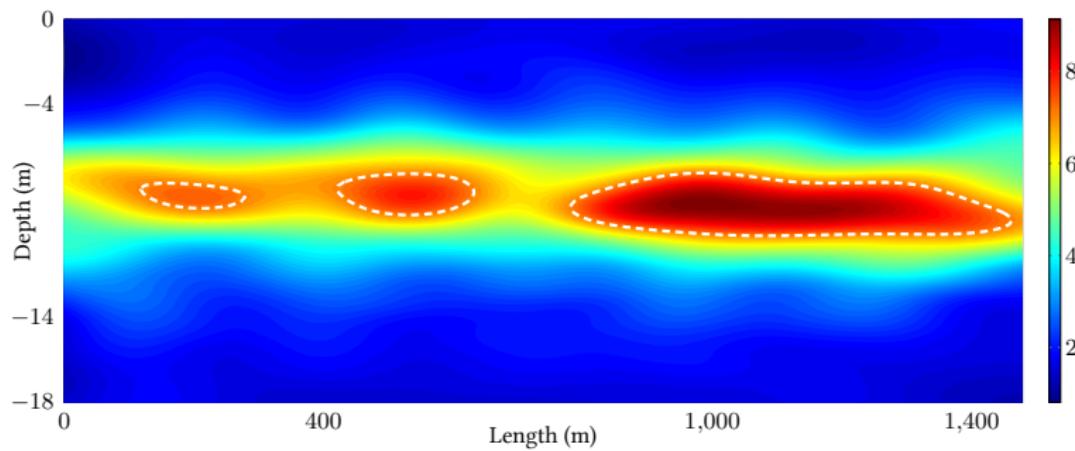
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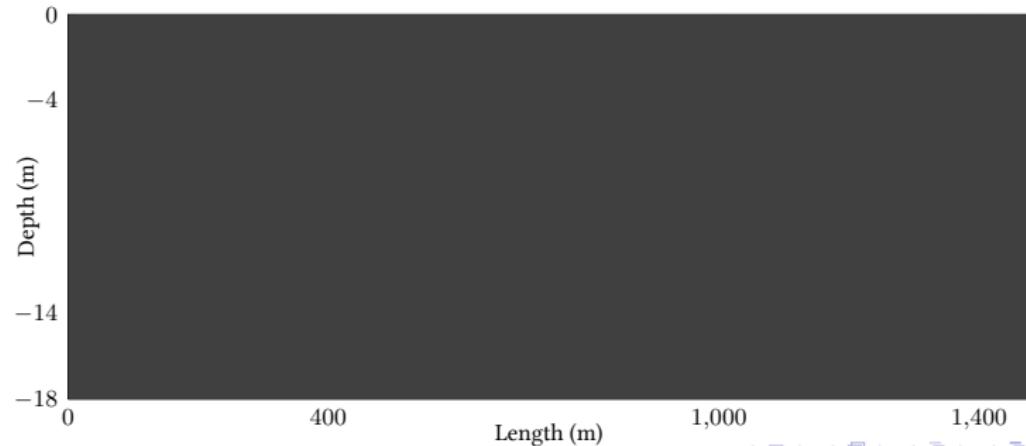
► Relaxed classification rules by an accuracy parameter ϵ (trades off sampling cost for accuracy)

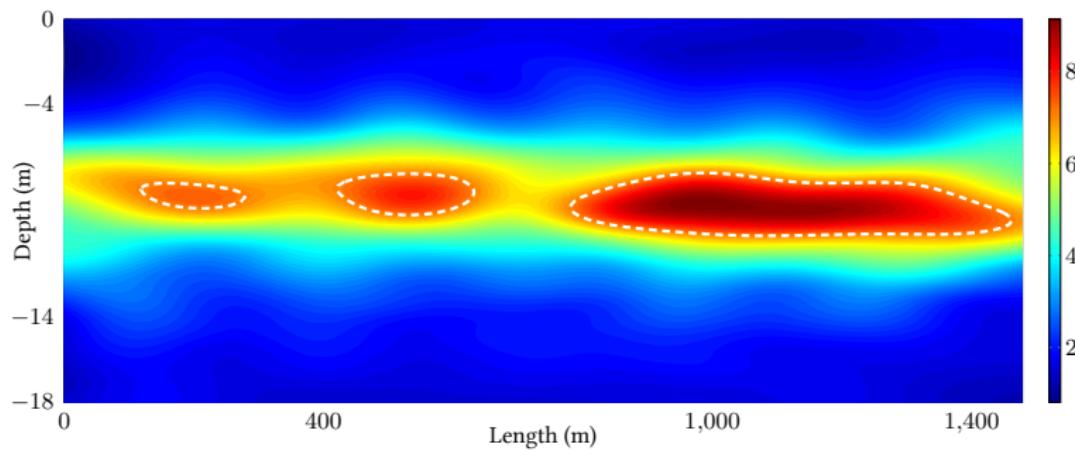




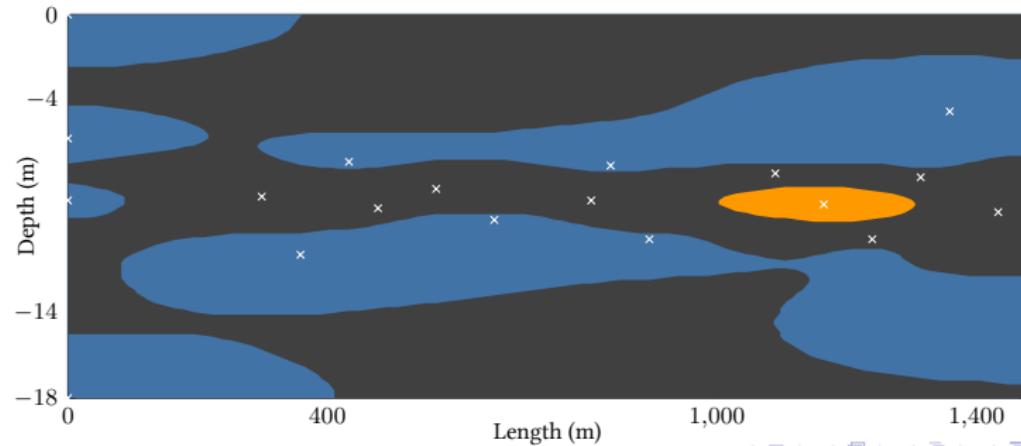


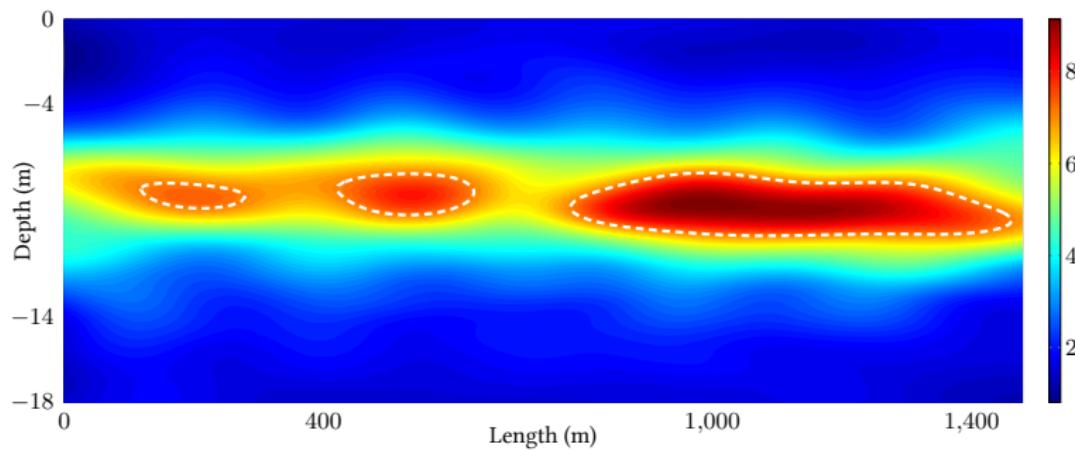
$t = 0$



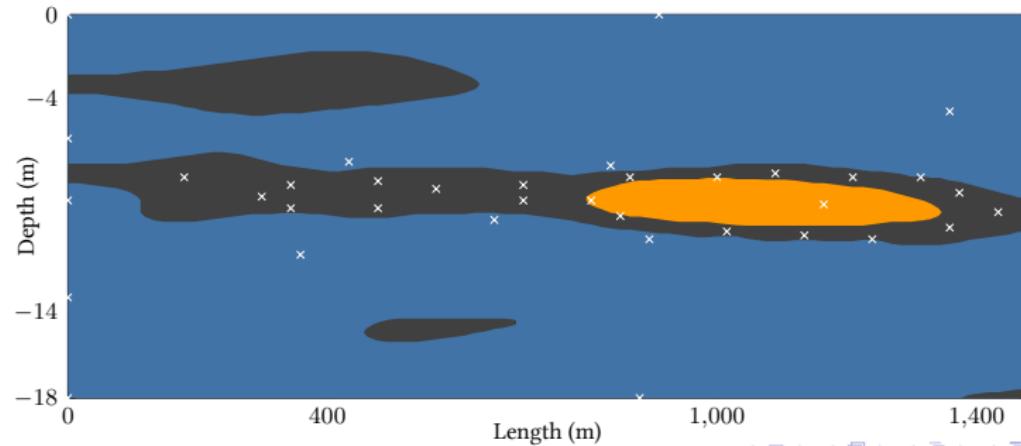


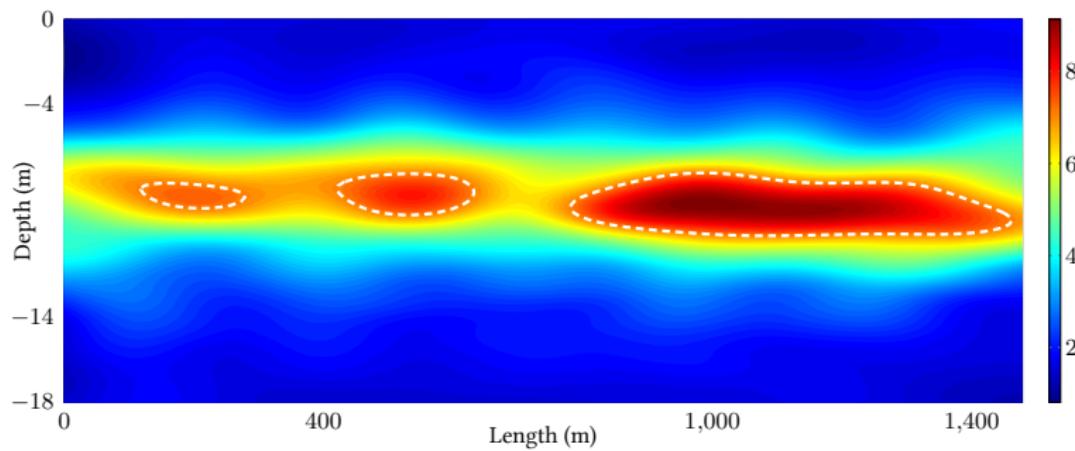
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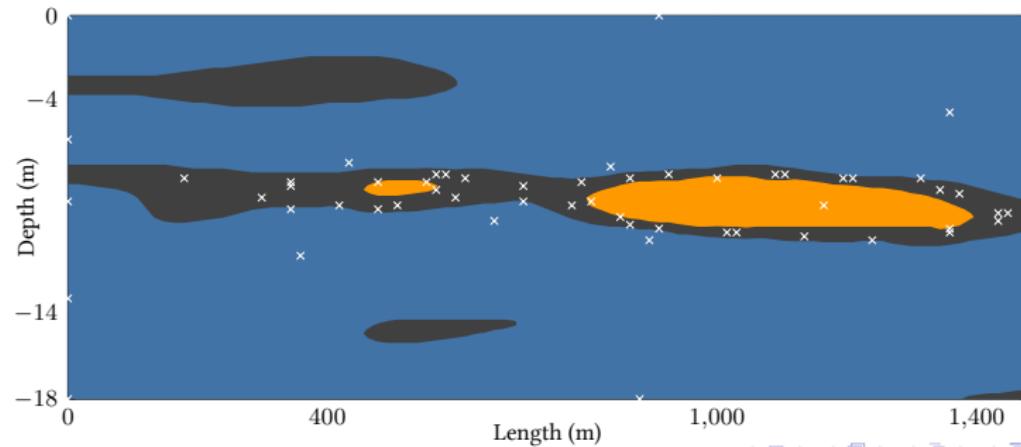


