Active Learning for Level Set Estimation

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IJCAI '13

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*, [...]"
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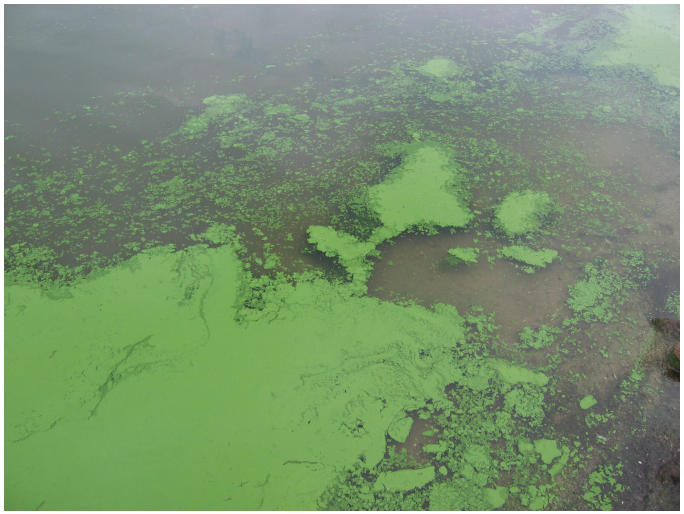
www.limnobotics.ch



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

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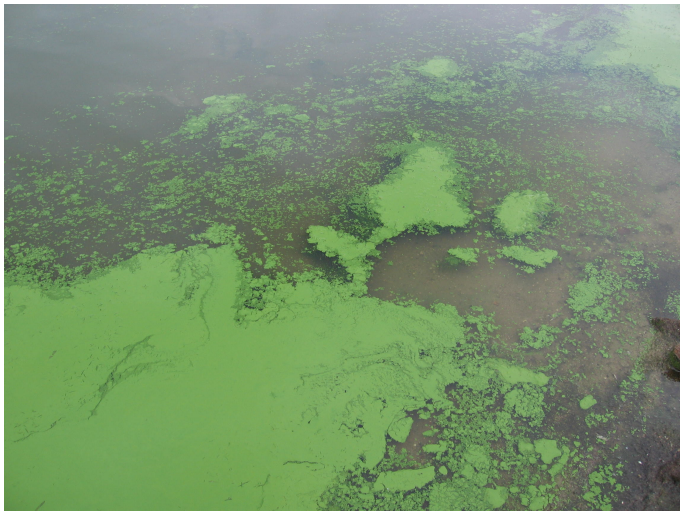

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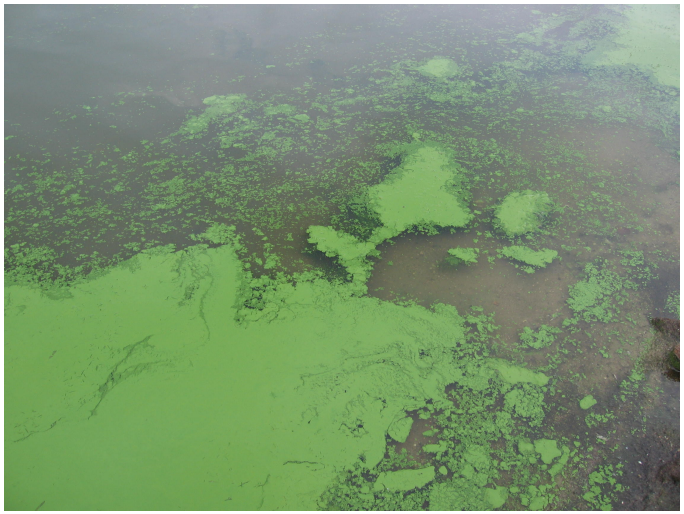

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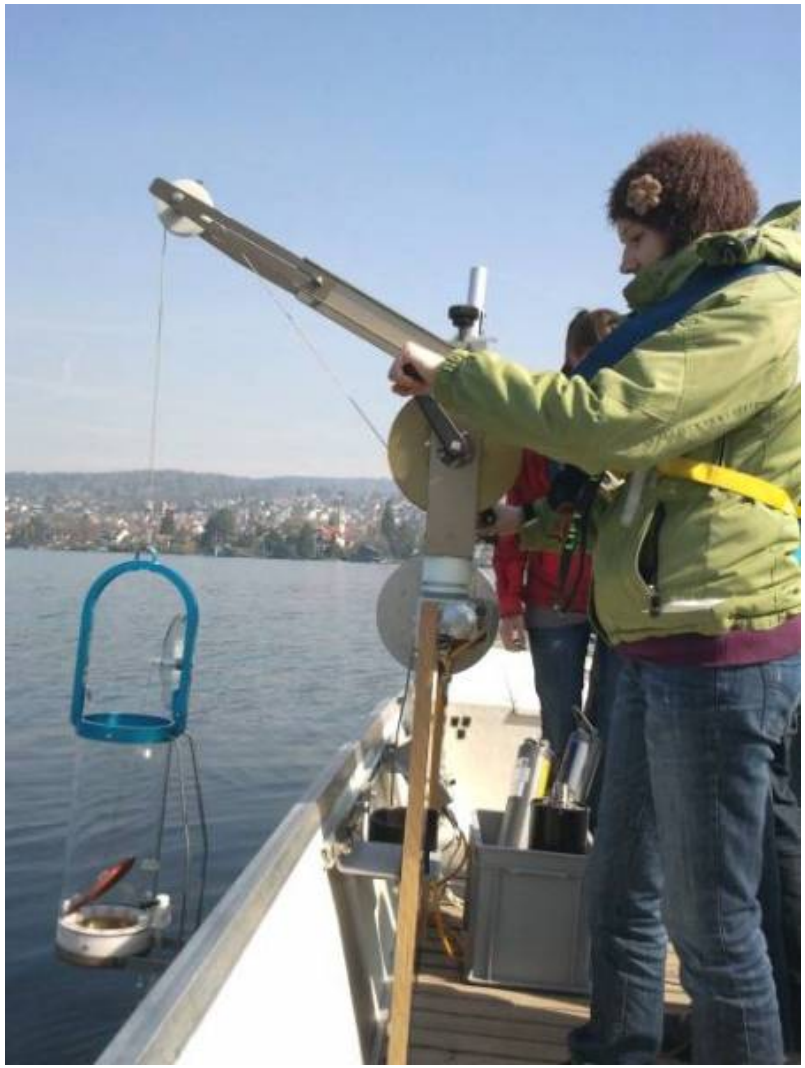
"Microcystins [...] are cyanotoxins and can be very toxic for plants and animals including humans. Their hepatotoxicity may cause serious damage to the liver."

— *Wikipedia*



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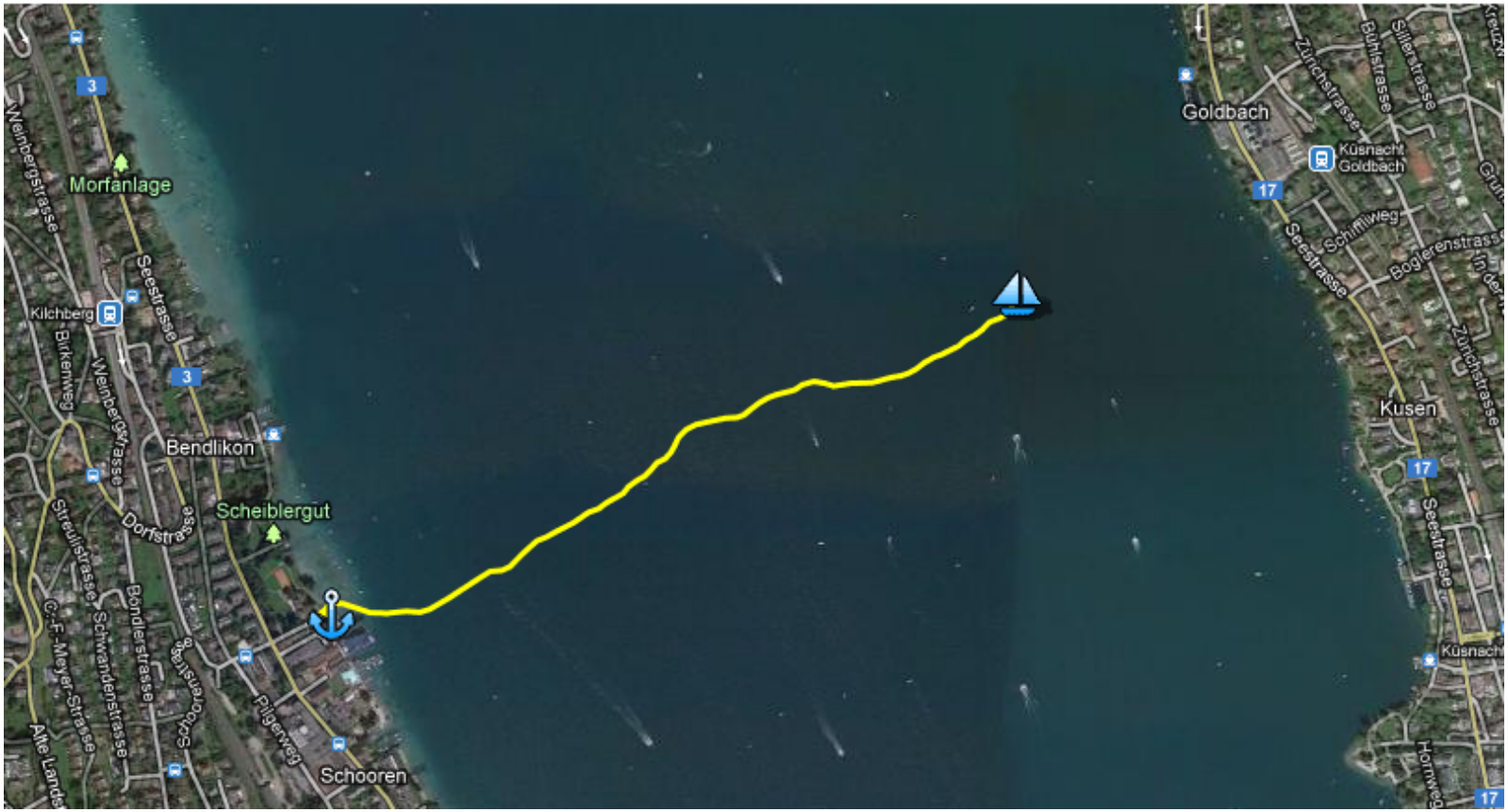