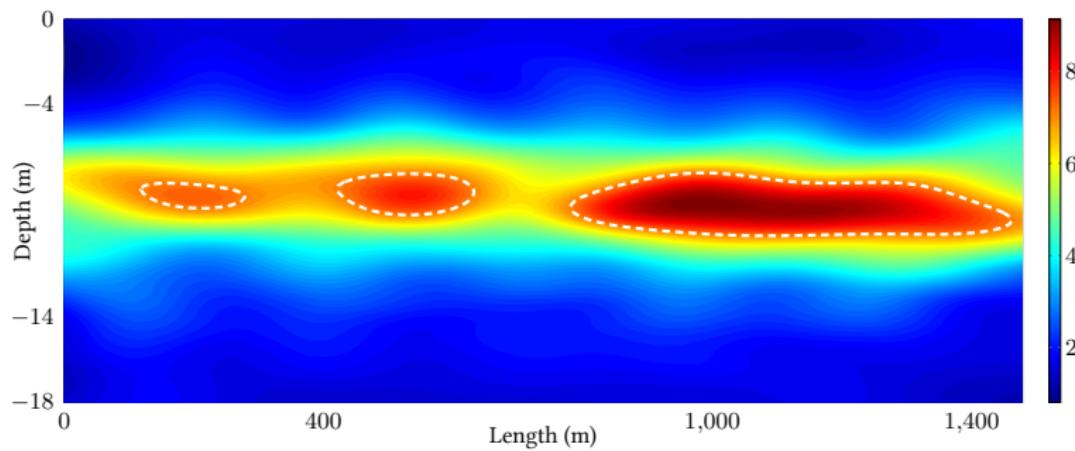
$t = 40$



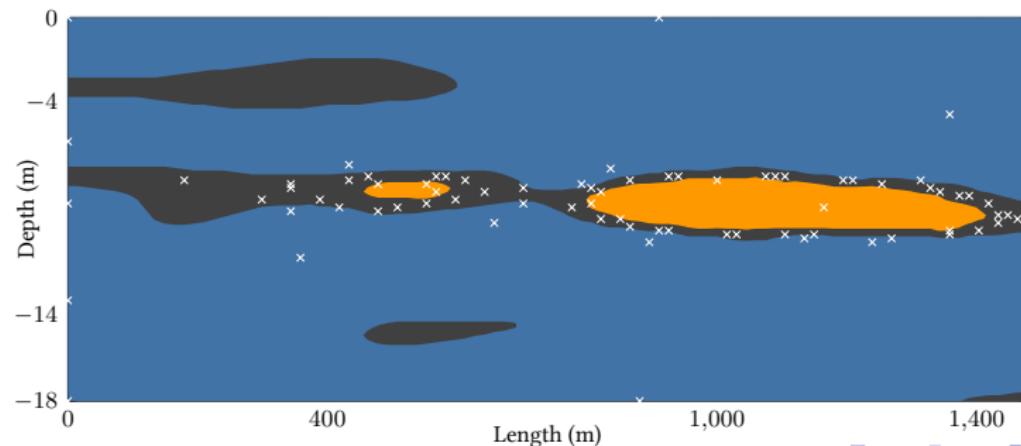


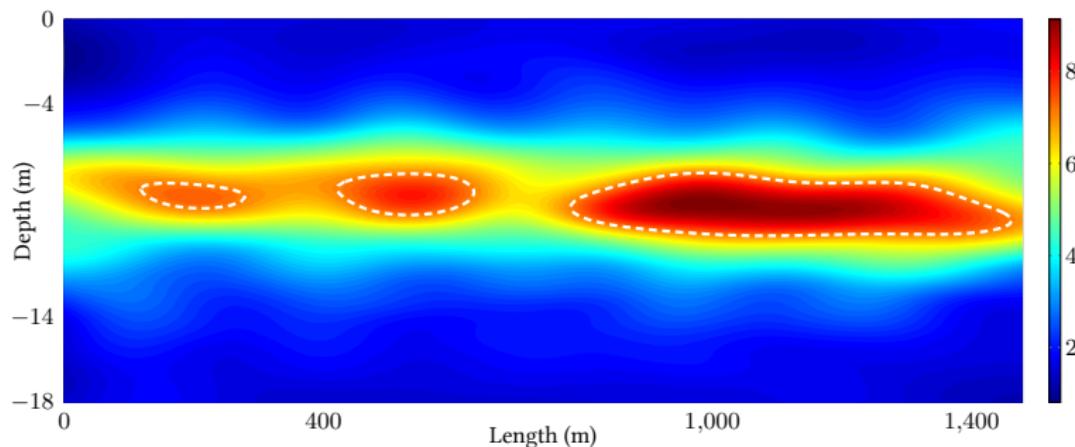
$t = 60$



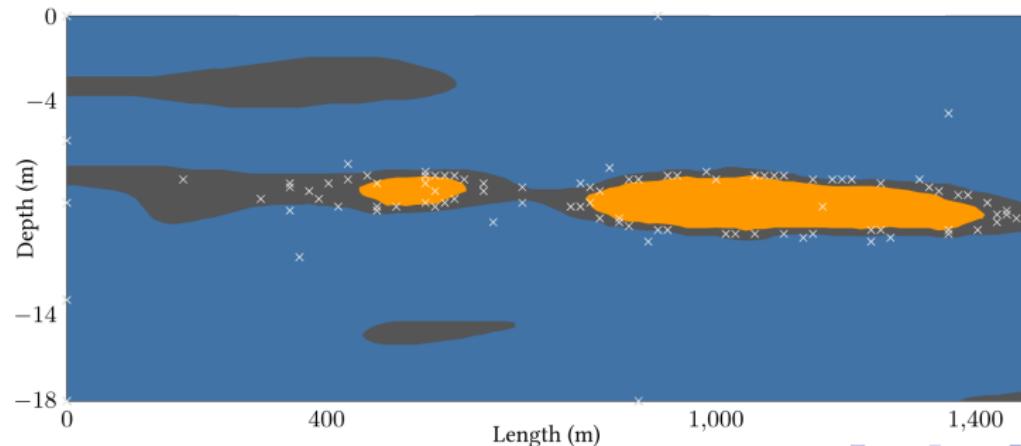


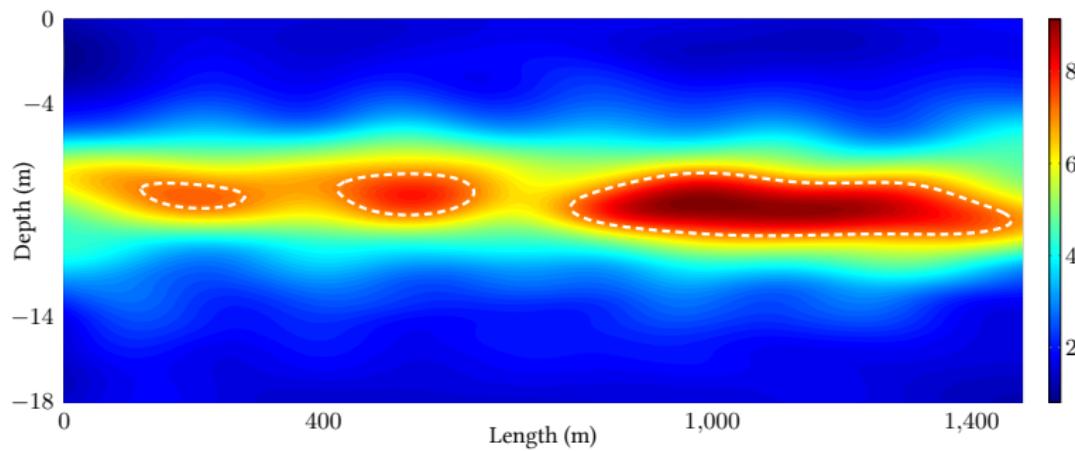
$t = 80$



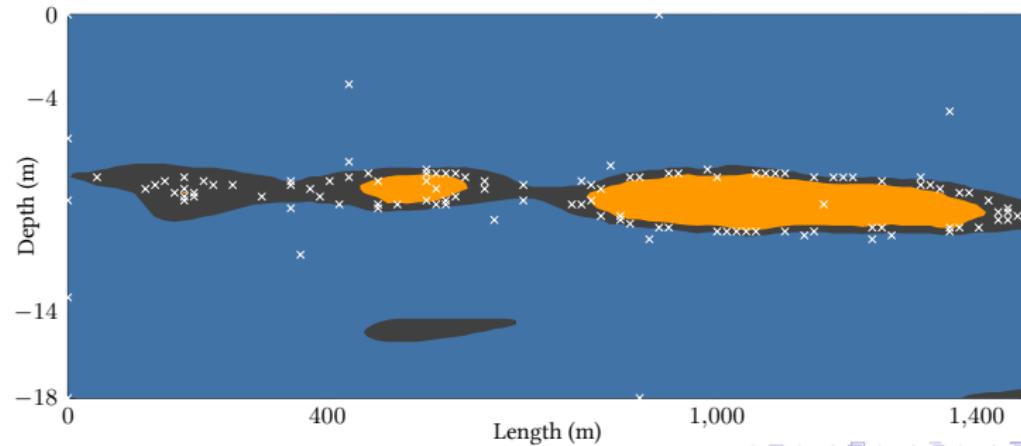


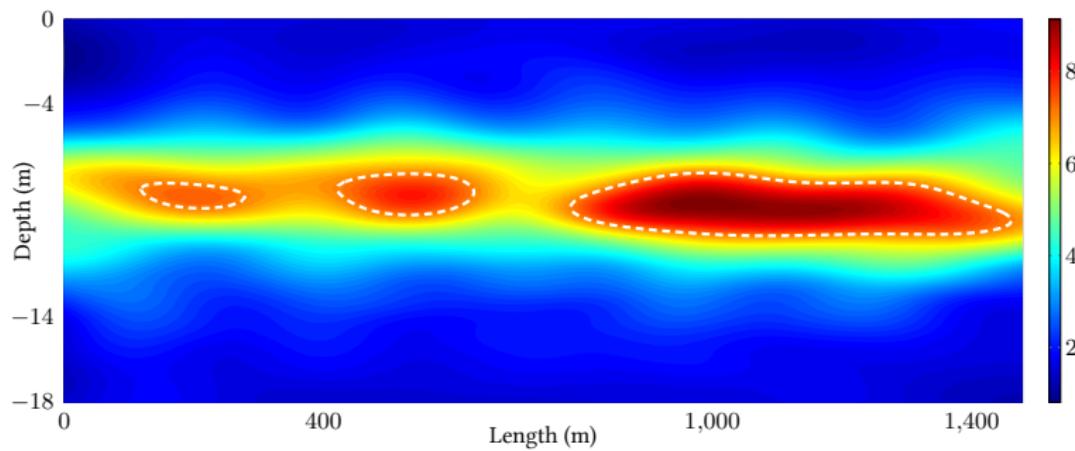
$t = 100$



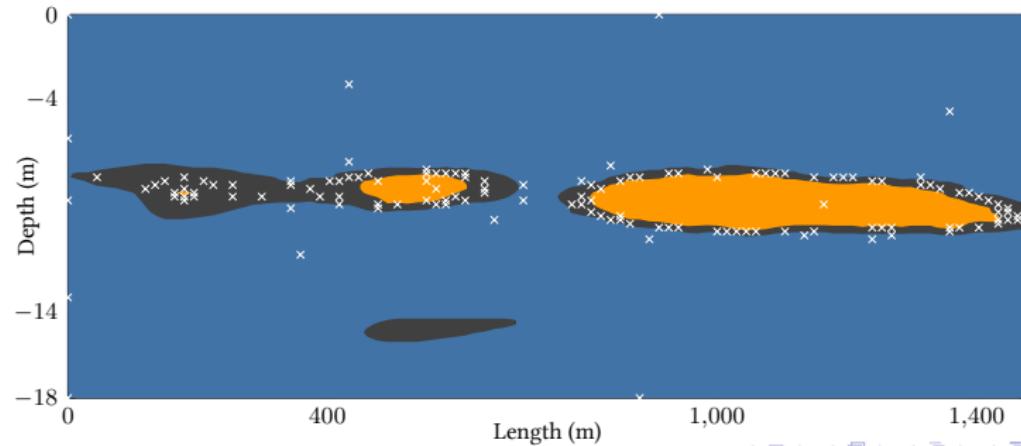


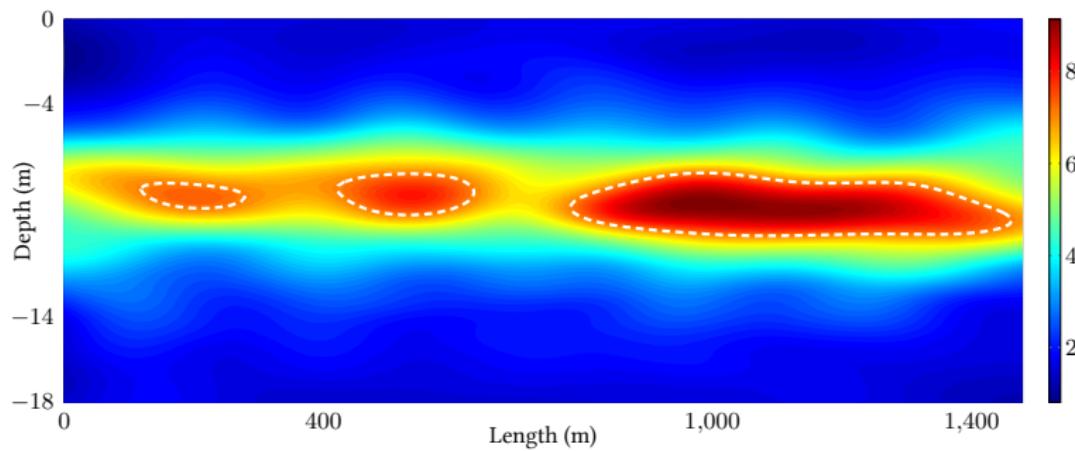
$t = 120$



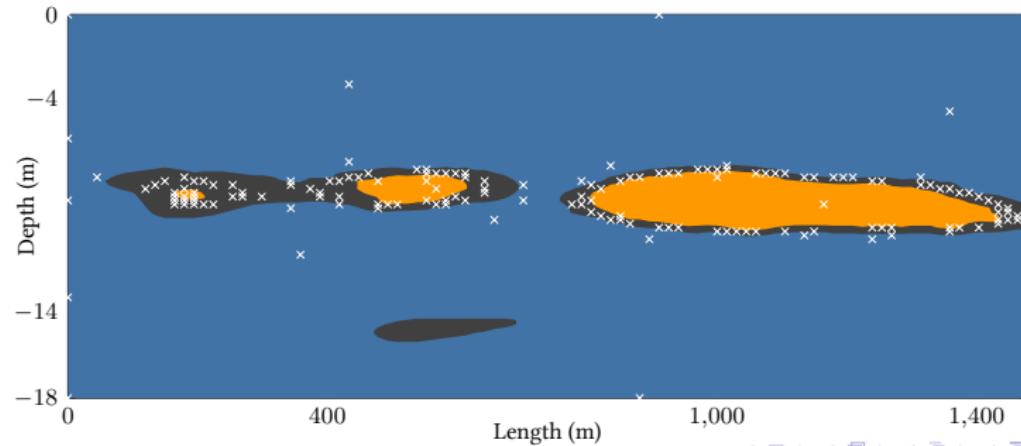


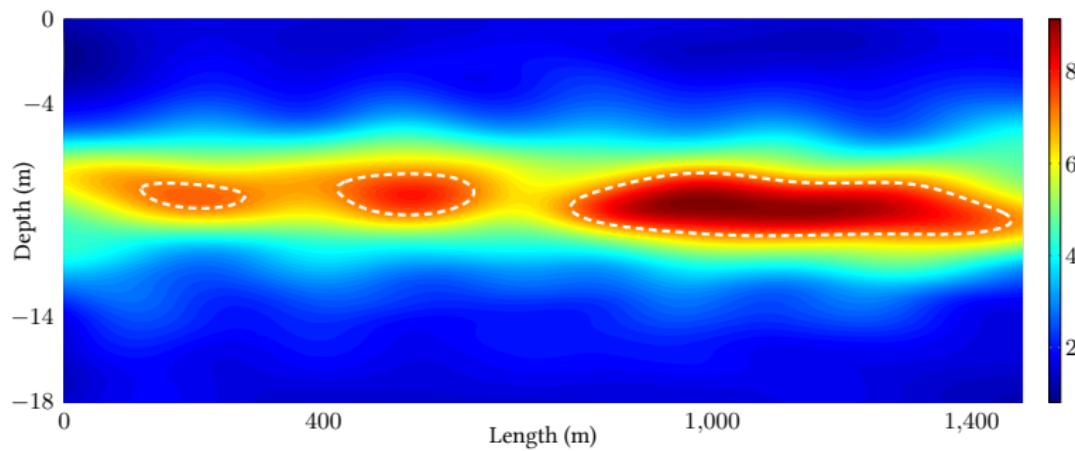
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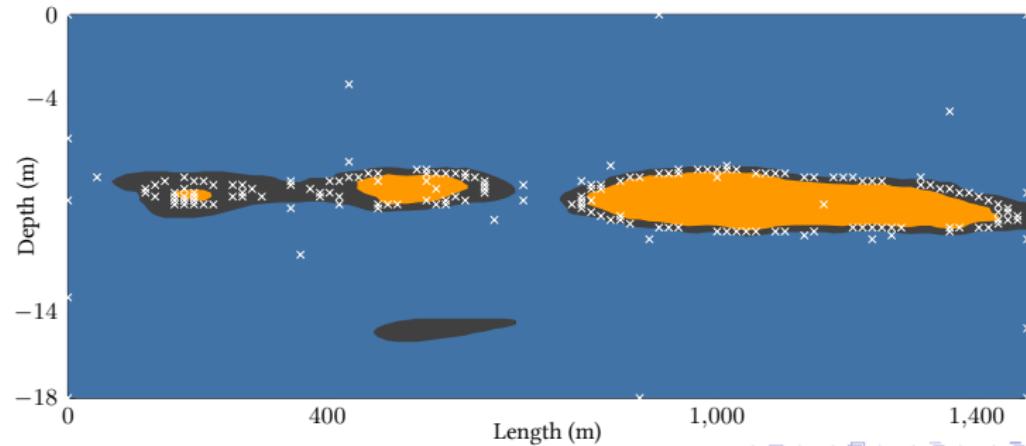


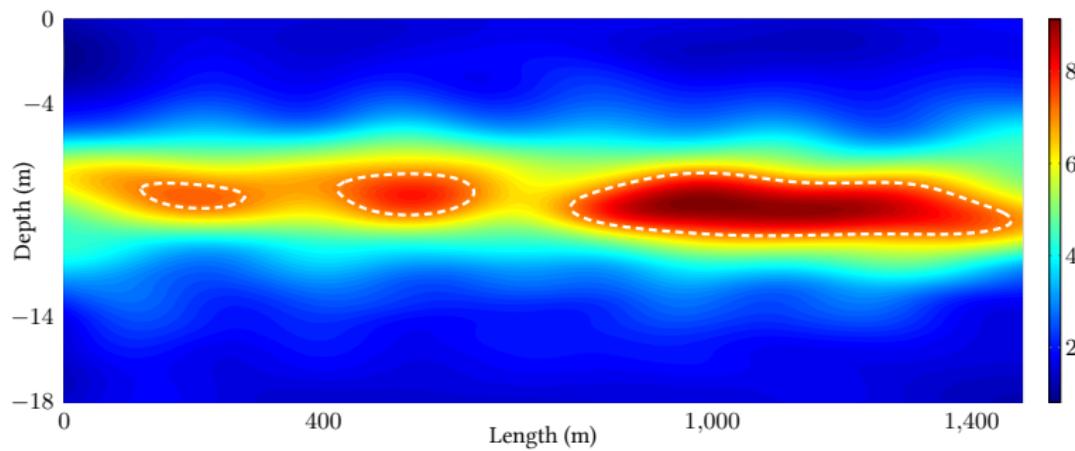
$t = 160$



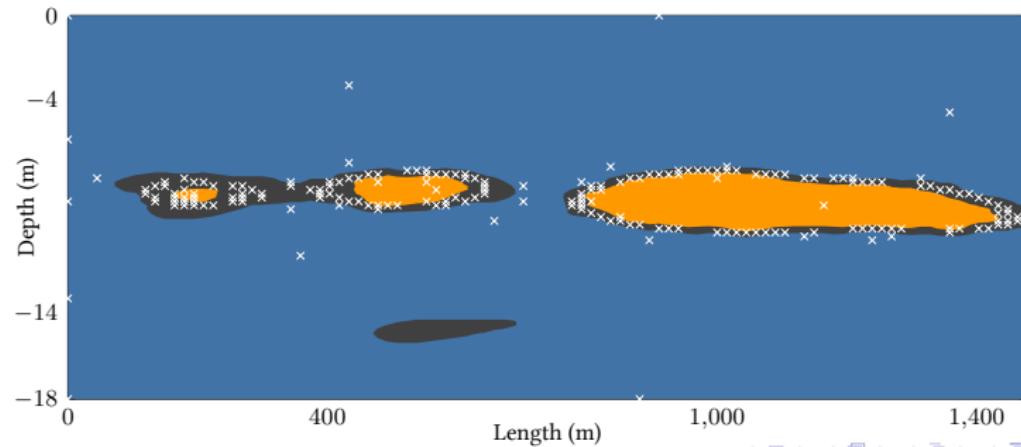


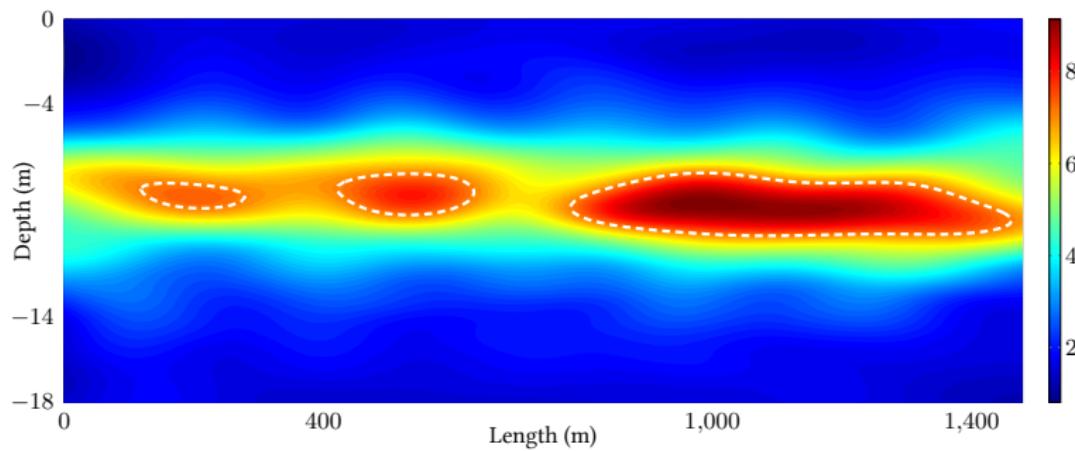
$t = 180$



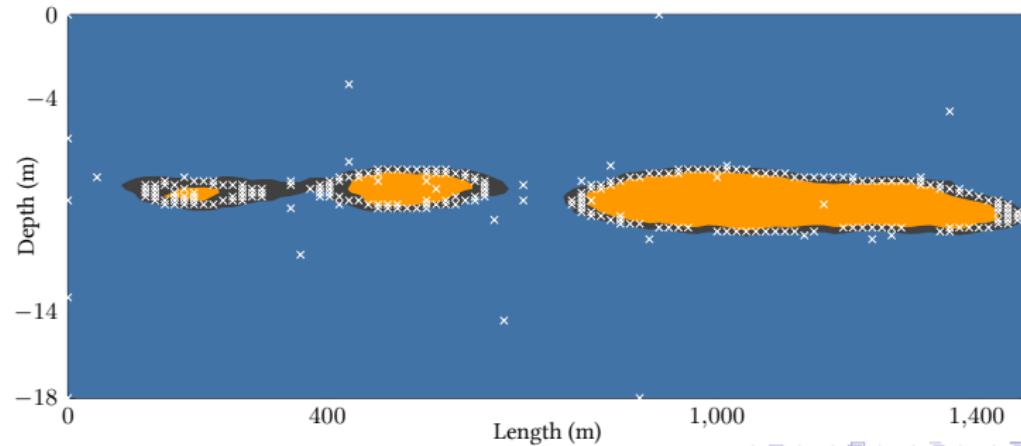


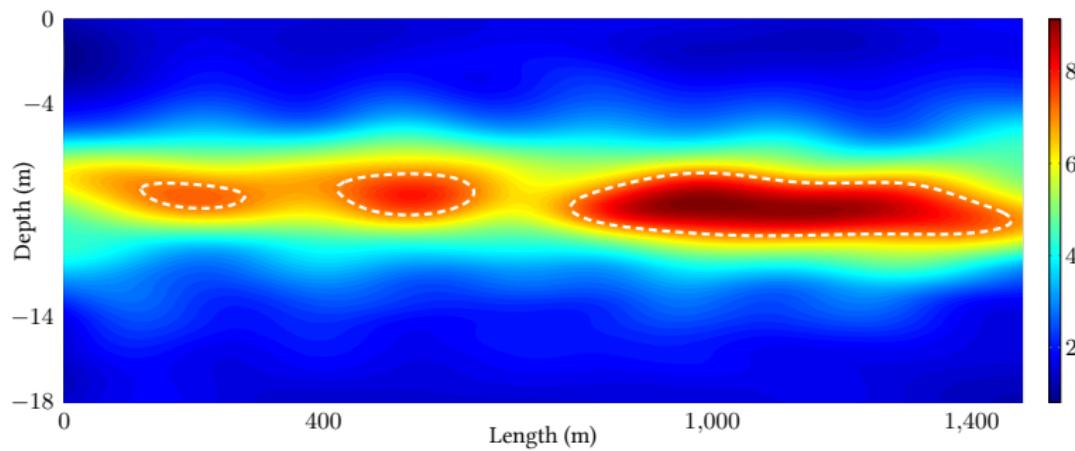
$t = 200$



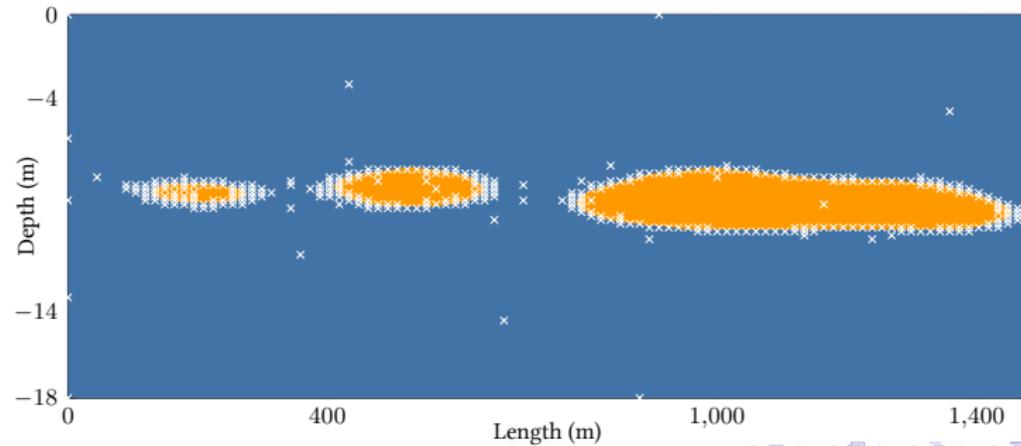


$t = 260$





$t = 354$



Theorem (Convergence of LSE)

For any $h \in \mathbb{R}$, $\delta \in (0, 1)$, and $\epsilon > 0$, if $\beta_t = 2 \log(|D| \pi^2 t^2 / (6\delta))$, LSE terminates after at most T iterations, where T is the smallest positive integer satisfying

$$\frac{T}{\beta_T \gamma_T} \geq \frac{C_1}{4\epsilon^2},$$

where $C_1 = 8/\log(1 + \sigma^{-2})$.

Furthermore, with probability at least $1 - \delta$, the algorithm returns an ϵ -accurate solution, that is

$$\Pr \left\{ \max_{\mathbf{x} \in D} \ell_h(\mathbf{x}) \leq \epsilon \right\} \geq 1 - \delta.$$

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If we choose β_t large enough, then:

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Experiments

1. LSE

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1. LSE
2. Maximum variance sampling:

$$\mathbf{x}_t = \operatorname{argmax}_{\mathbf{x} \in D} \sigma_{t-1}(\mathbf{x})$$

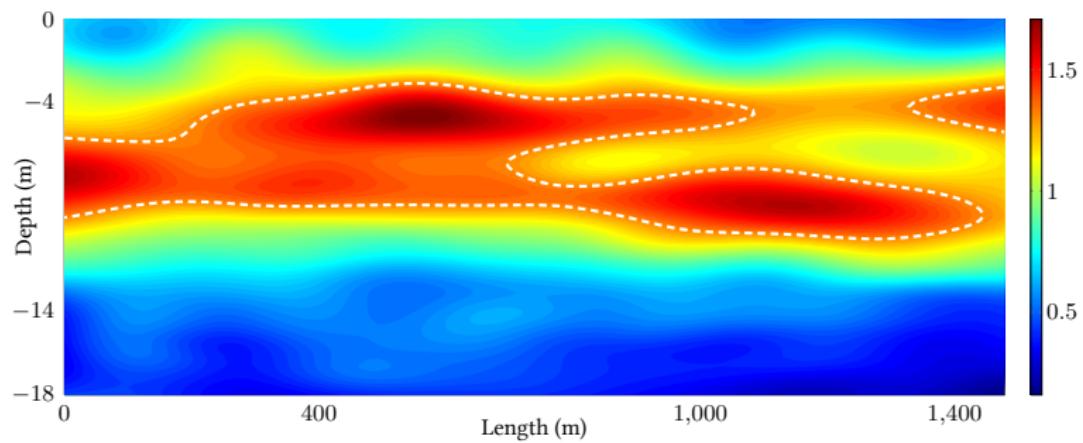
Experiments

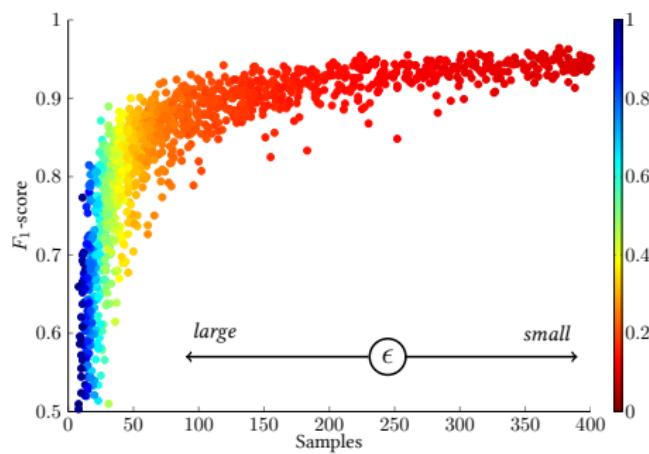
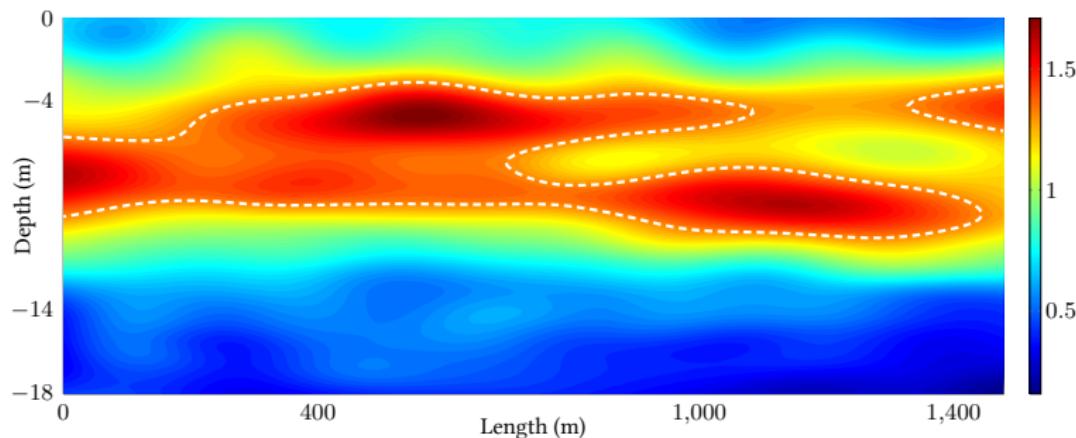
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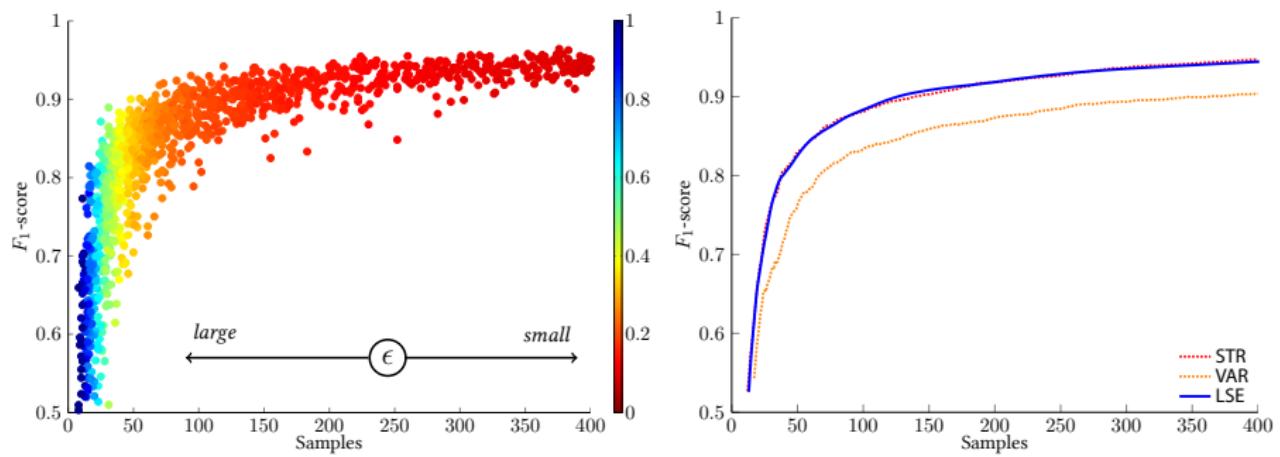
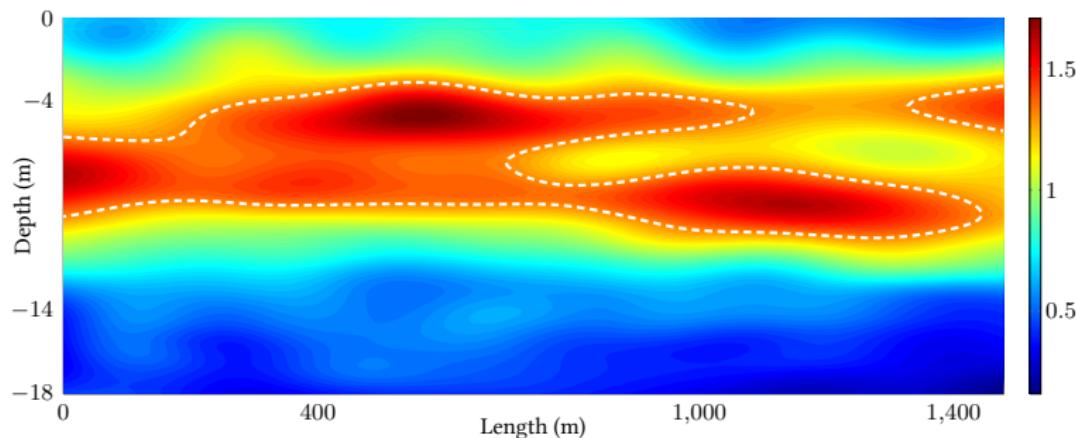
$$\mathbf{x}_t = \operatorname{argmax}_{\mathbf{x} \in D} \sigma_{t-1}(\mathbf{x})$$

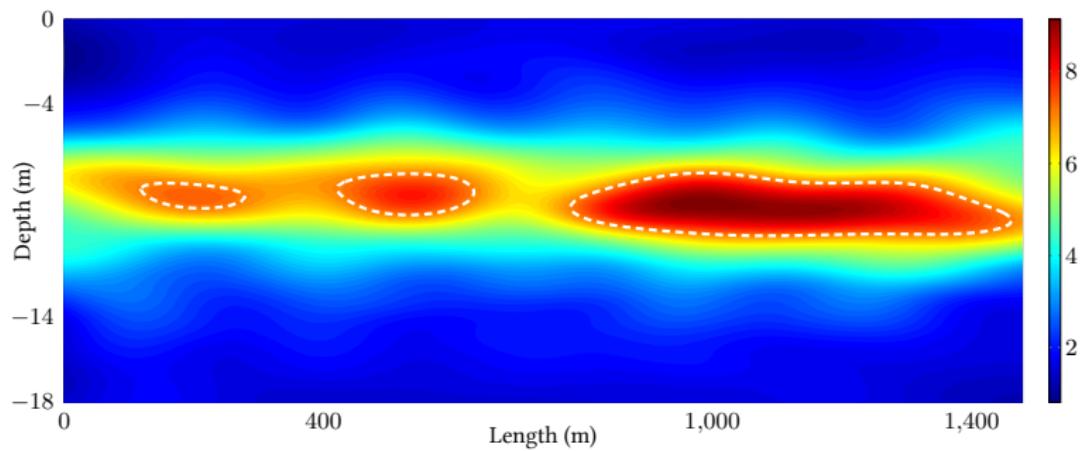
3. State of the art “straddle” heuristic (Bryan *et al.*, 2005):