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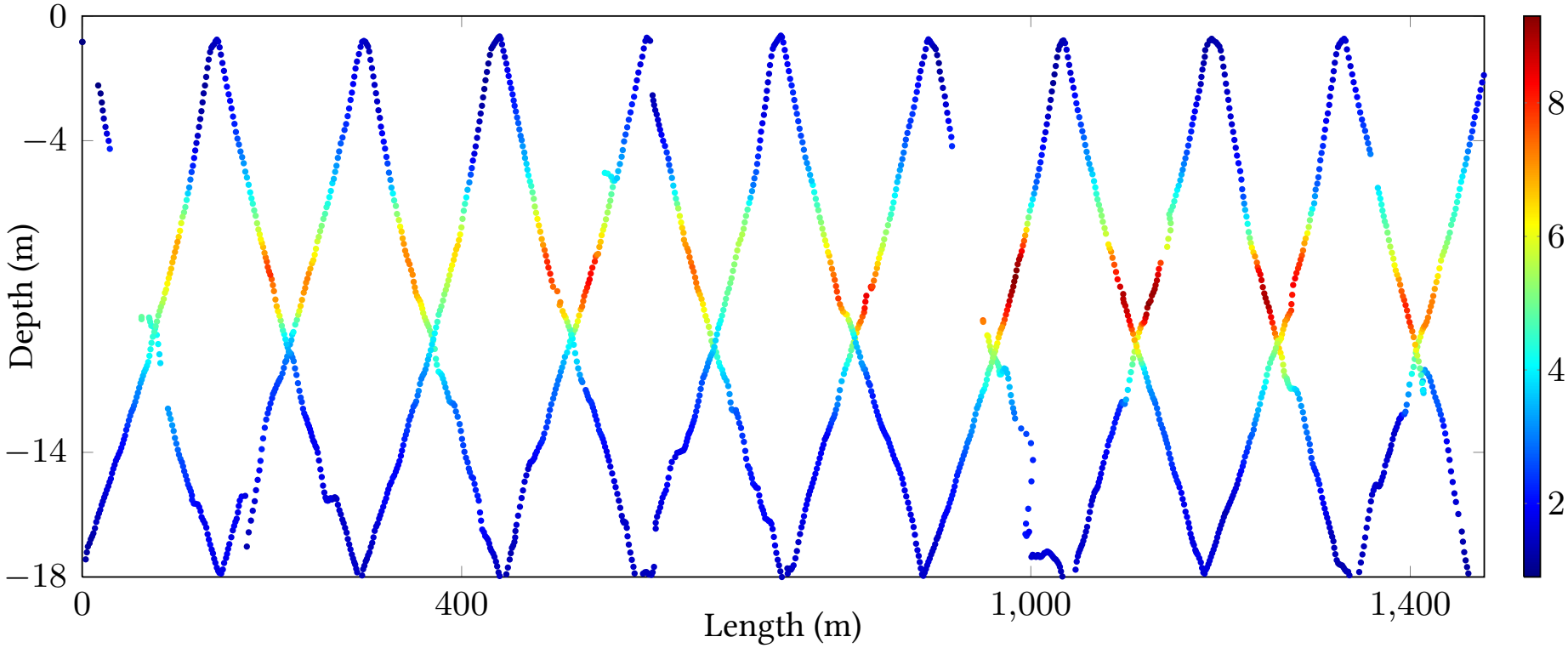
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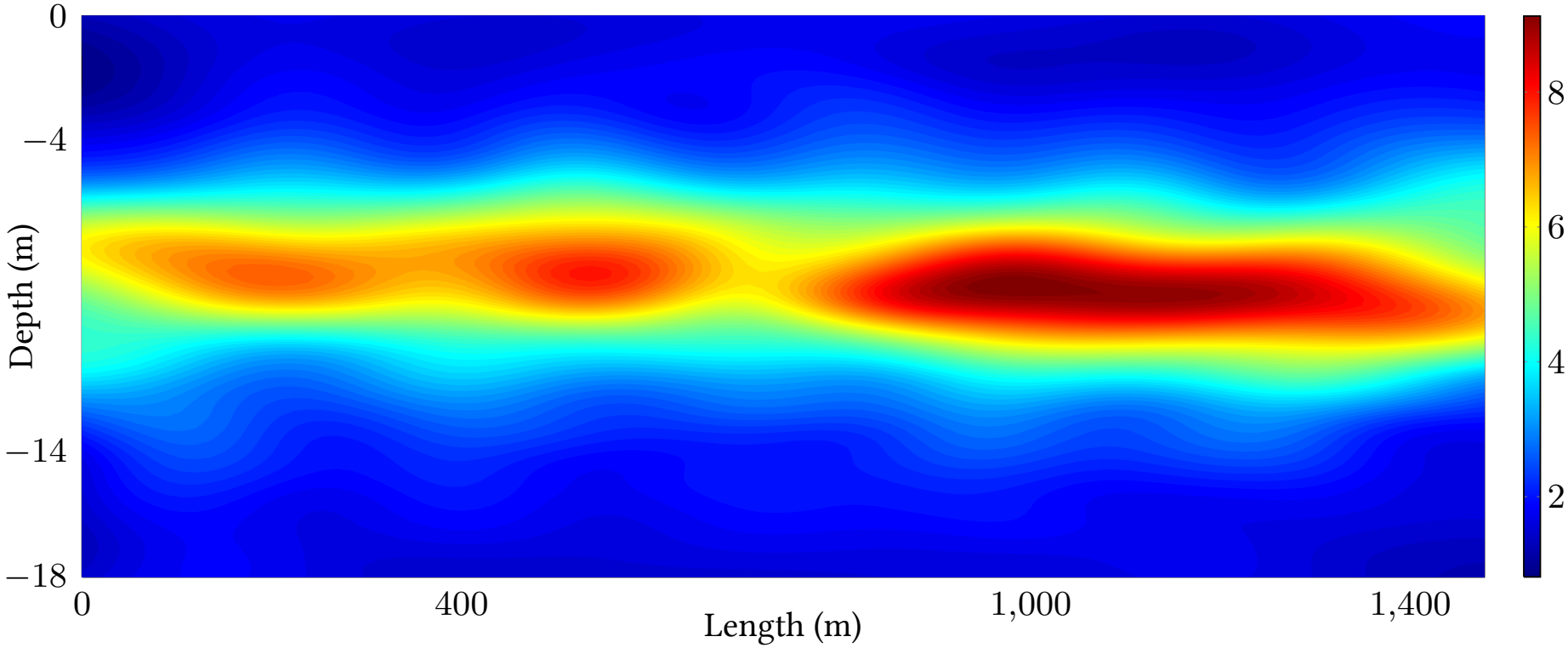
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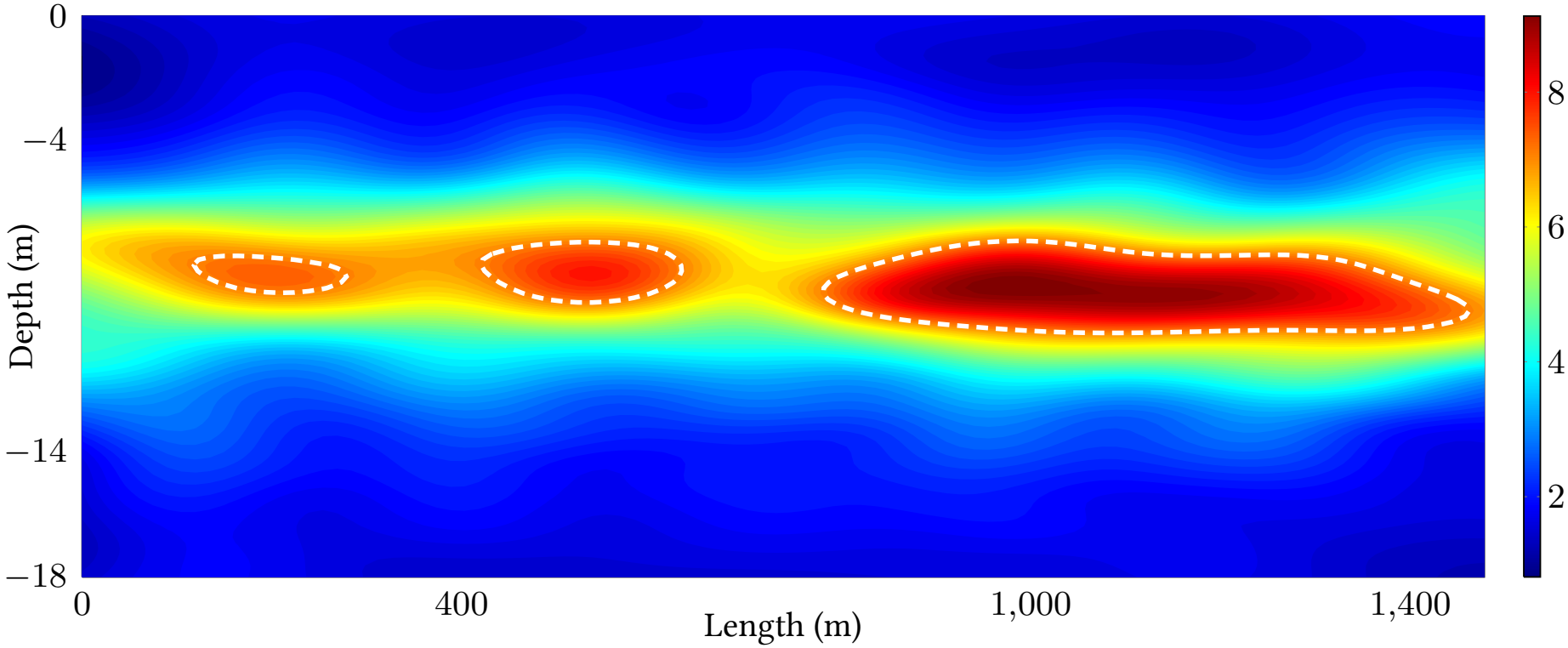
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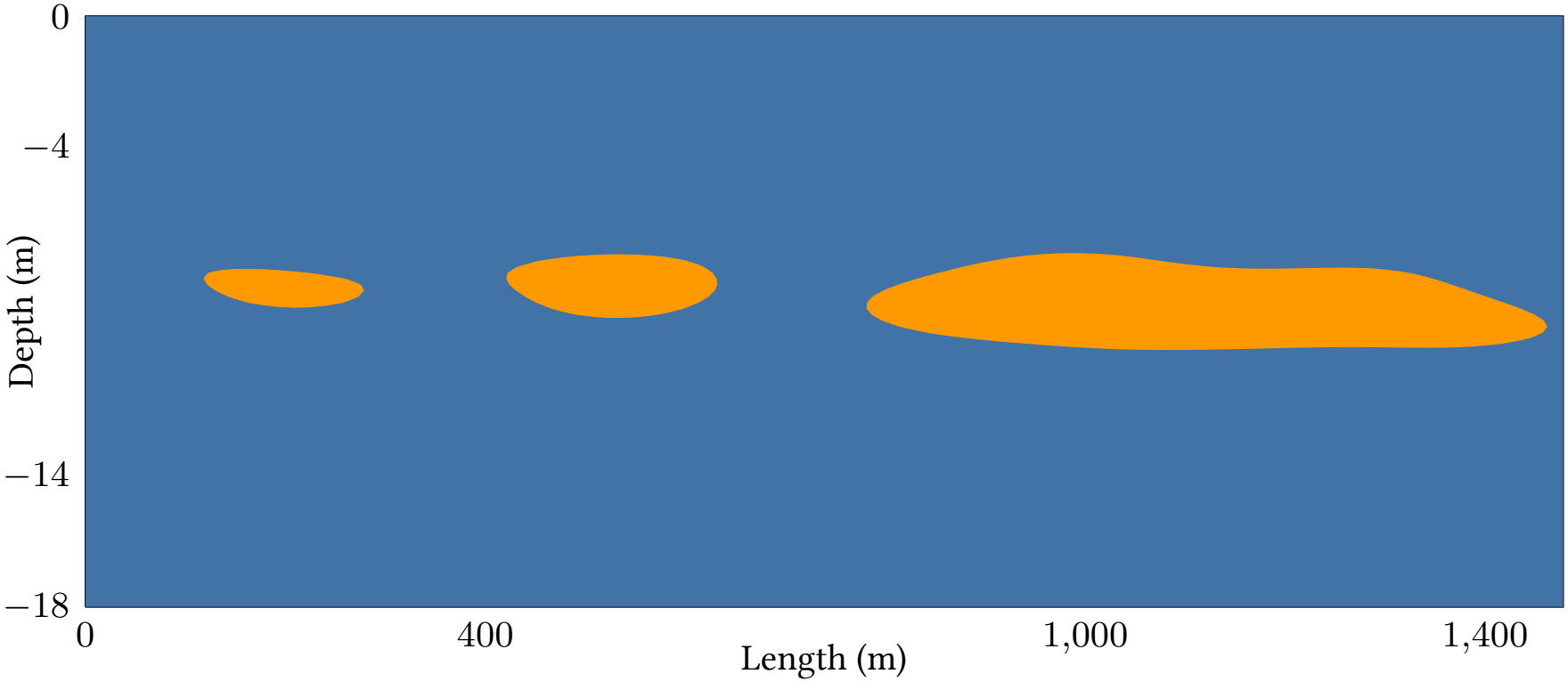
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- Update our estimate of f