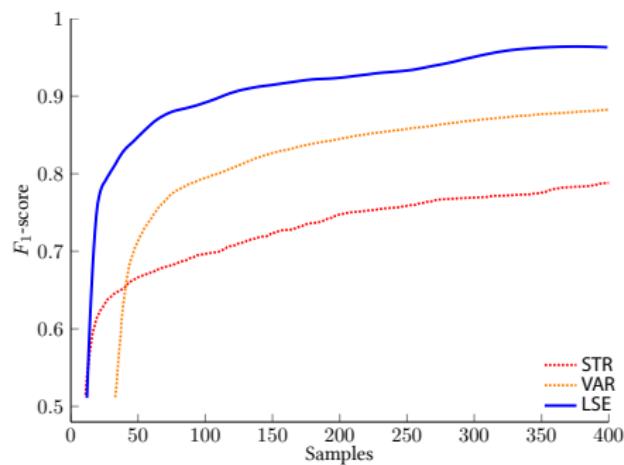
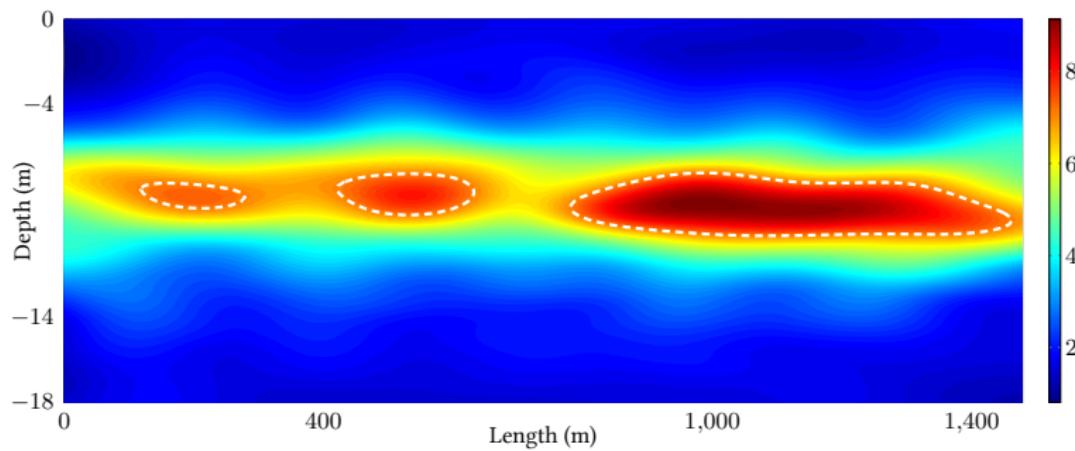
$$\mathbf{x}_t \approx \operatorname{argmax}_{\mathbf{x} \in D} a_{t-1}(\mathbf{x}) \quad (\text{for } \beta_t^{1/2} = 1.96)$$











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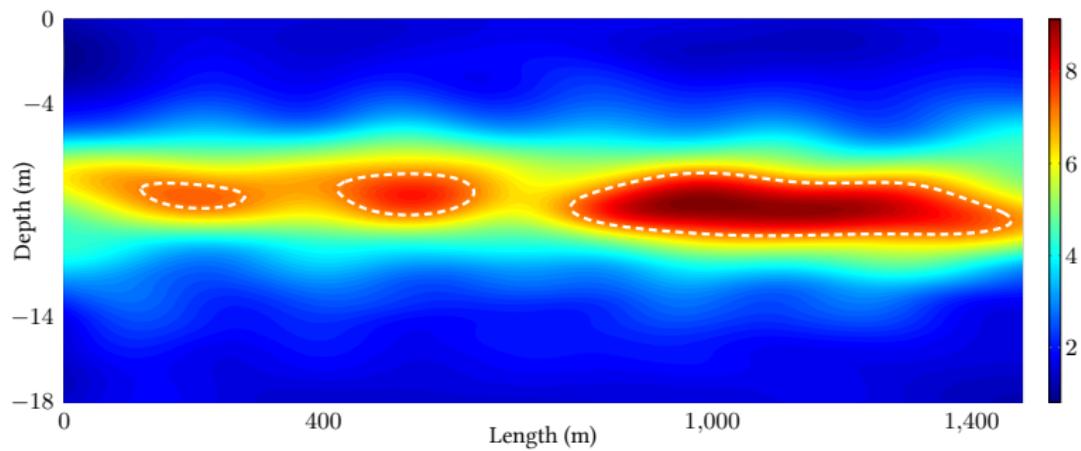
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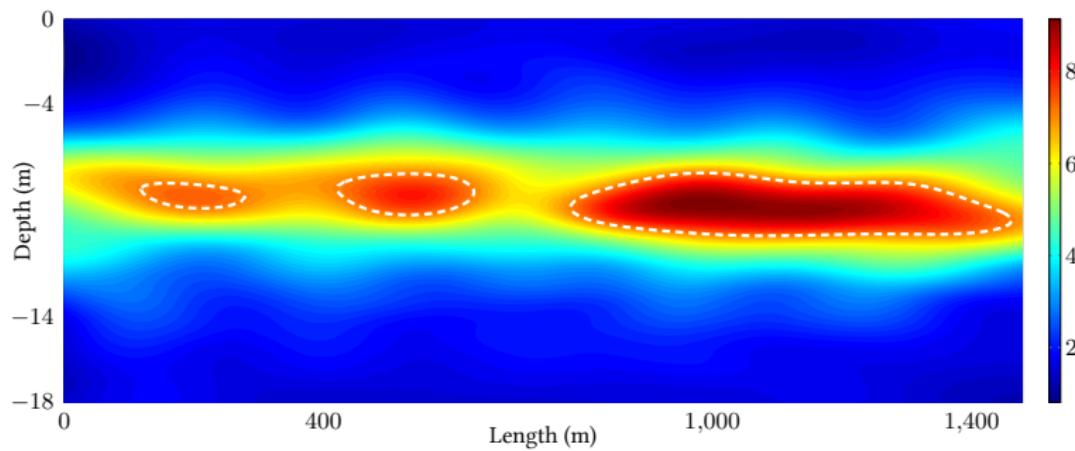
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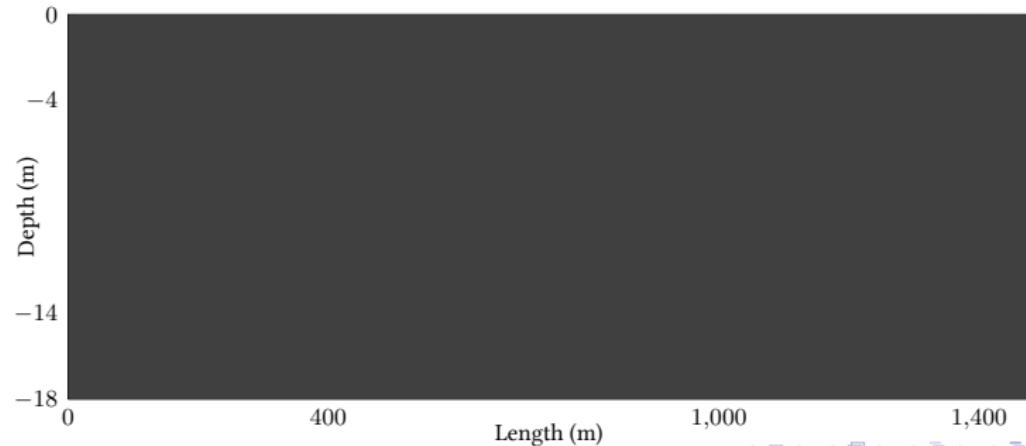
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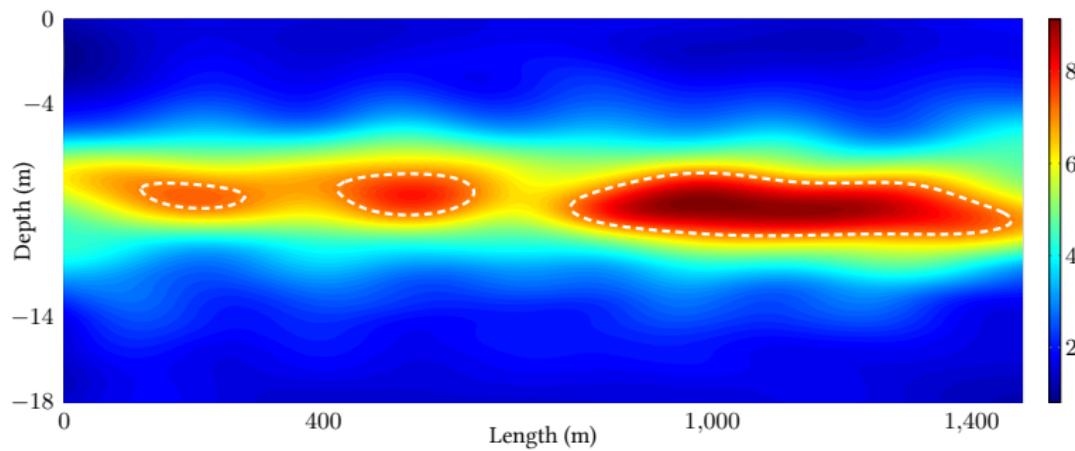
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 - ▶ h is now an estimated quantity → modified classification rules



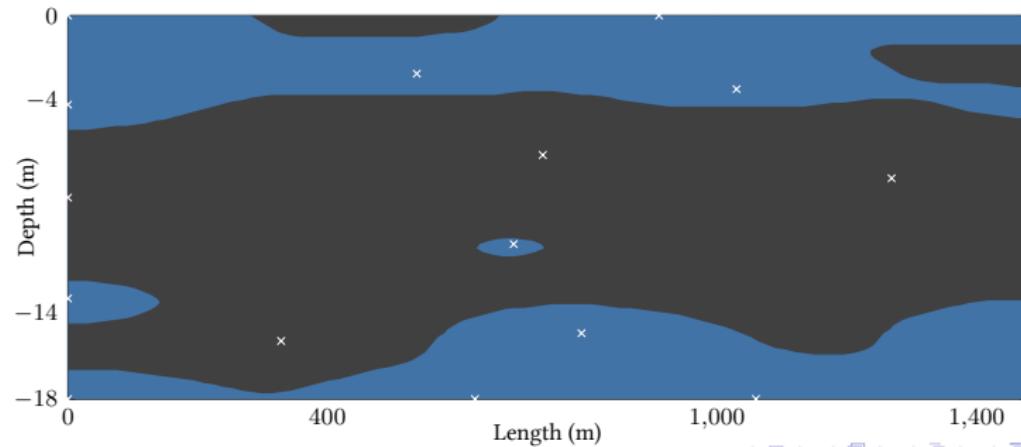


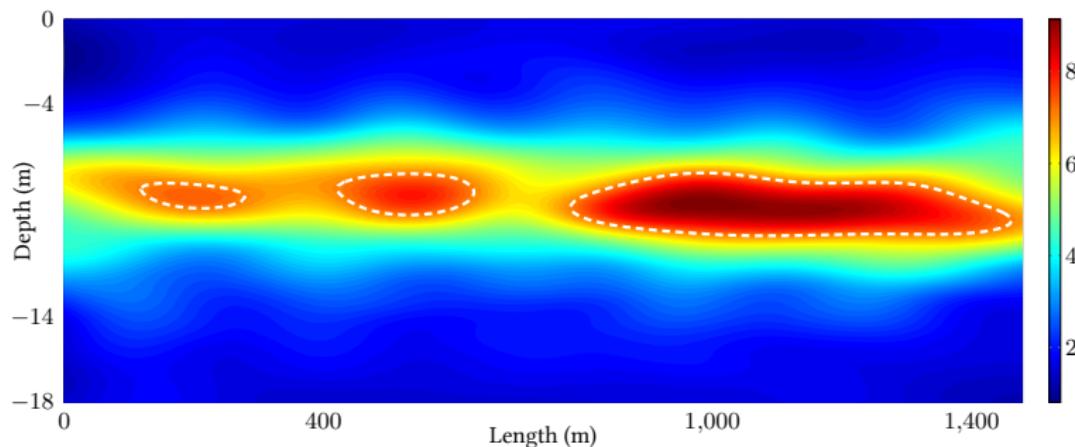
$t = 0$



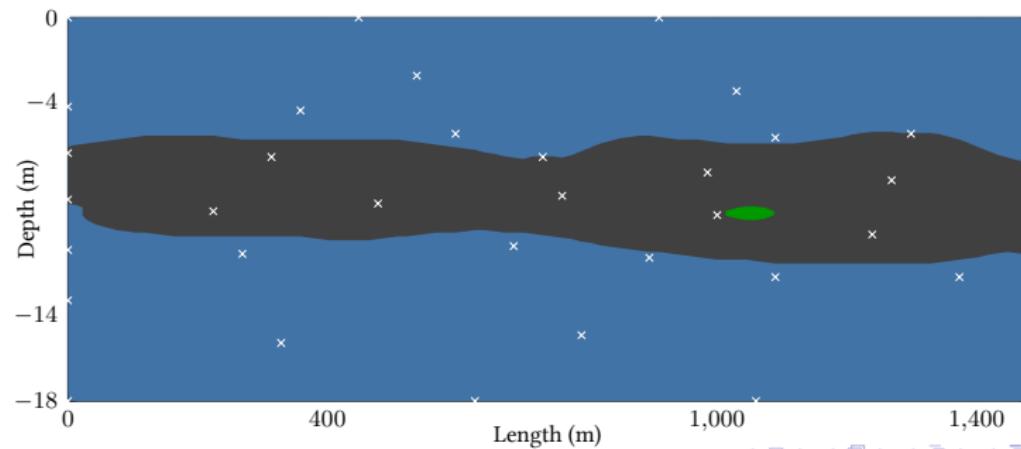


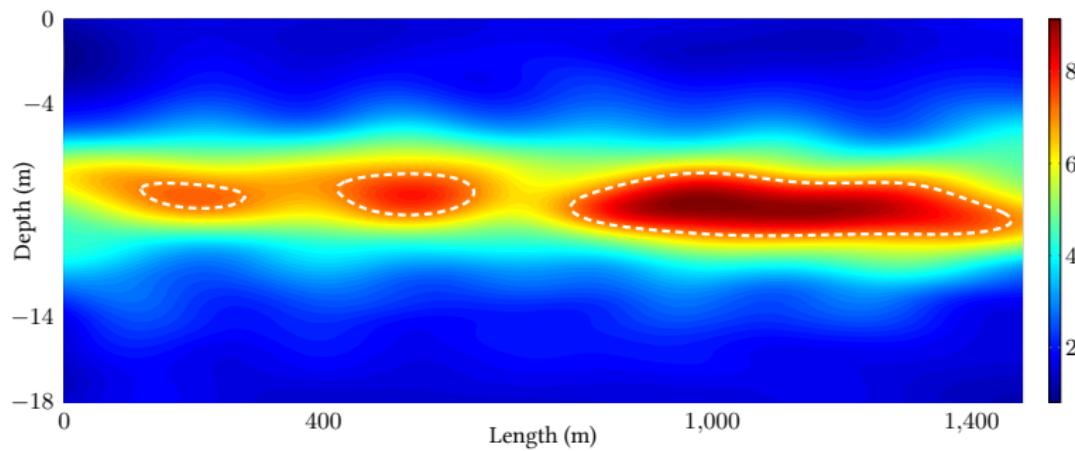
$t = 20$



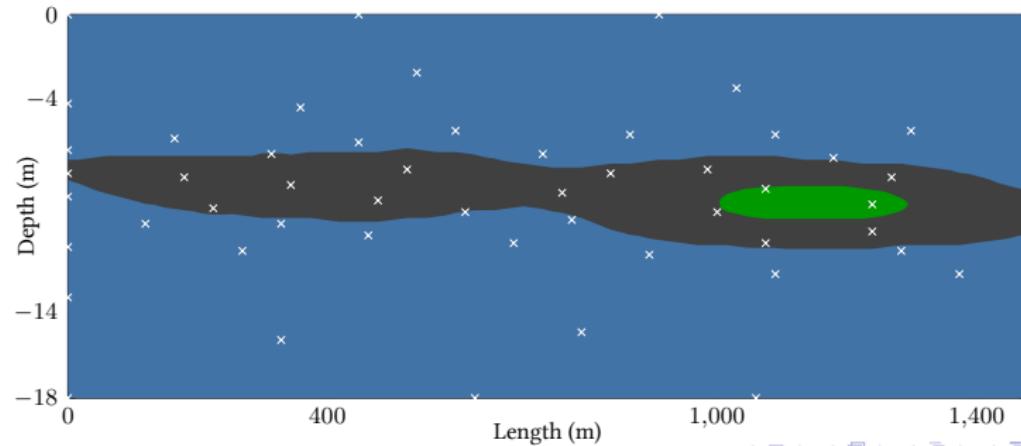


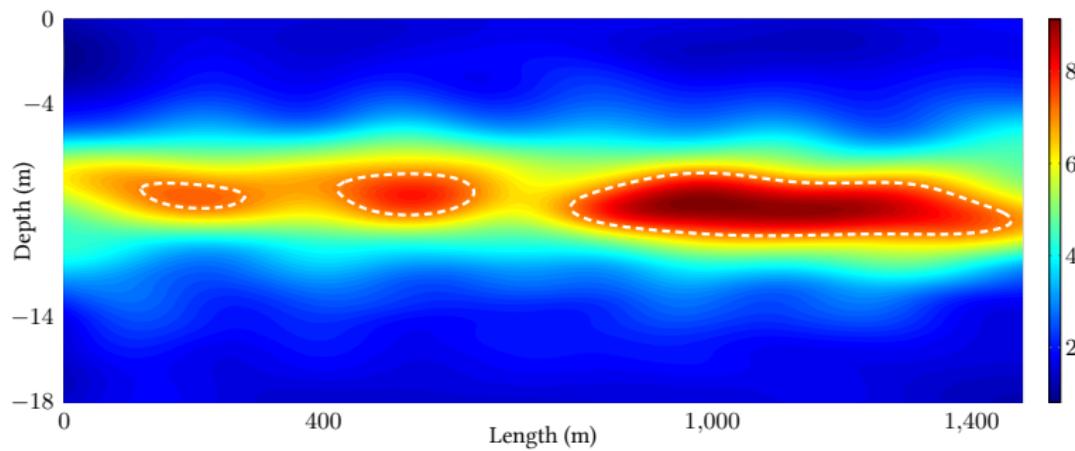
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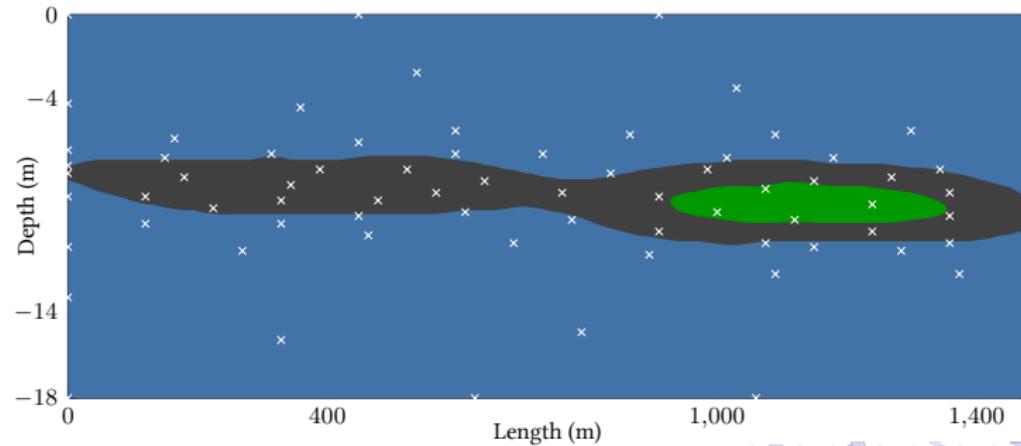


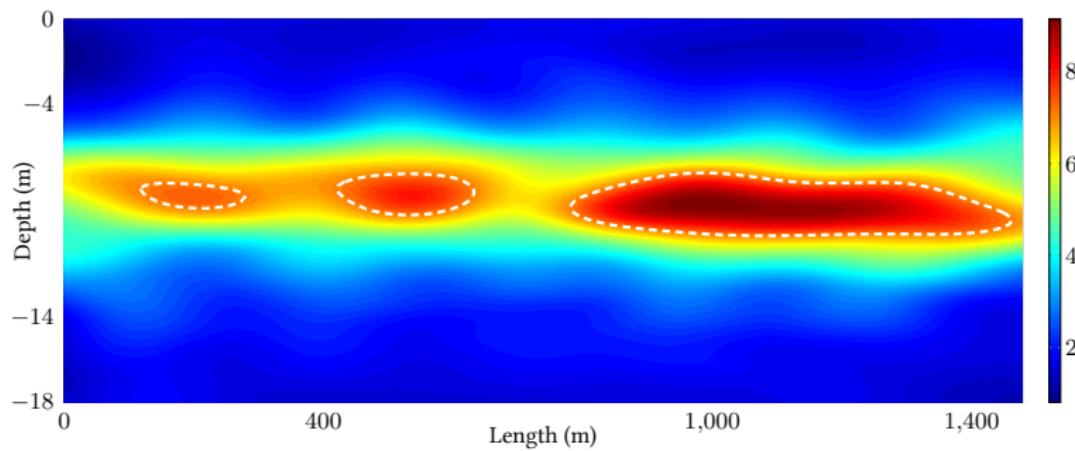
$t = 60$



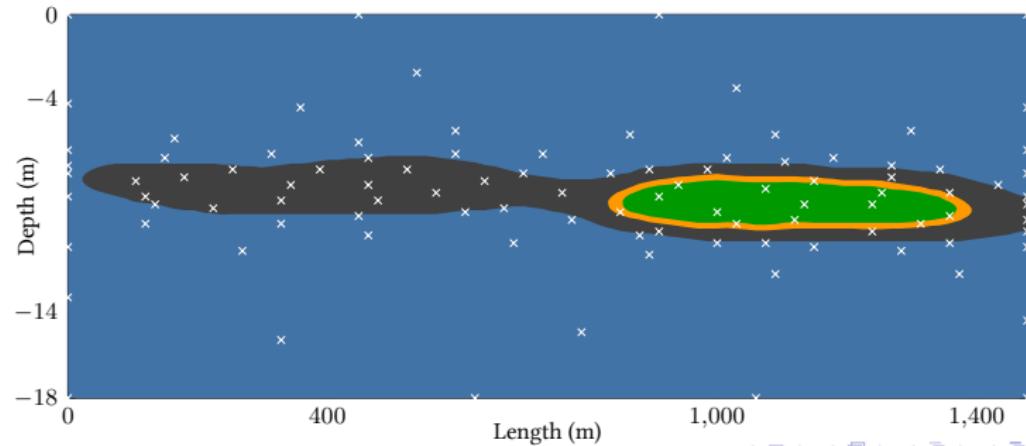


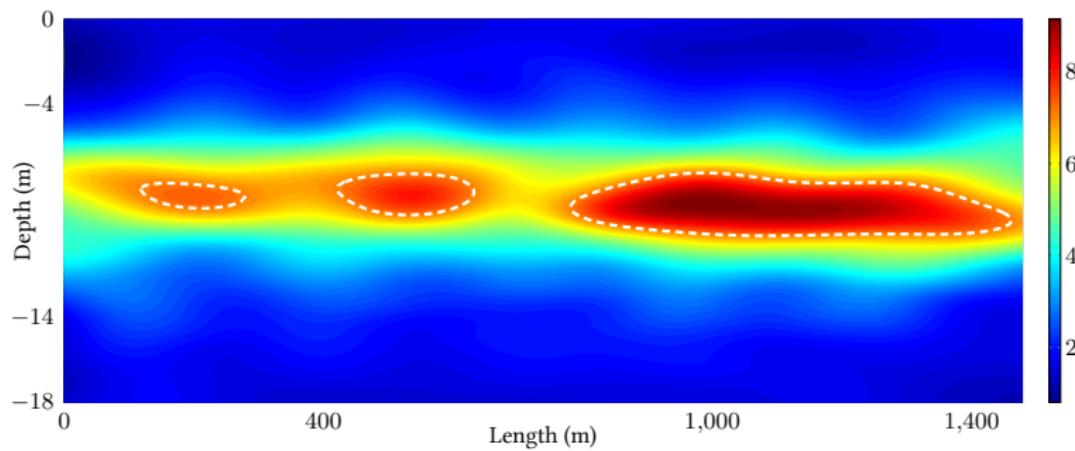
$t = 80$



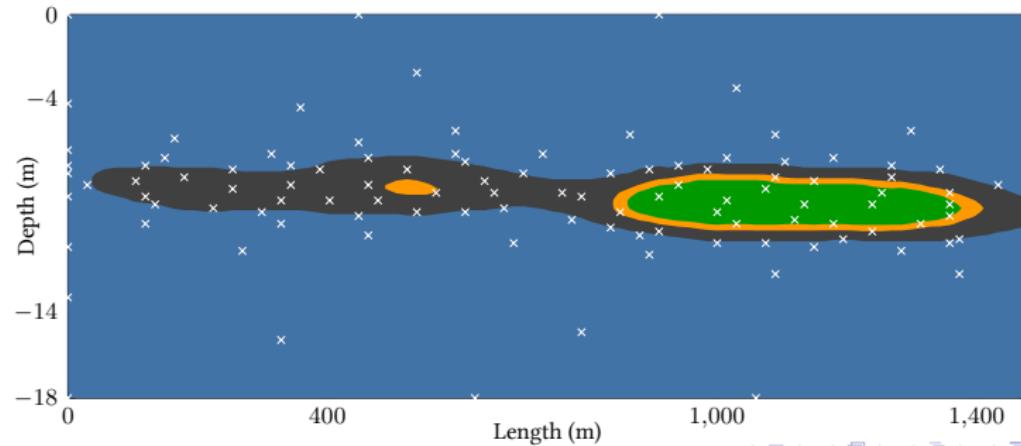


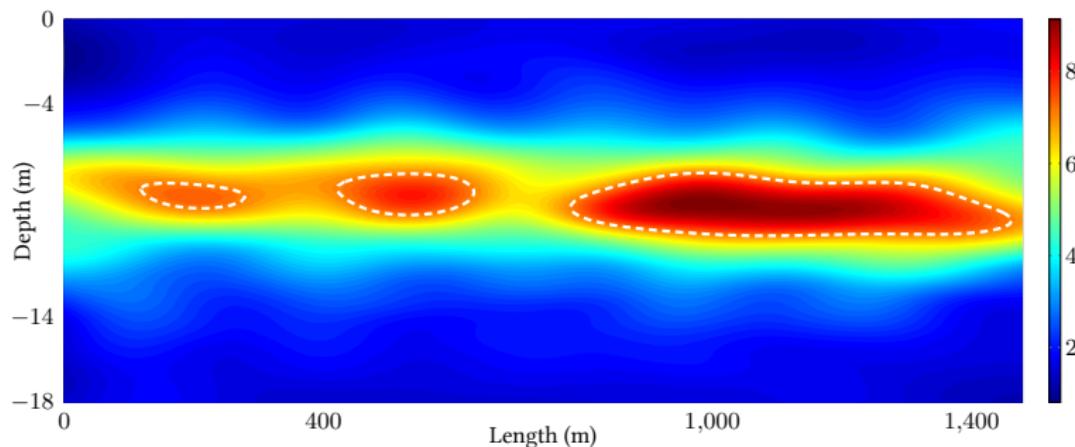
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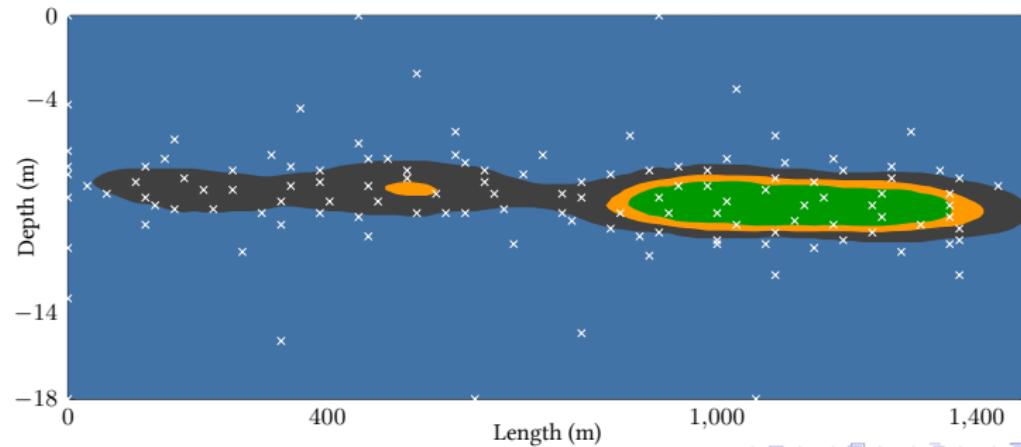