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Gaussian processes to the rescue!

Gaussian processes

- **Nonpaparametric**: impose "smoothness" assumptions via kernel $k(\boldsymbol{x}, \boldsymbol{x}')$

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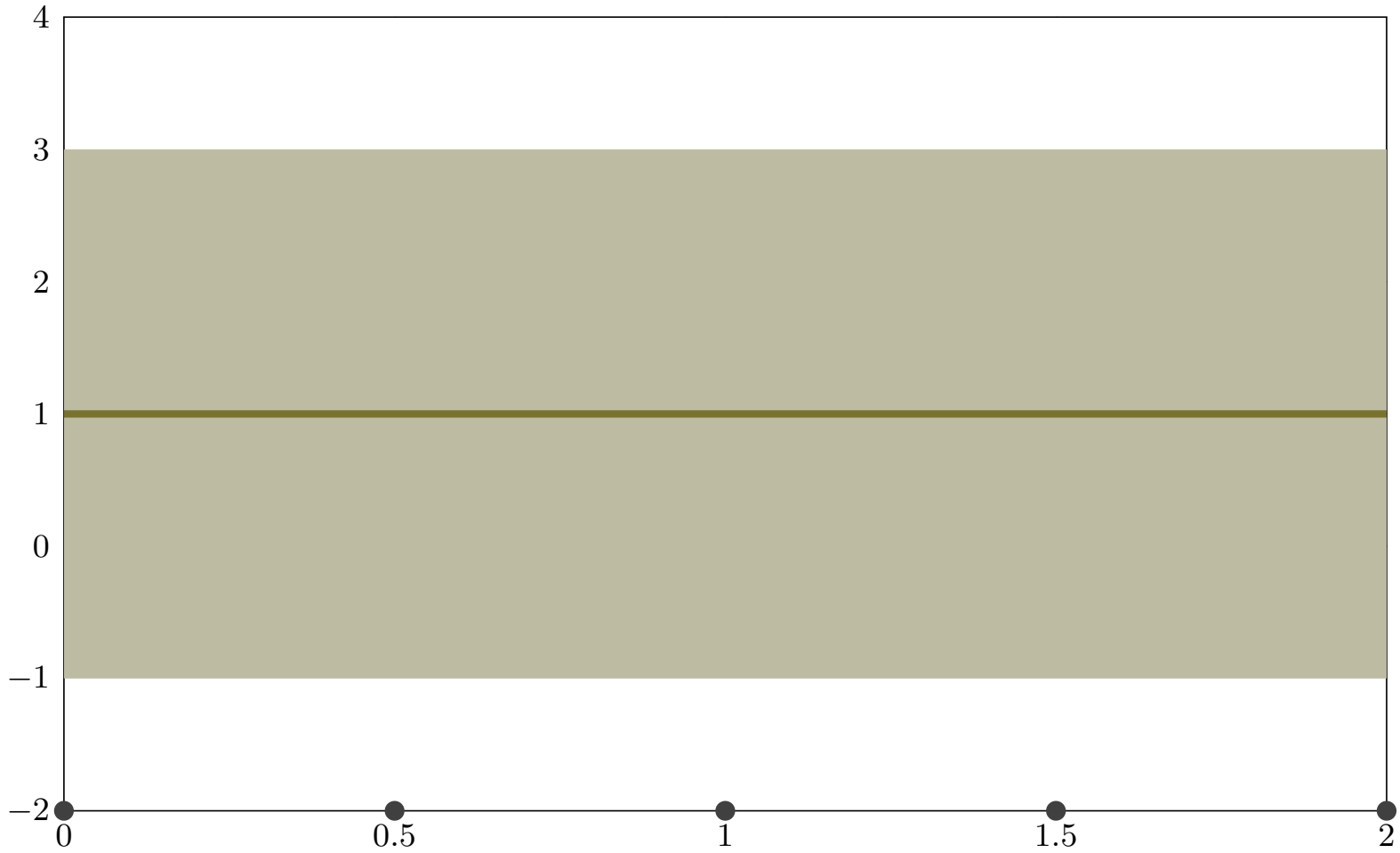