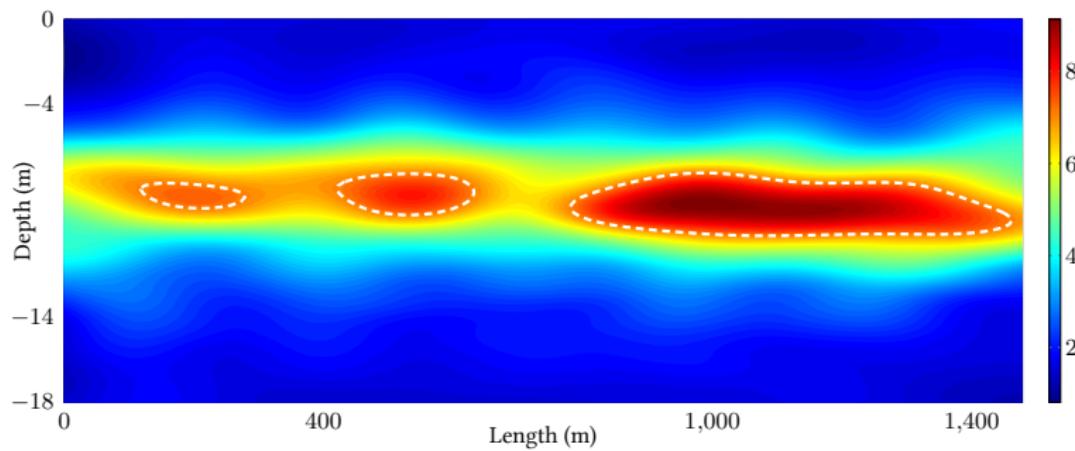
$t = 120$



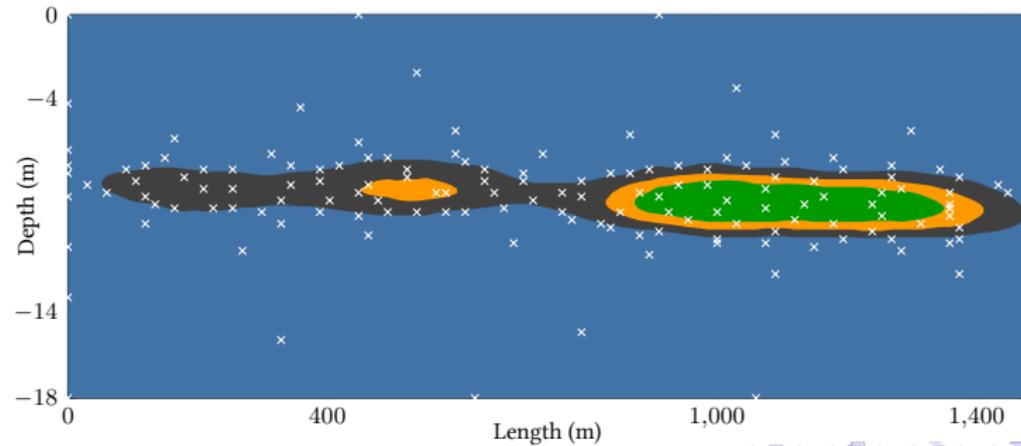


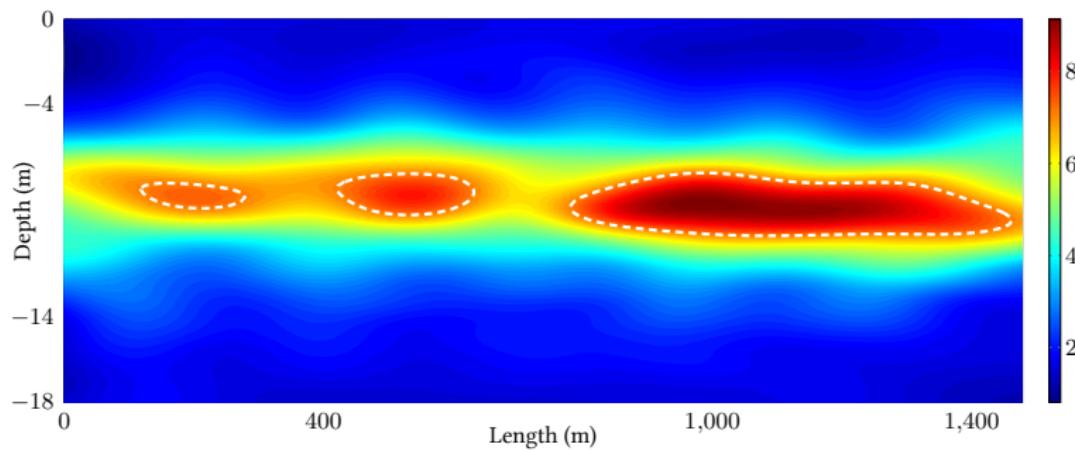
$t = 140$



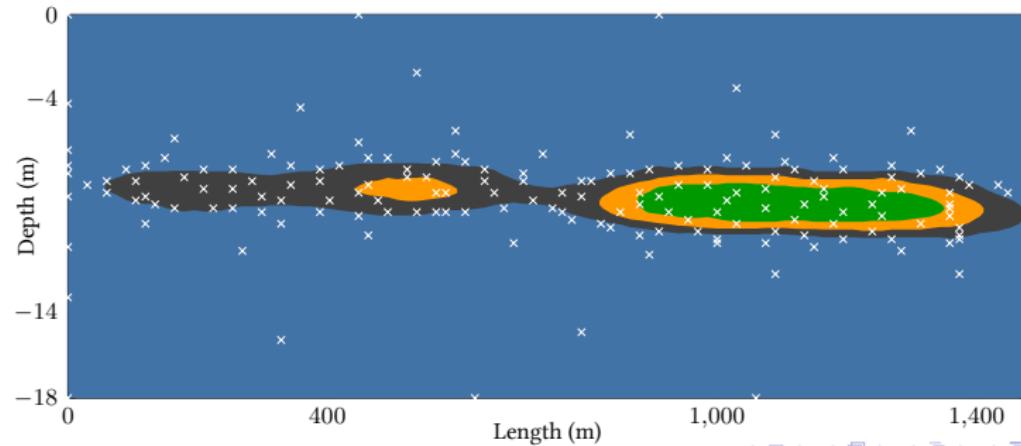


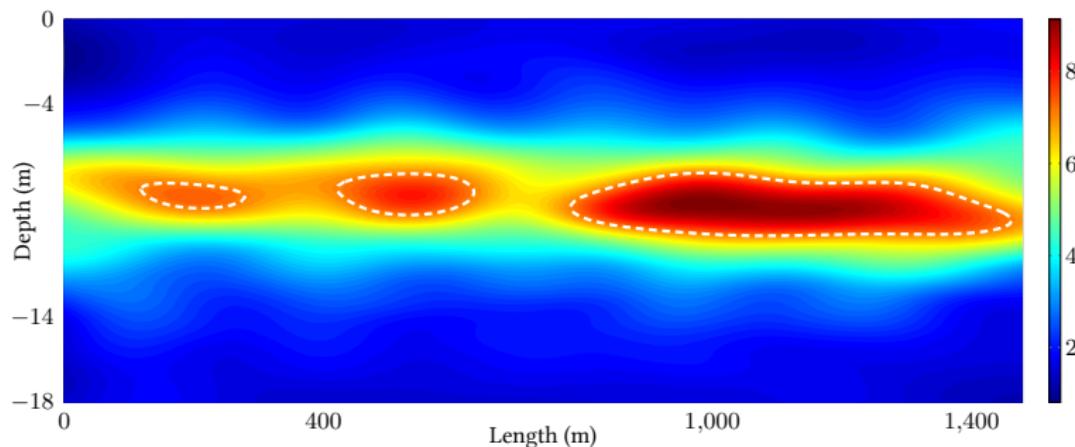
$t = 160$



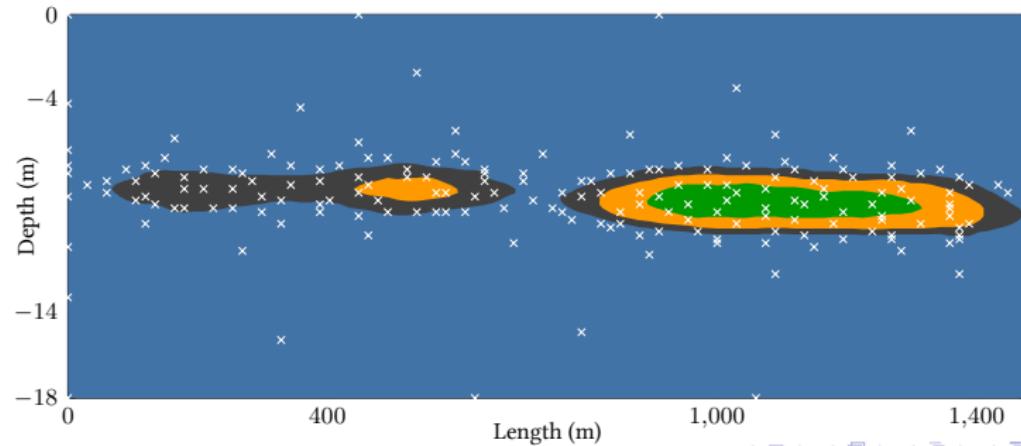


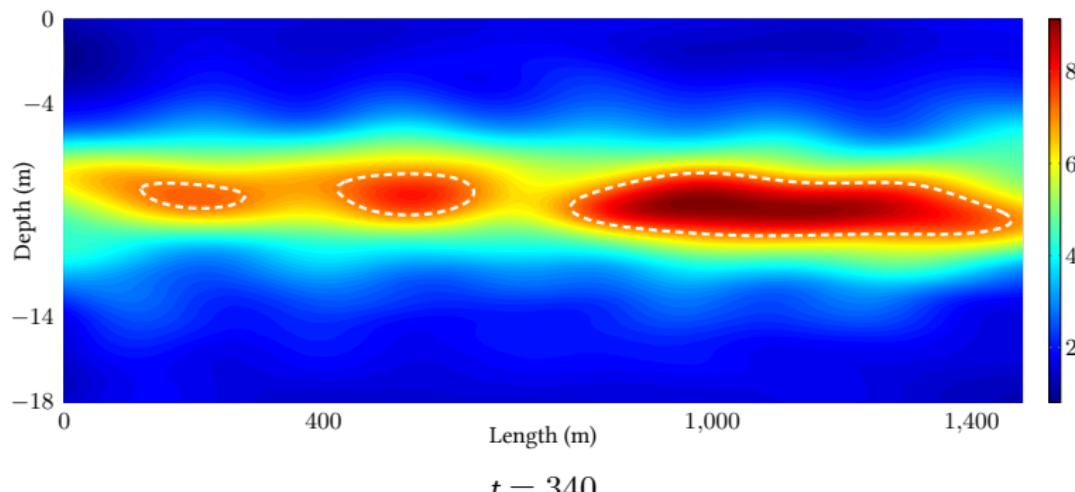
$t = 180$



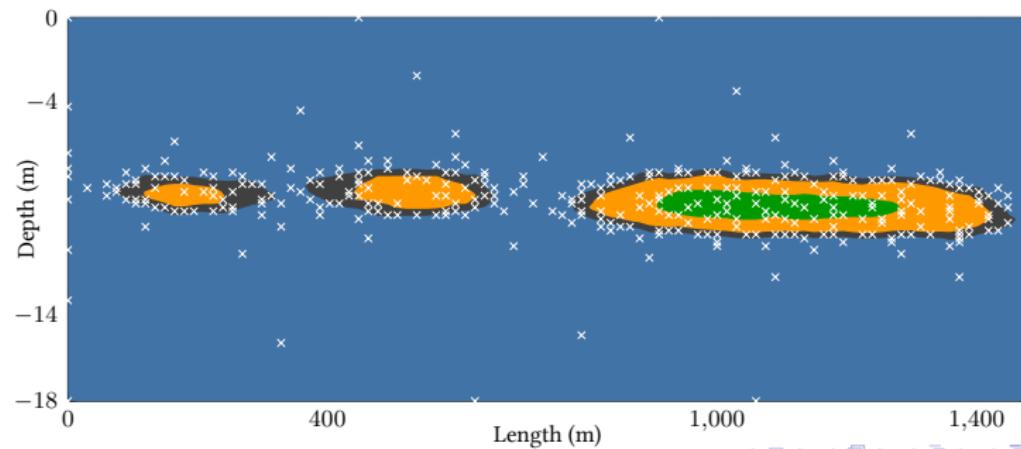


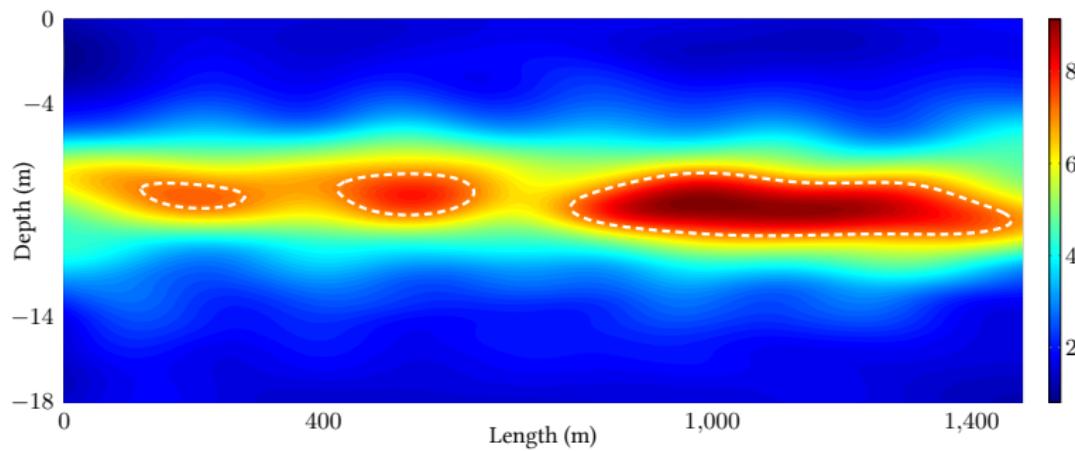
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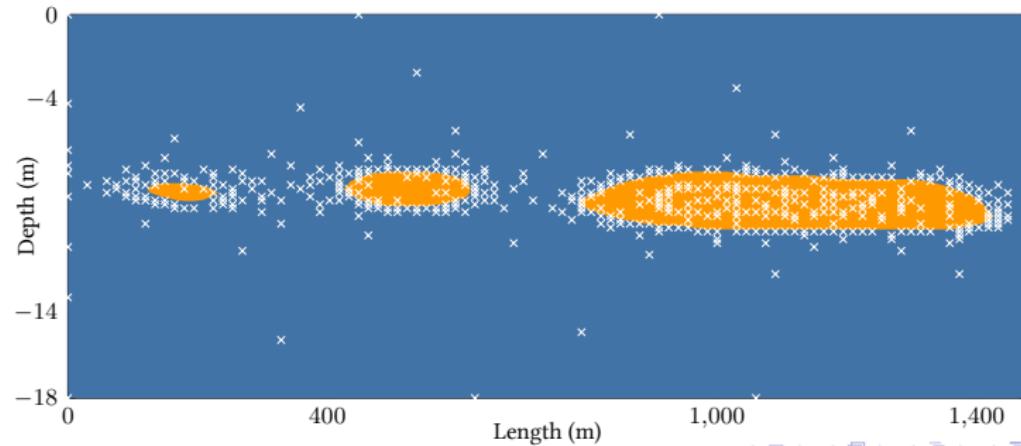


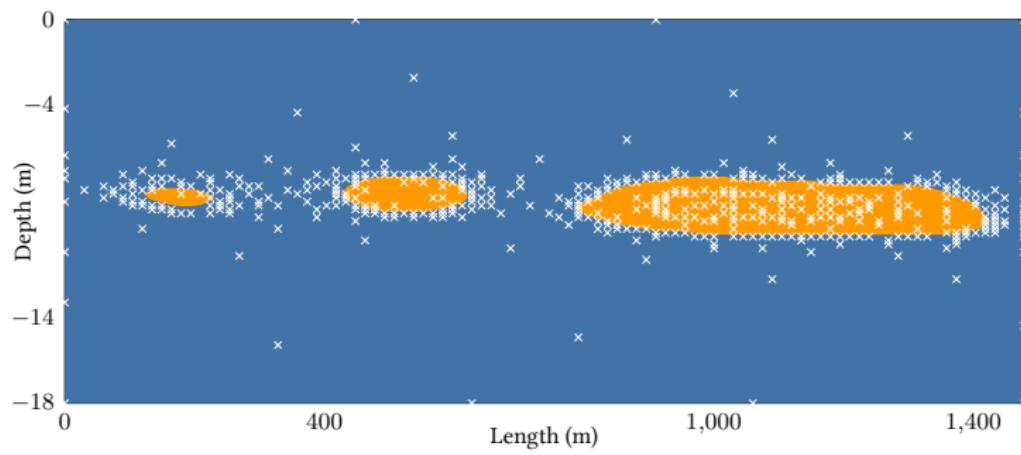
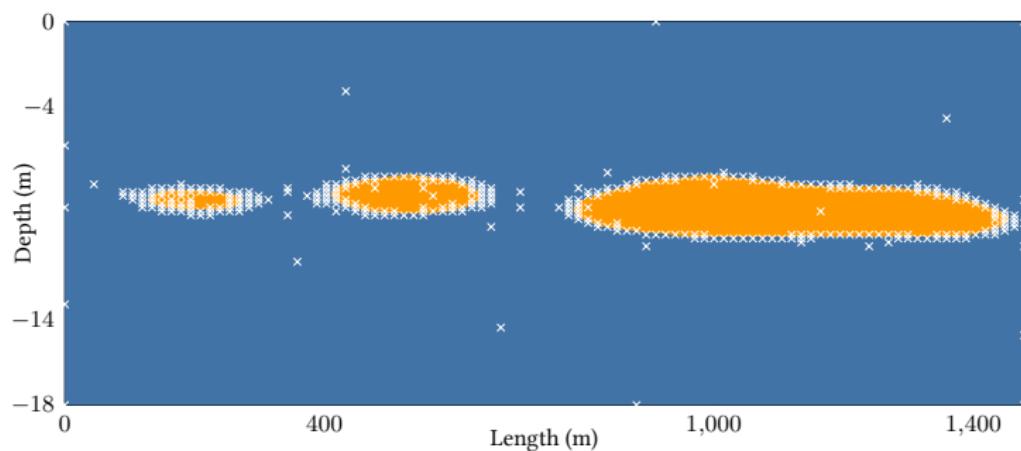
$t = 340$