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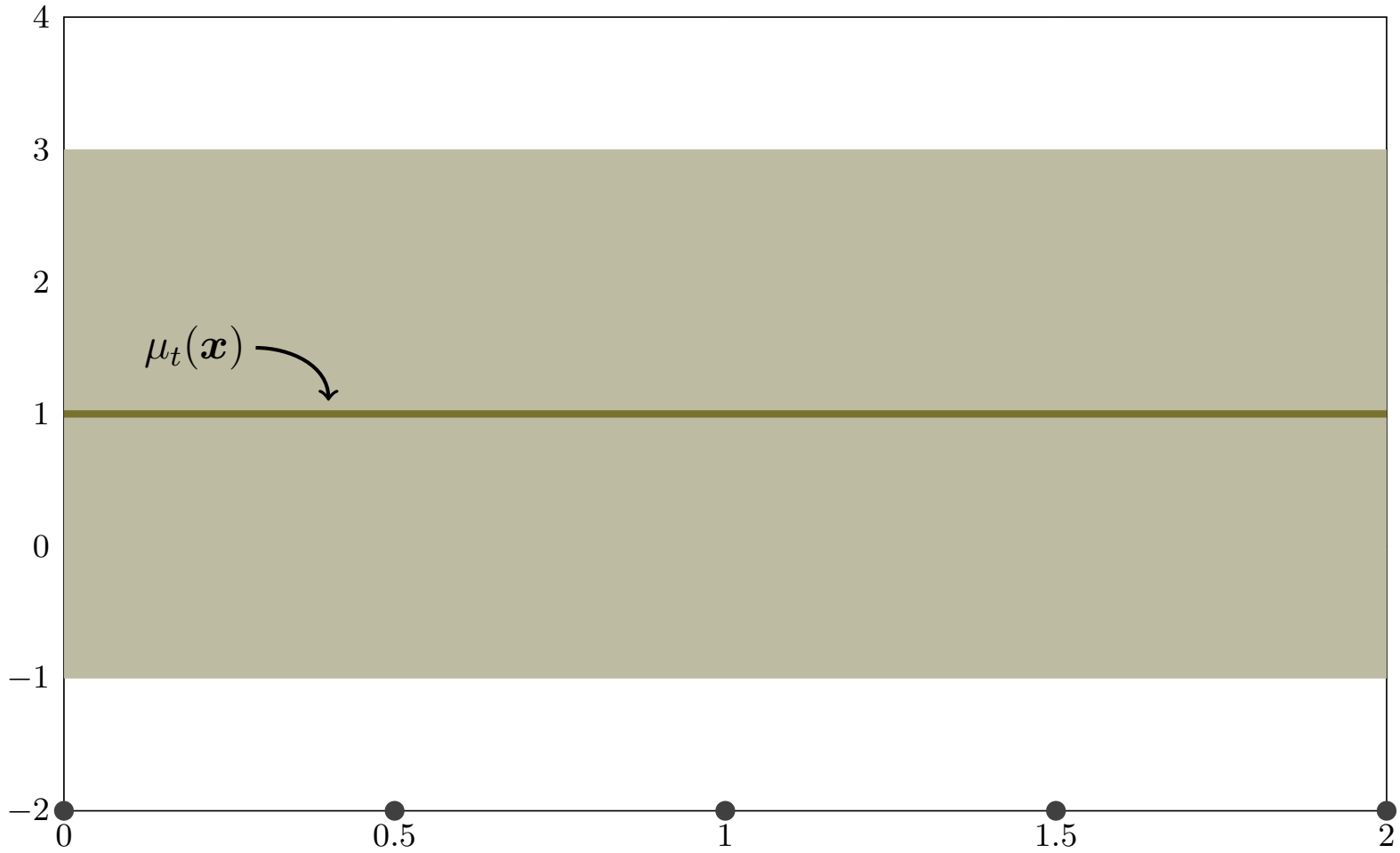

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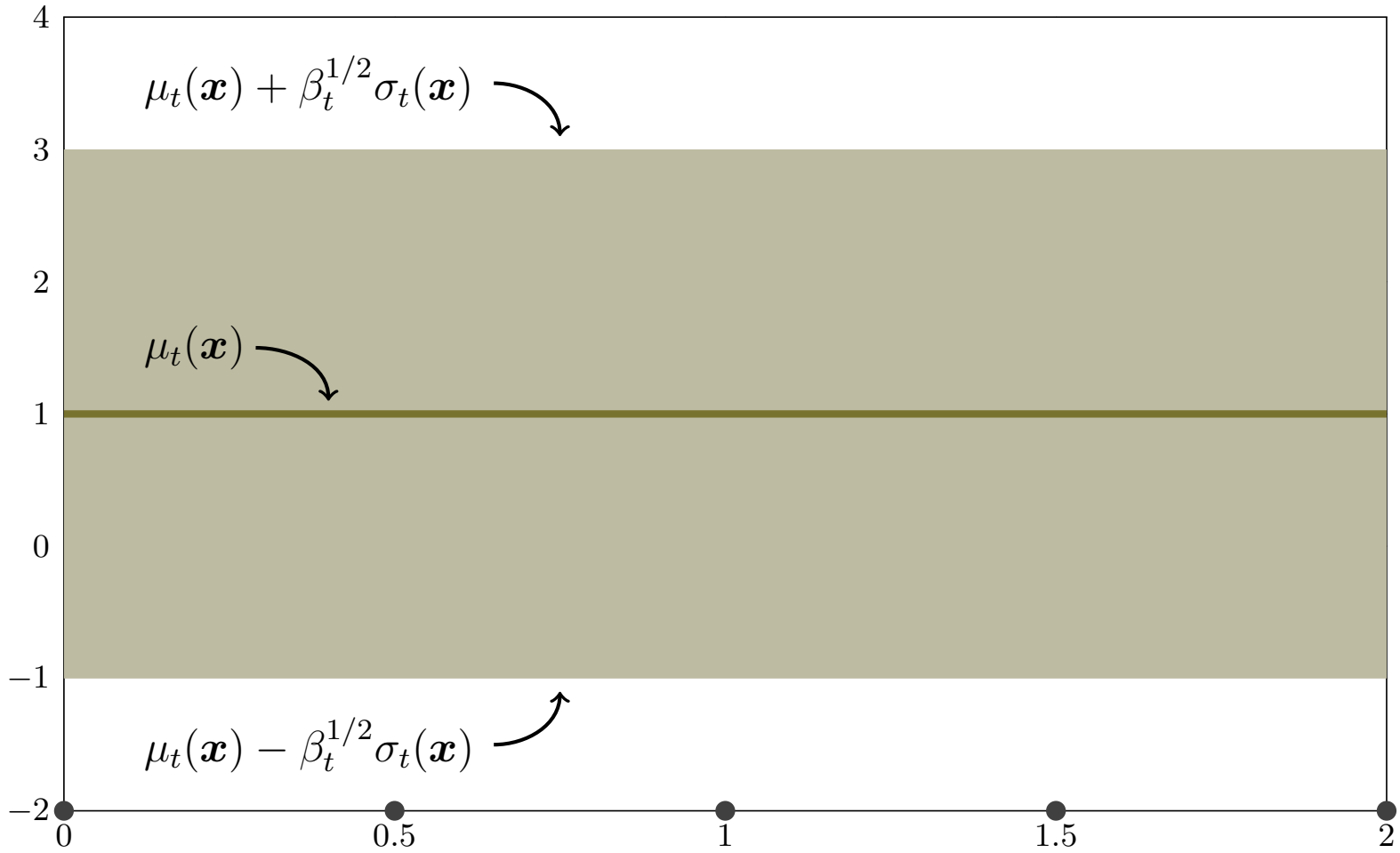