$t = 486$



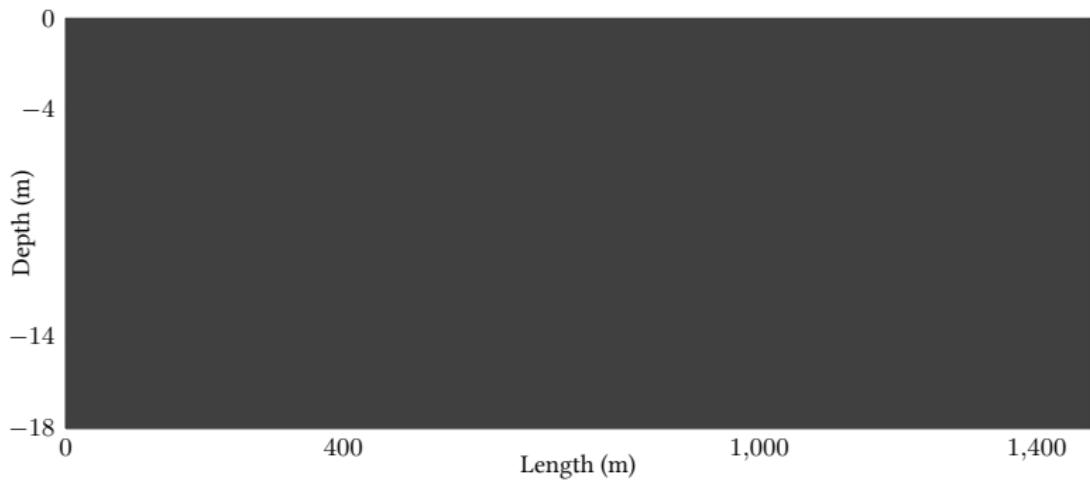


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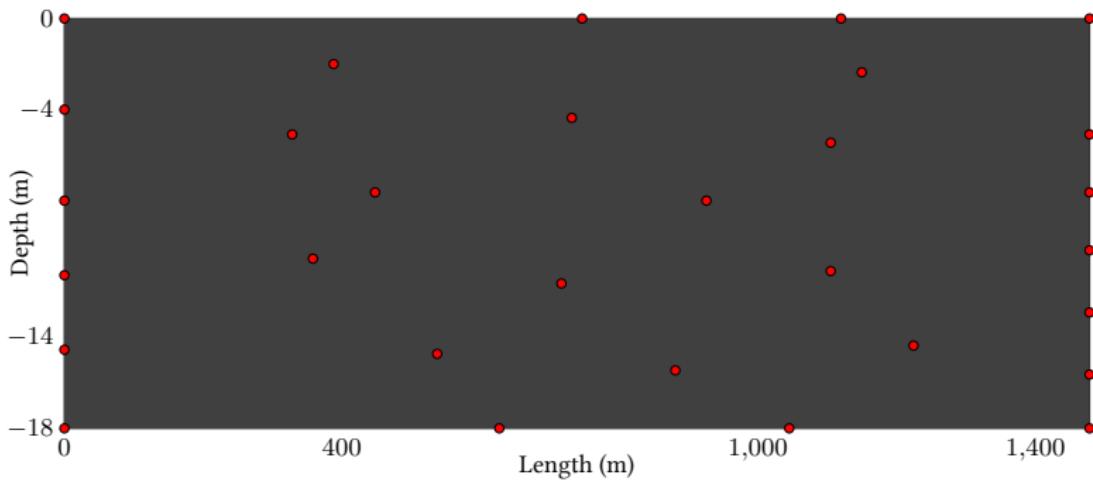
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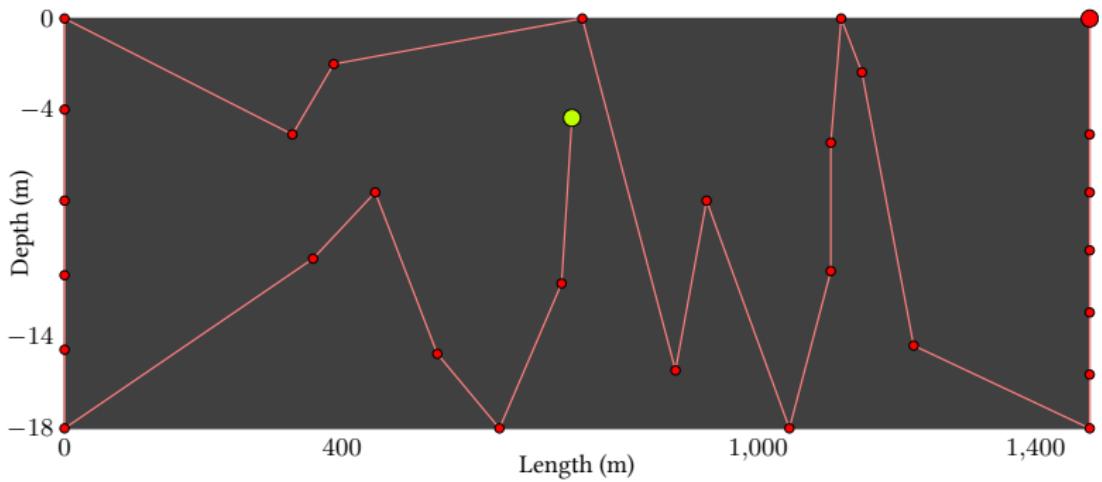
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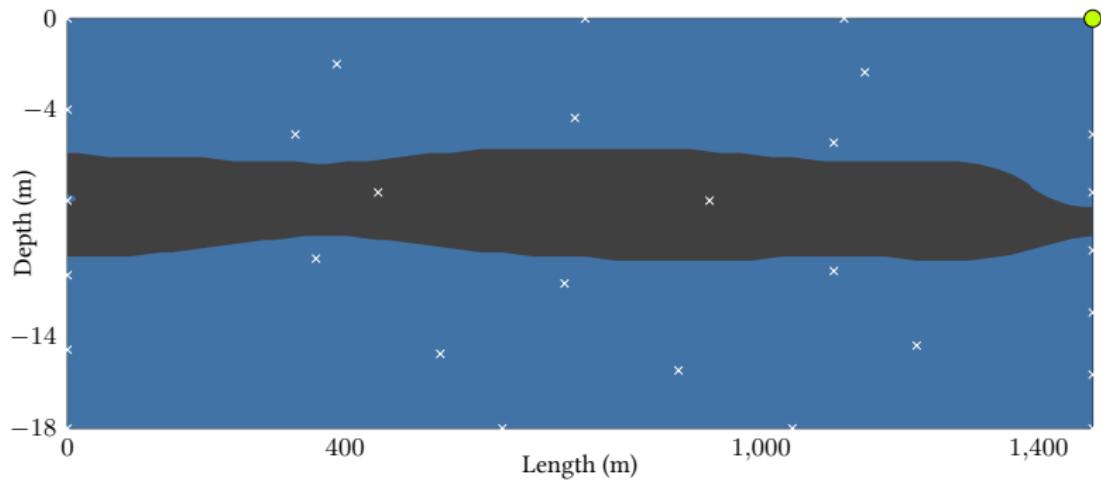
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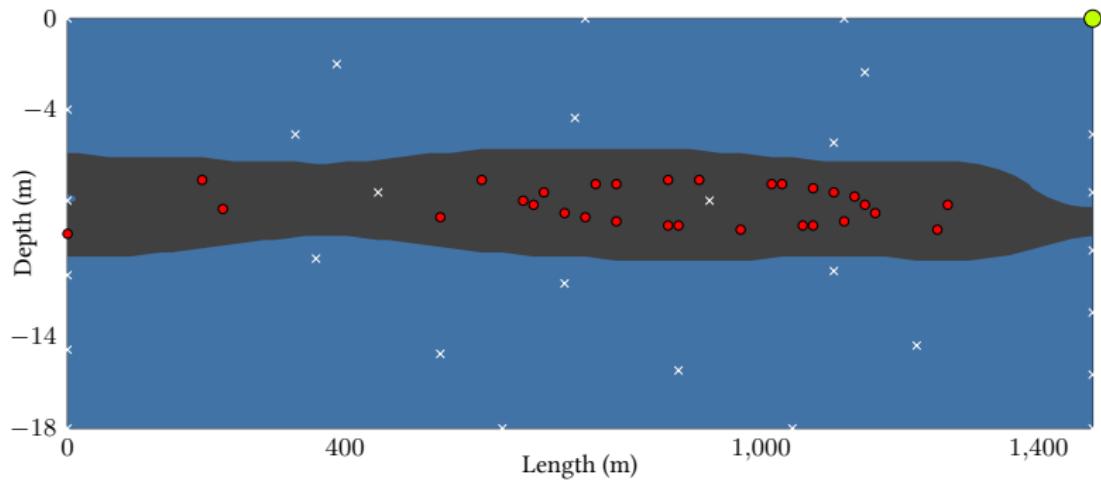
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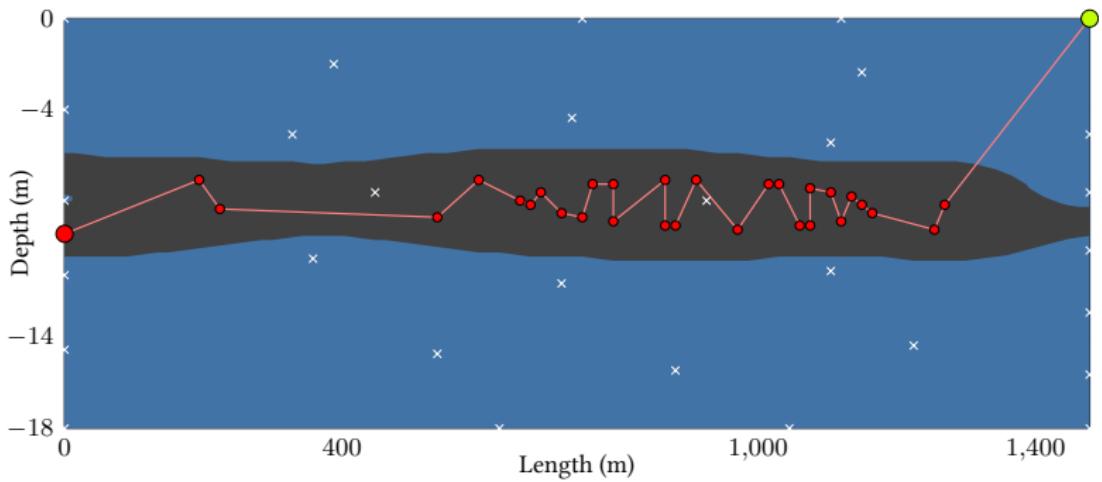
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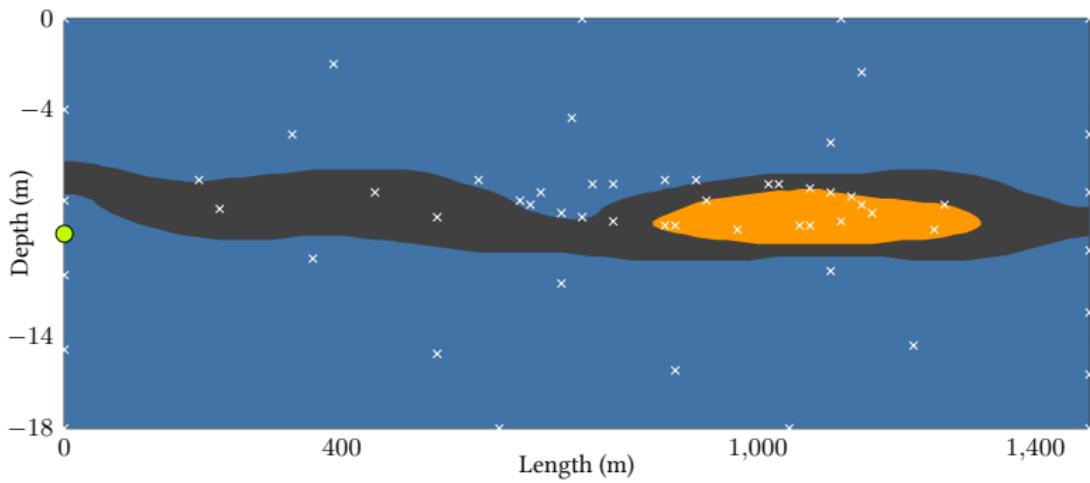
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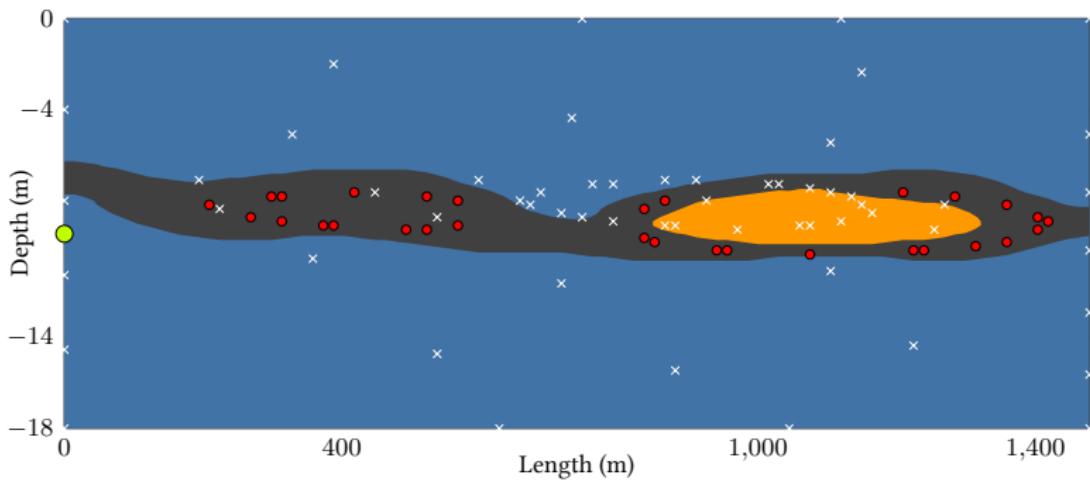
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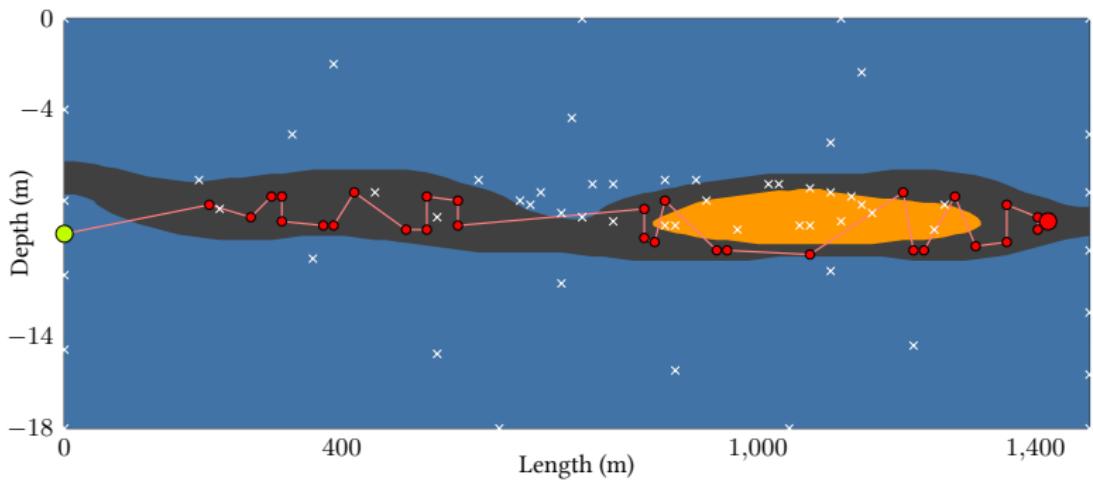
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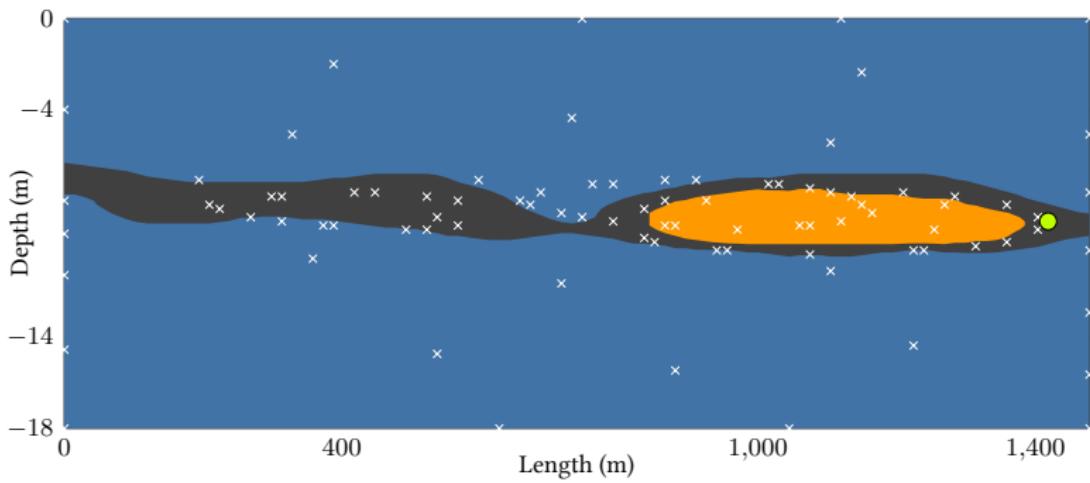
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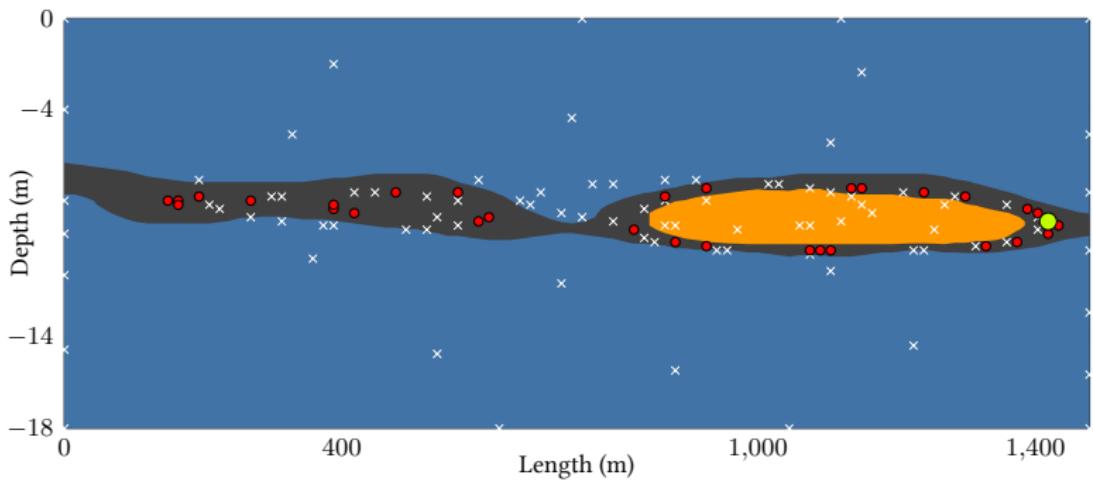
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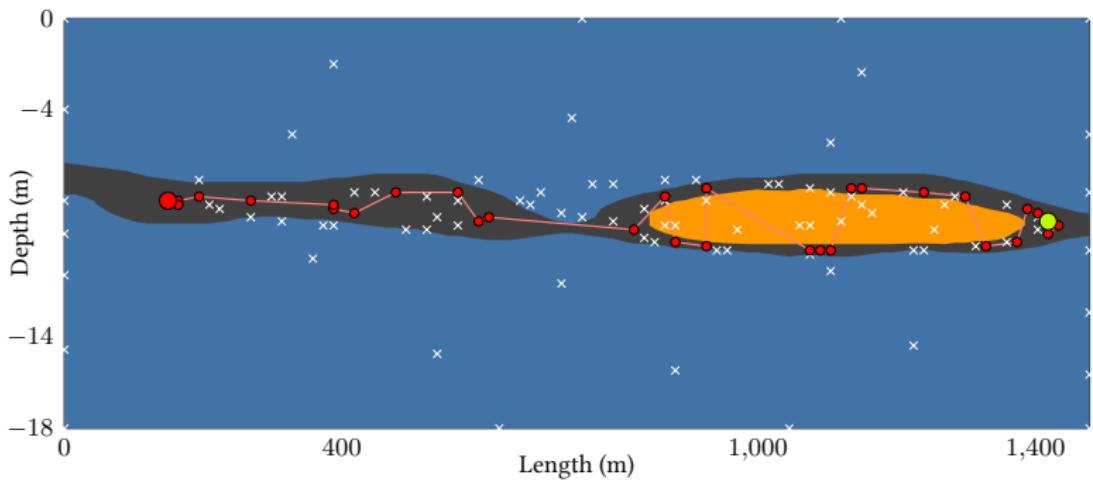
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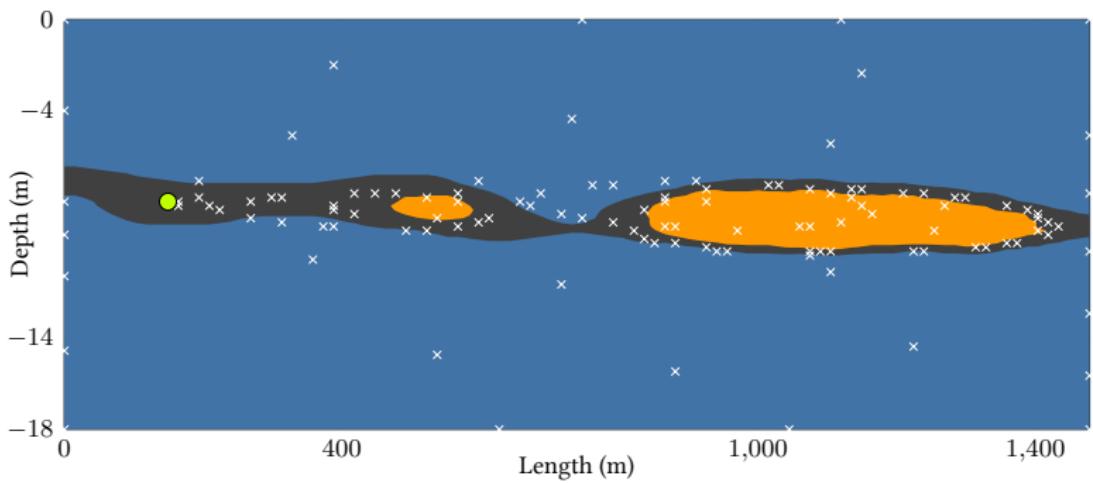
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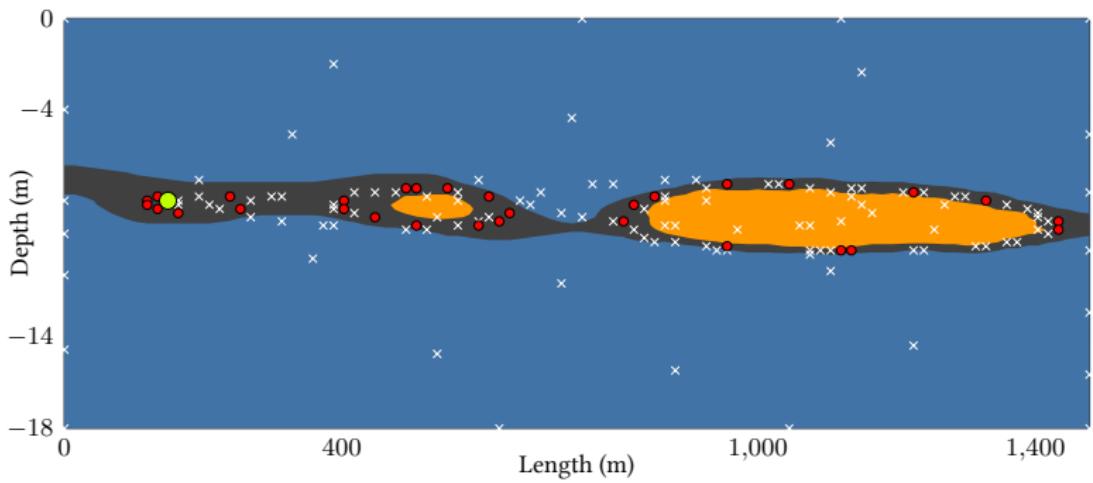
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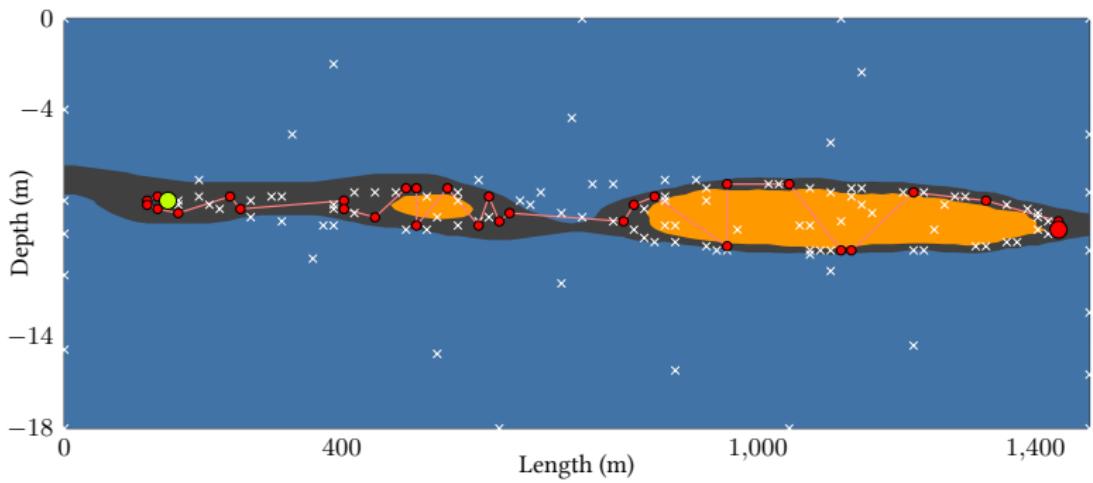
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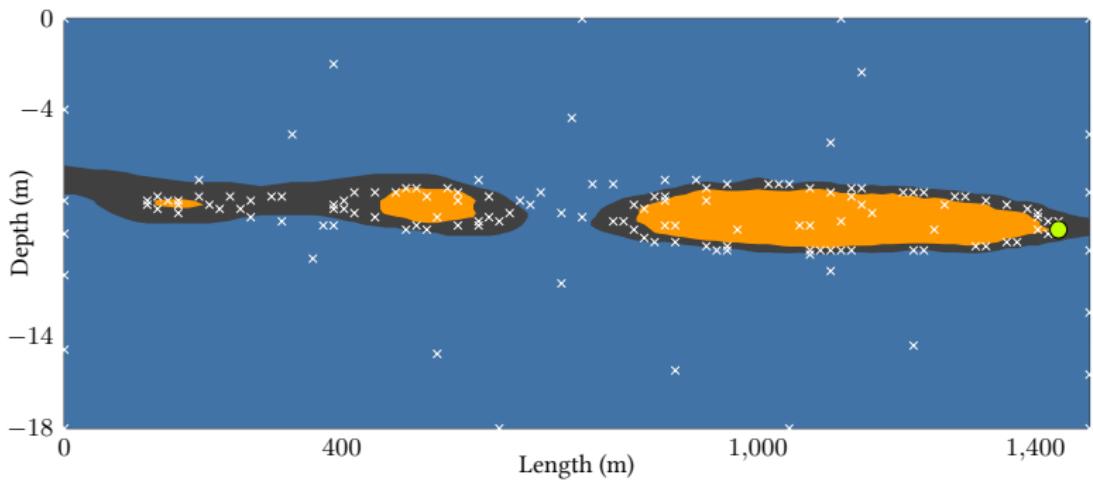
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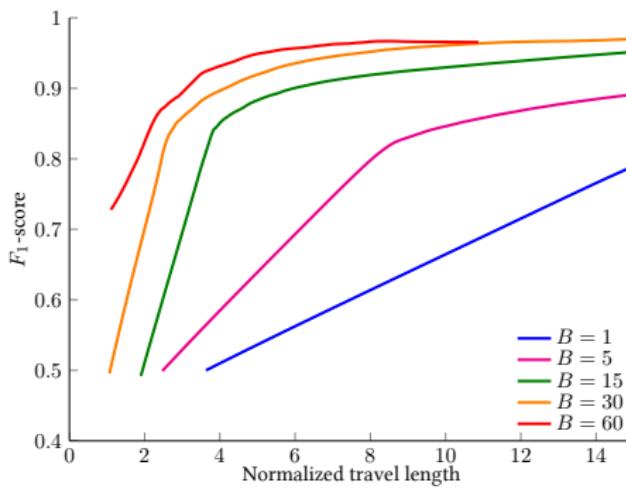
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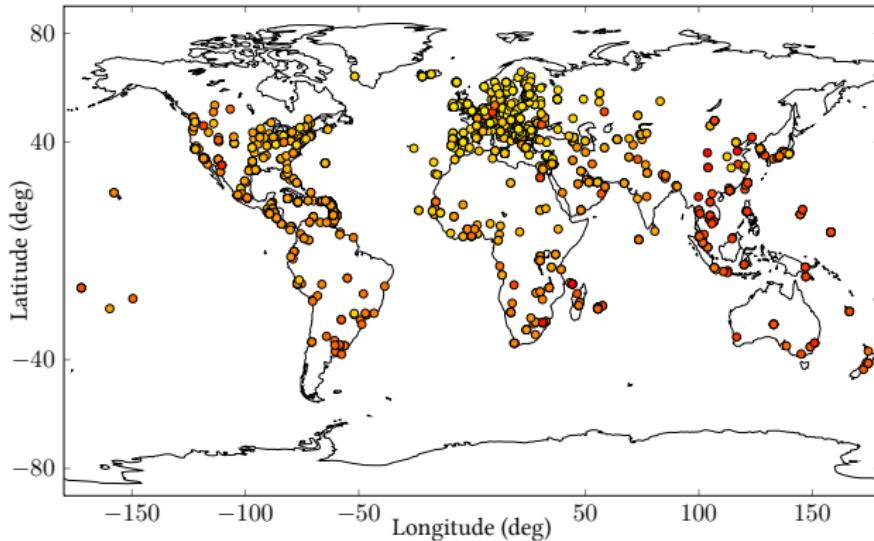
Come to the poster session for more...