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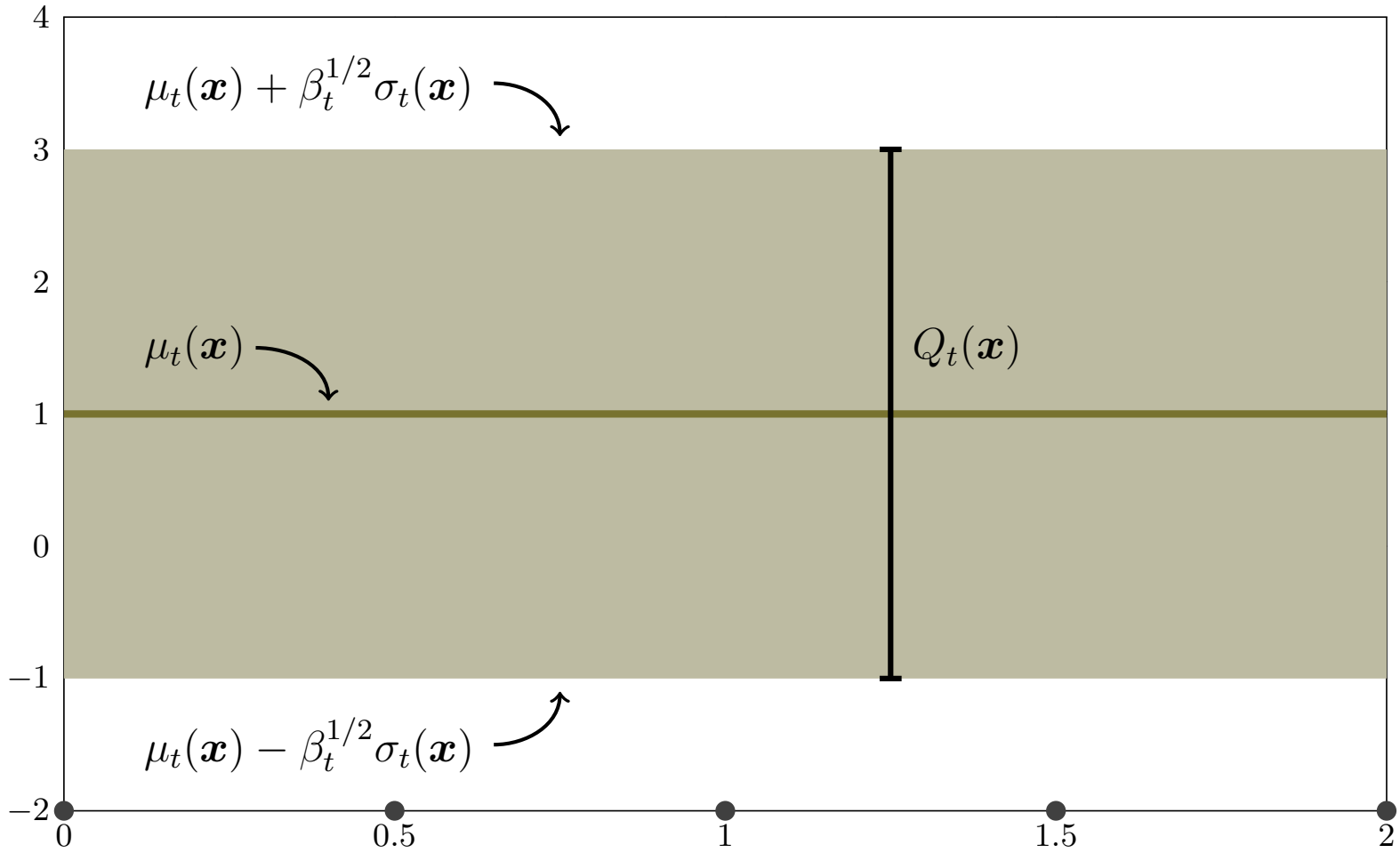

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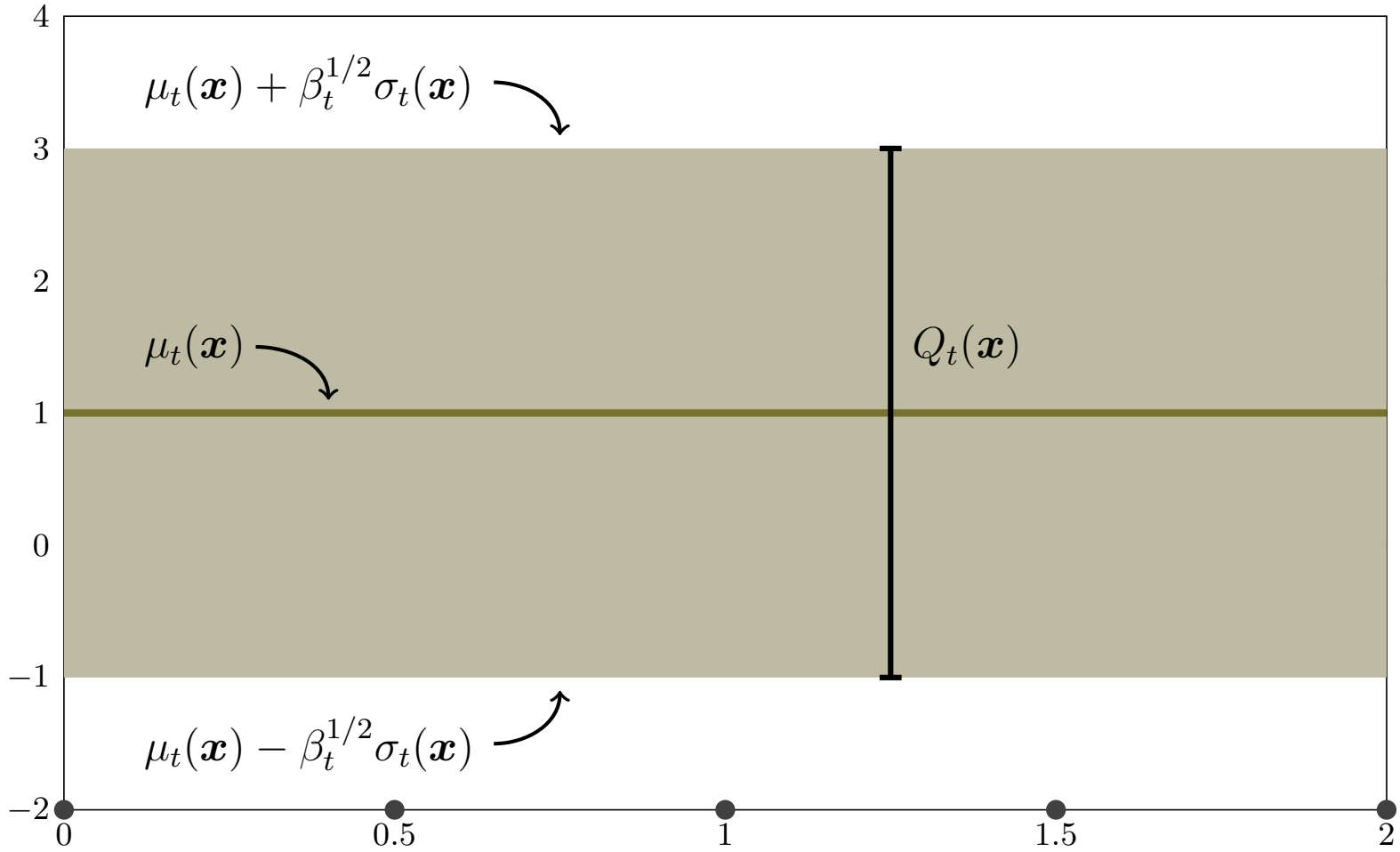

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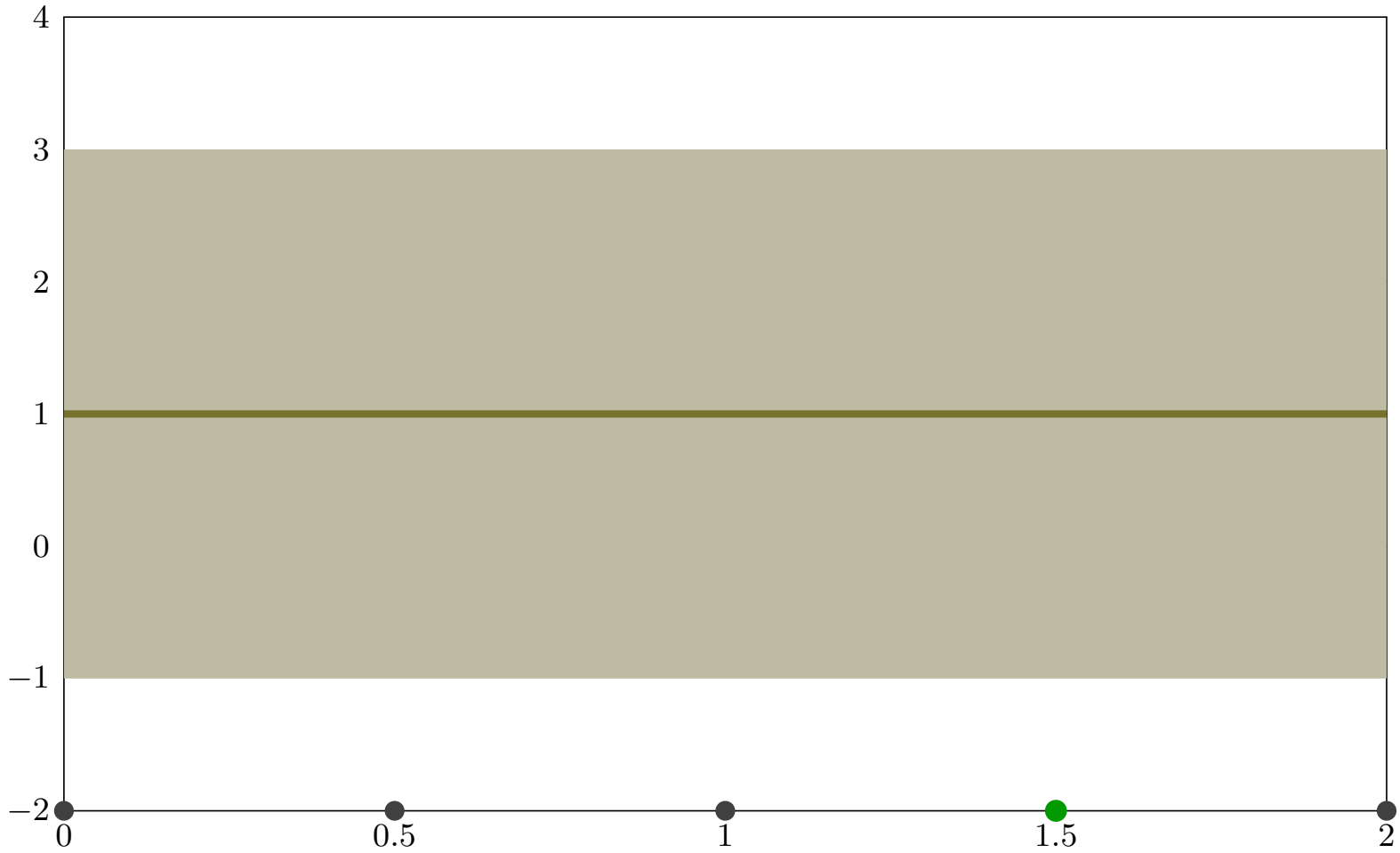

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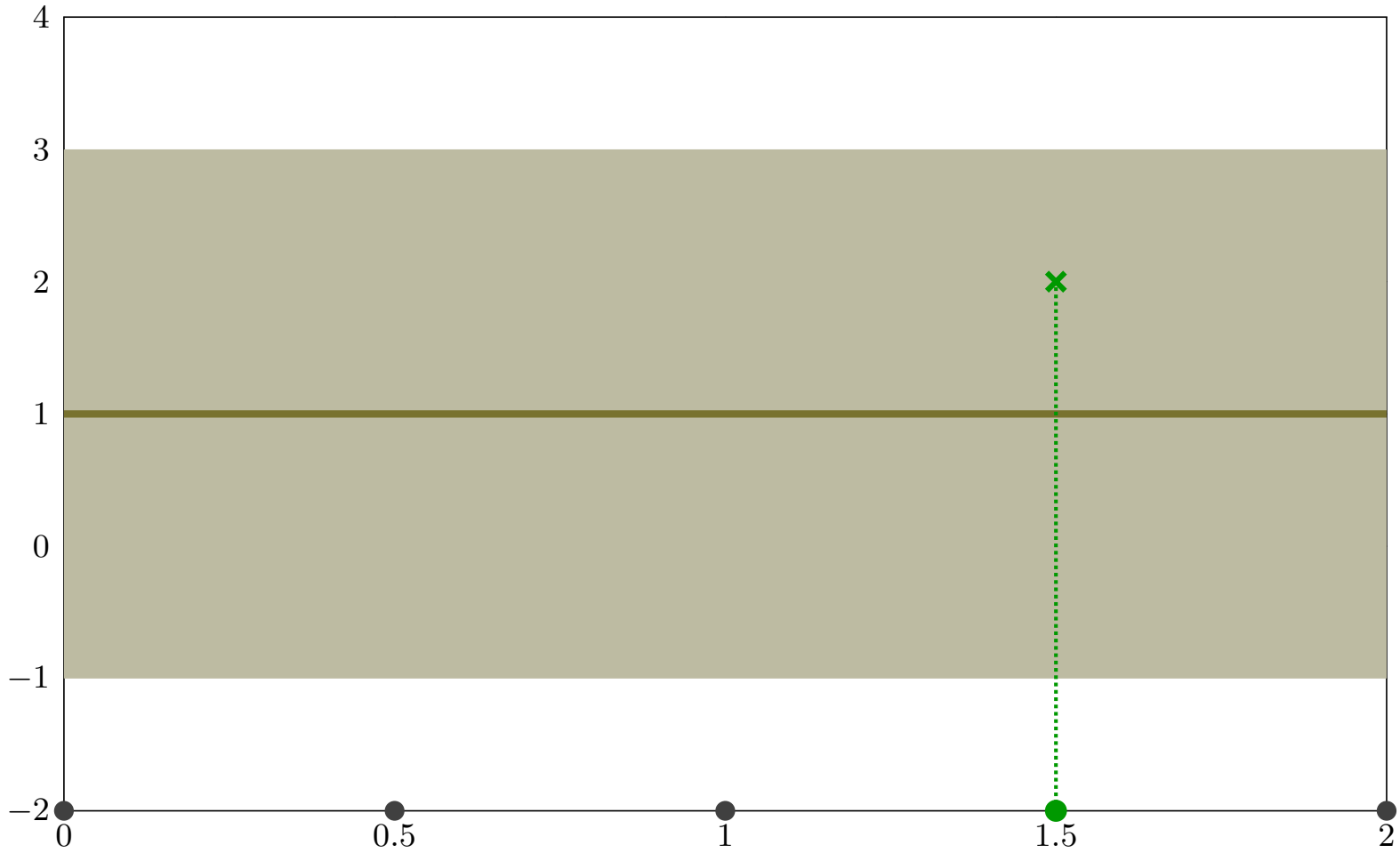

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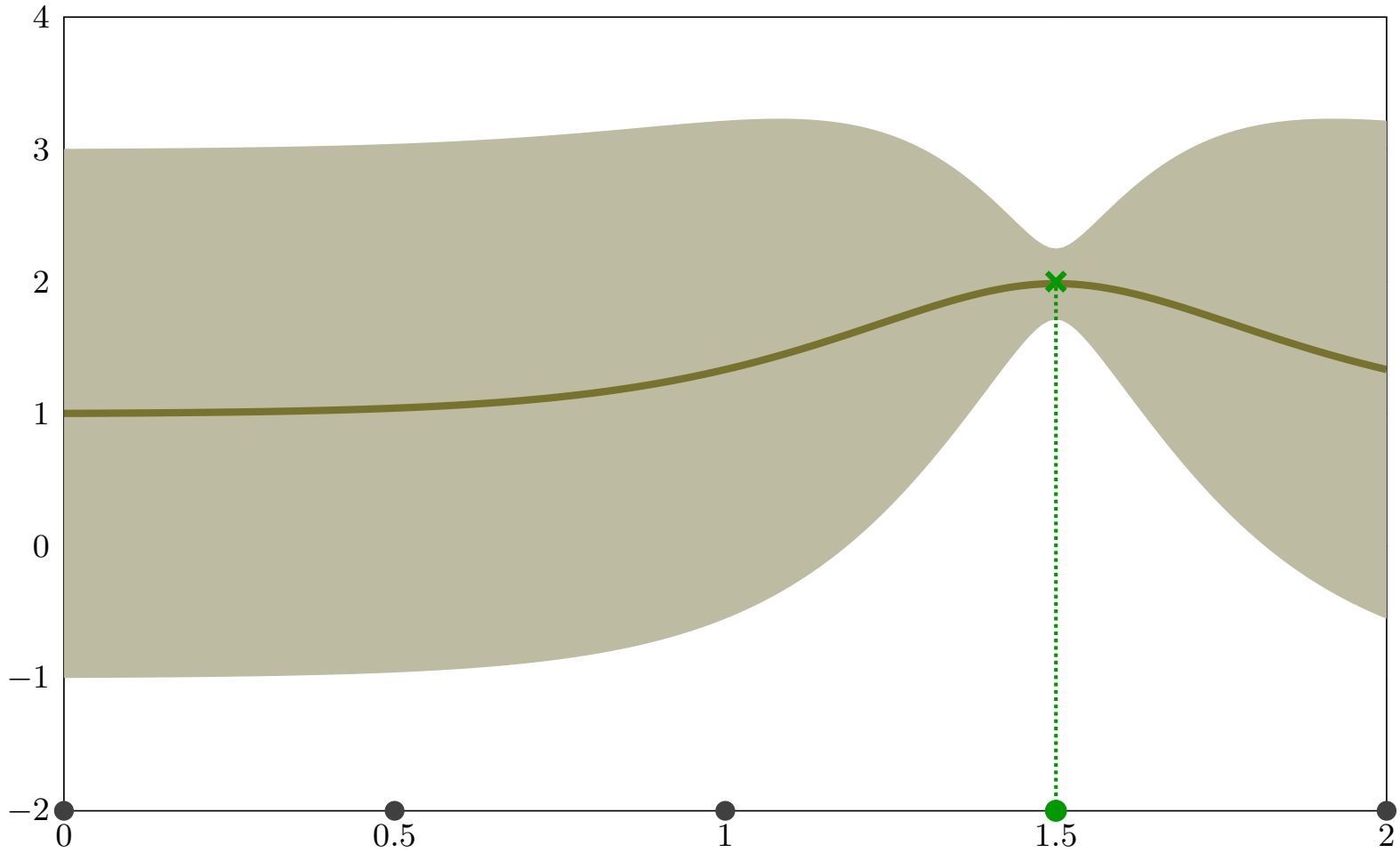