Come to the poster session for more...

- ▶ ...theory: sample complexity bounds in more detail

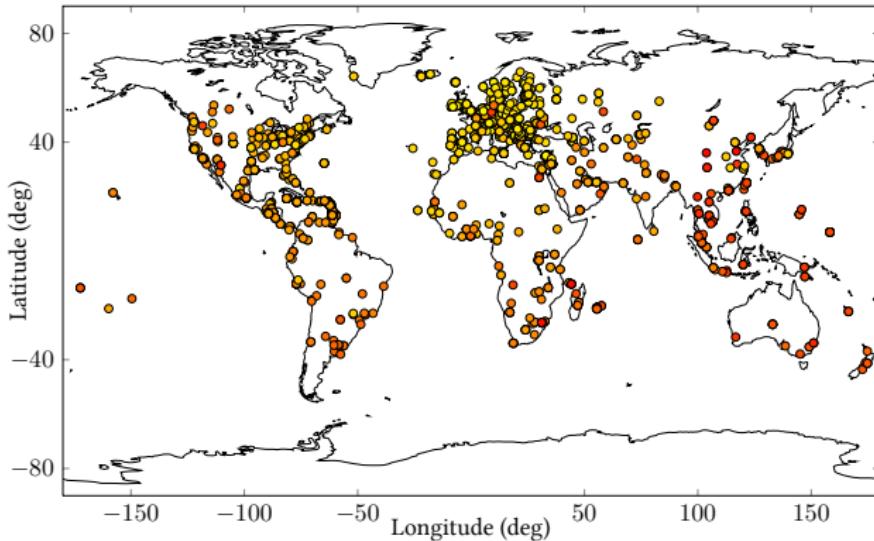
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- ▶ ...results: why does LSE greatly outperform “straddle” in some cases?

Summary

- ▶ LSE algorithm:

Summary

► LSE algorithm:

► Theoretical guarantees

Theorem (Convergence of LSE)

For any $\hbar \in \mathbb{R}$, $\delta \in (0, 1)$, and $\epsilon > 0$, if $\beta_0 = 2 \log(D\pi^2)^2/(6\delta)$, LSE terminates after at most T iterations, where T is the smallest positive integer satisfying

$$\frac{T}{\beta_0 \gamma} \geq \frac{C_1}{4\epsilon^2}$$

where $C_1 = 8/\log(1 + \sigma^{-2})$.

Furthermore, with probability at least $1 - \delta$, the algorithm returns an ϵ -accurate solution, that is

$$\Pr \left\{ \max_{\mathbf{x} \in \mathcal{D}} \ell_k(\mathbf{x}) \leq \epsilon \right\} \geq 1 - \delta.$$

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- ▶ Competitive with the state-of-the-art in practice (sometimes considerably superior)

Theorem (Convergence of LSE)

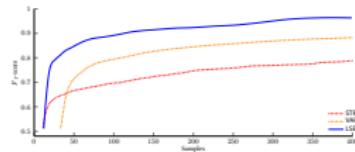
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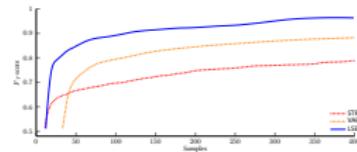
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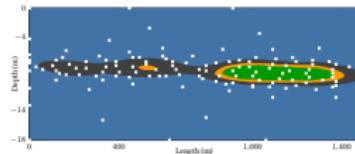
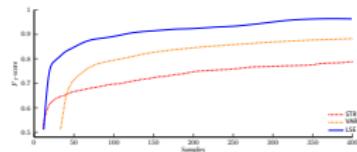
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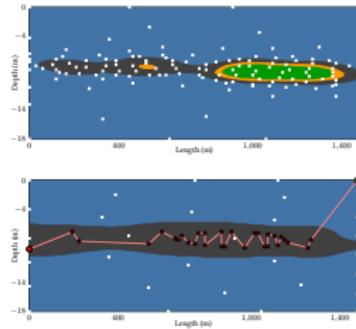
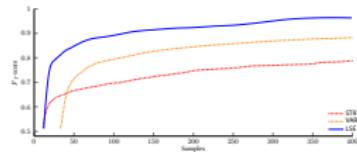
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- ▶ Look out for algae when swimming in Lake Zurich! 😊

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