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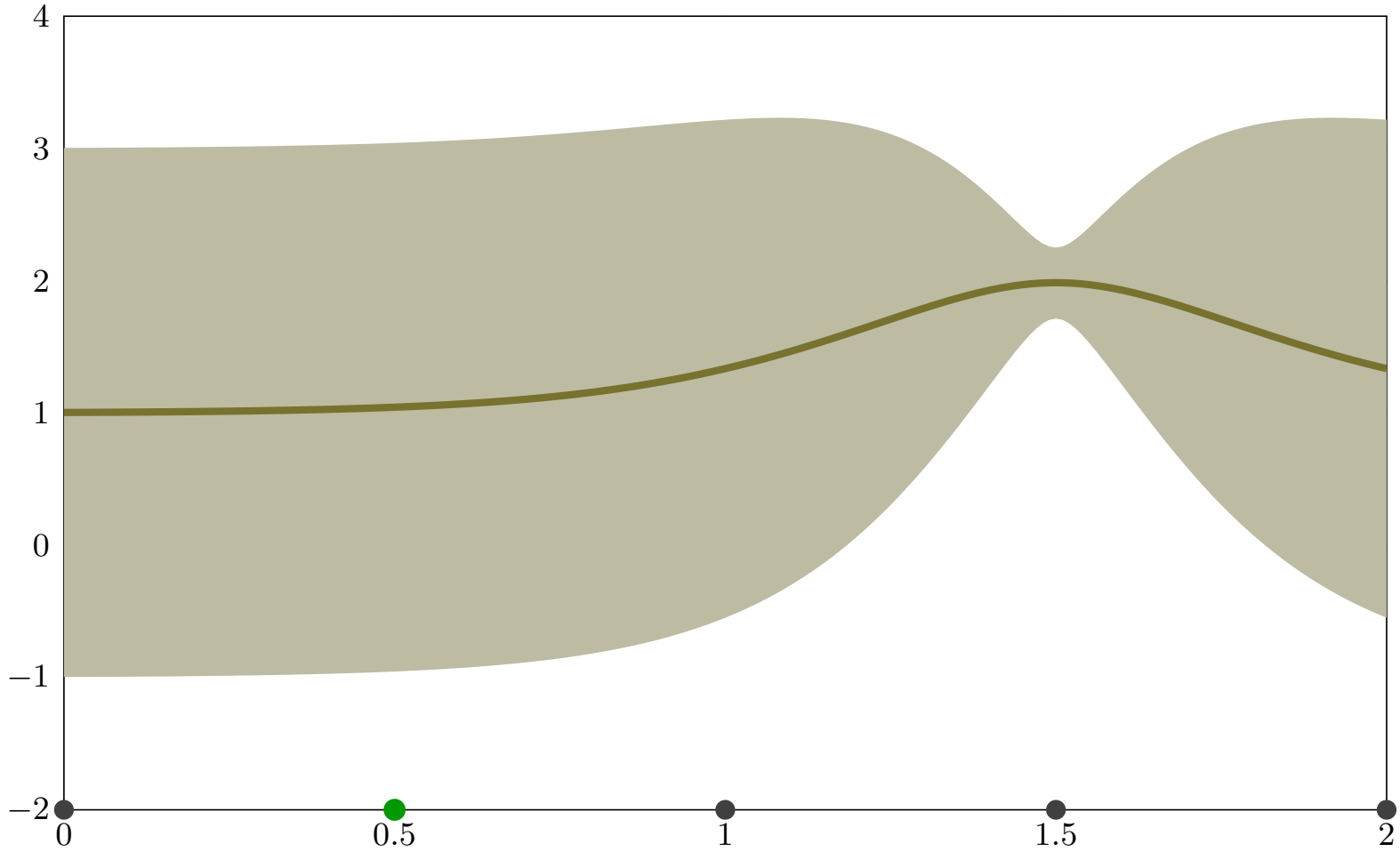

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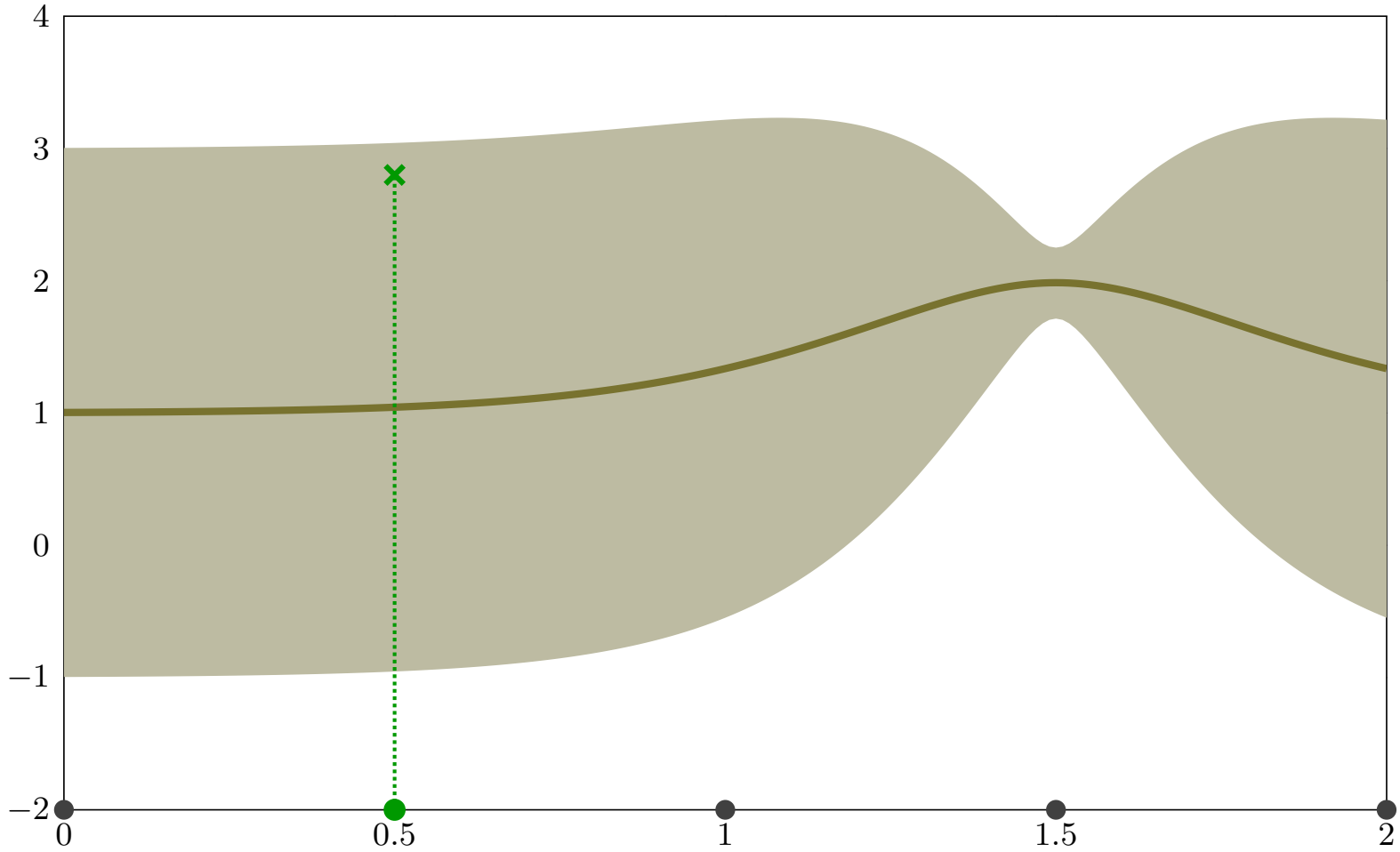

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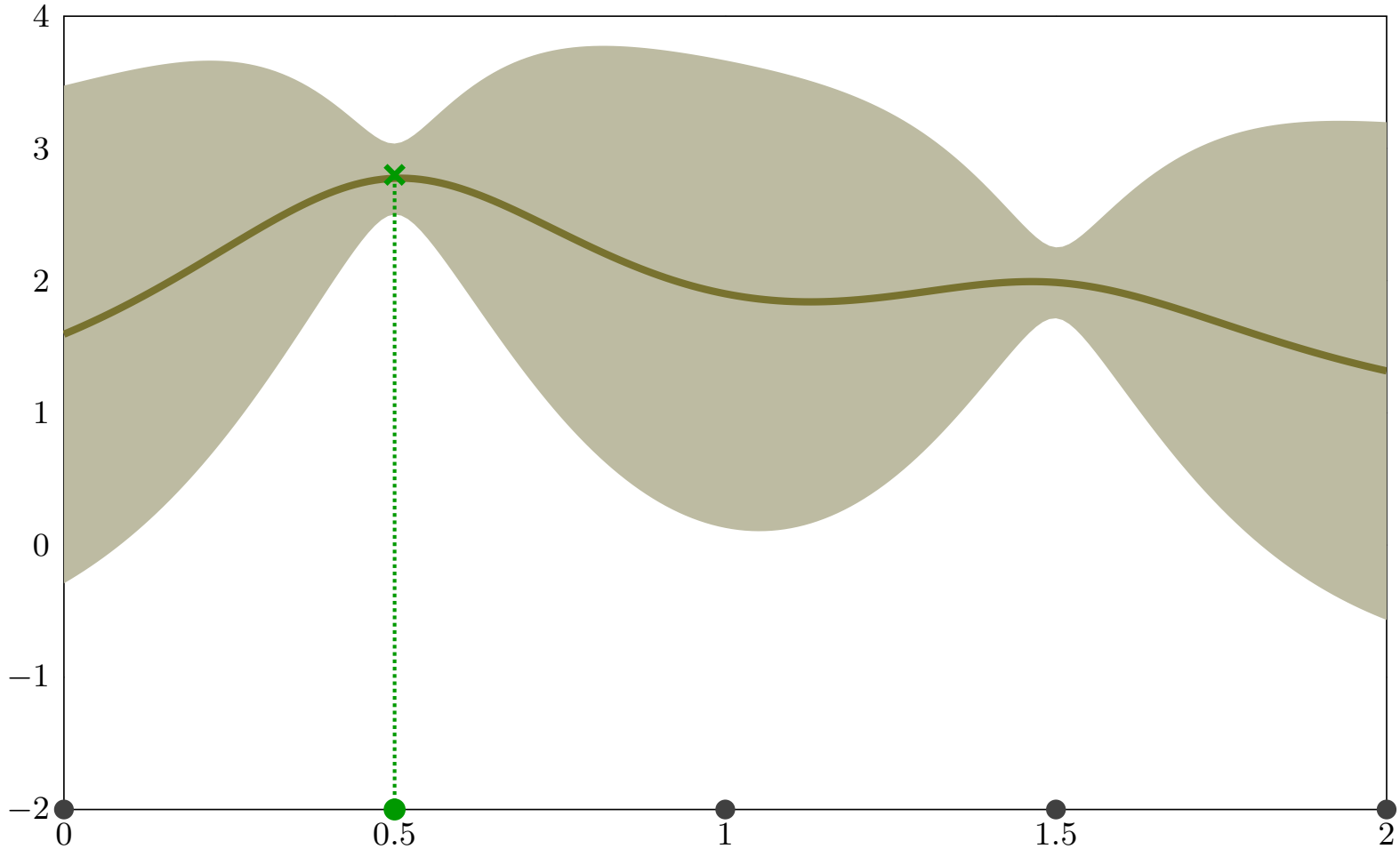

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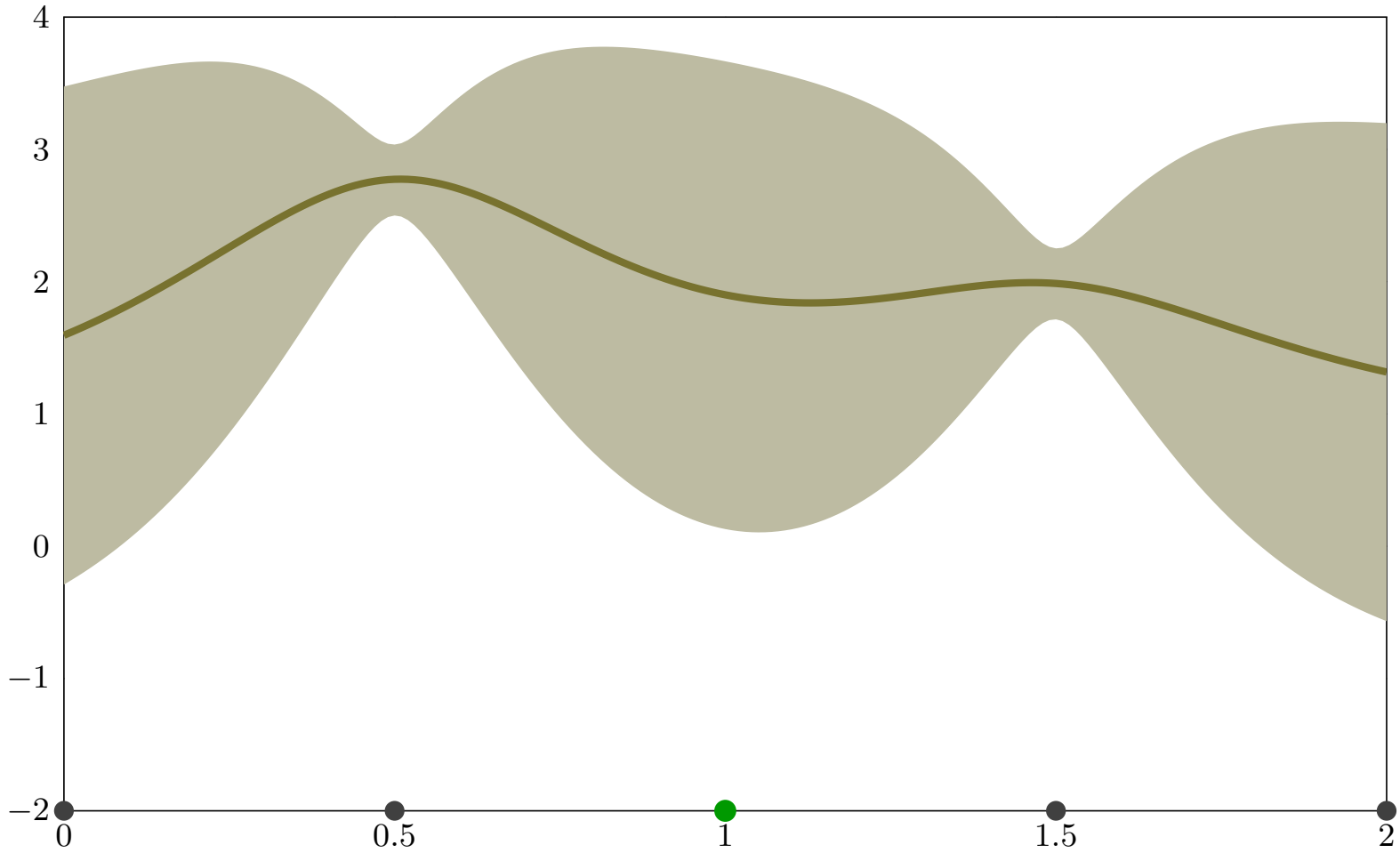

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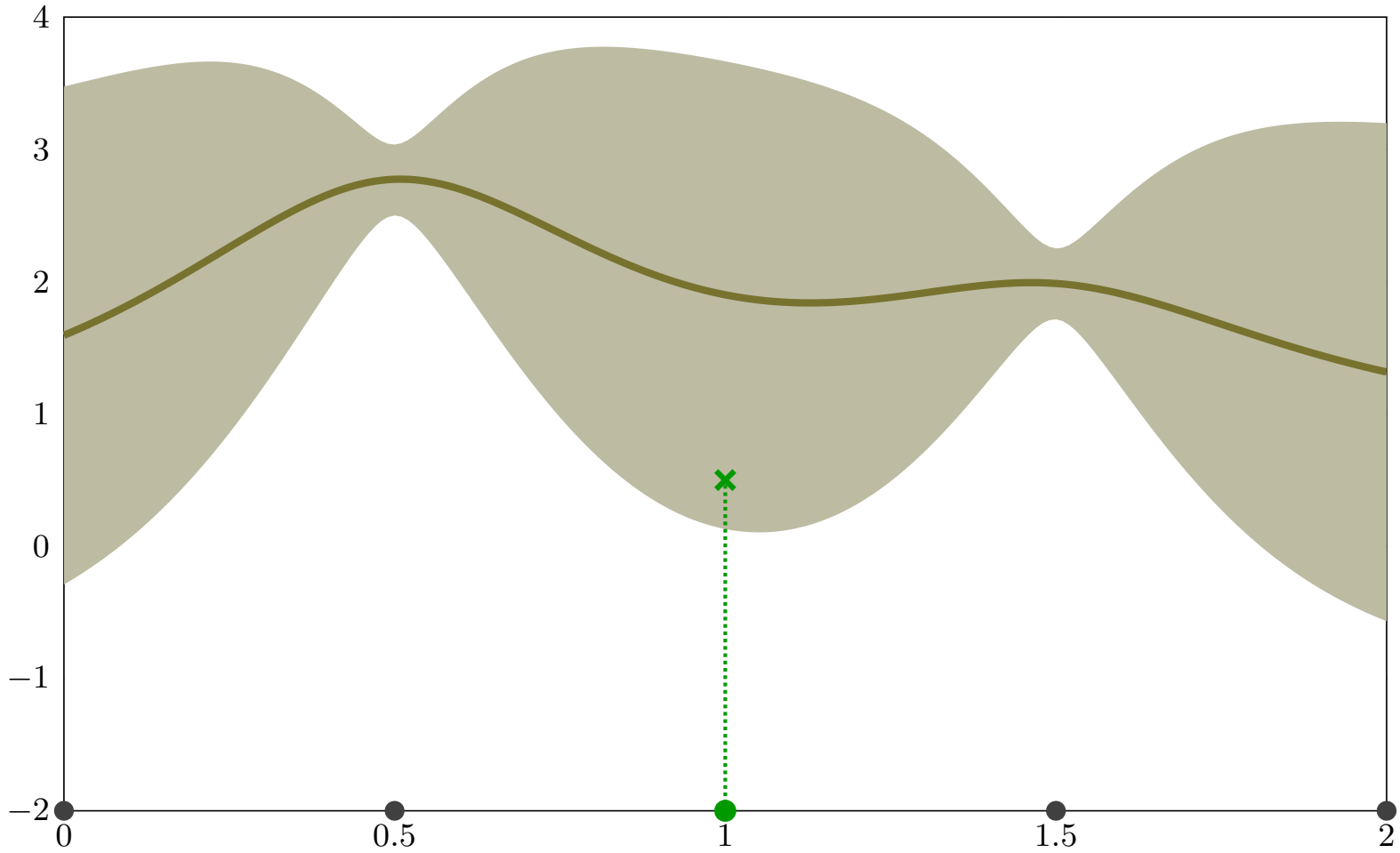

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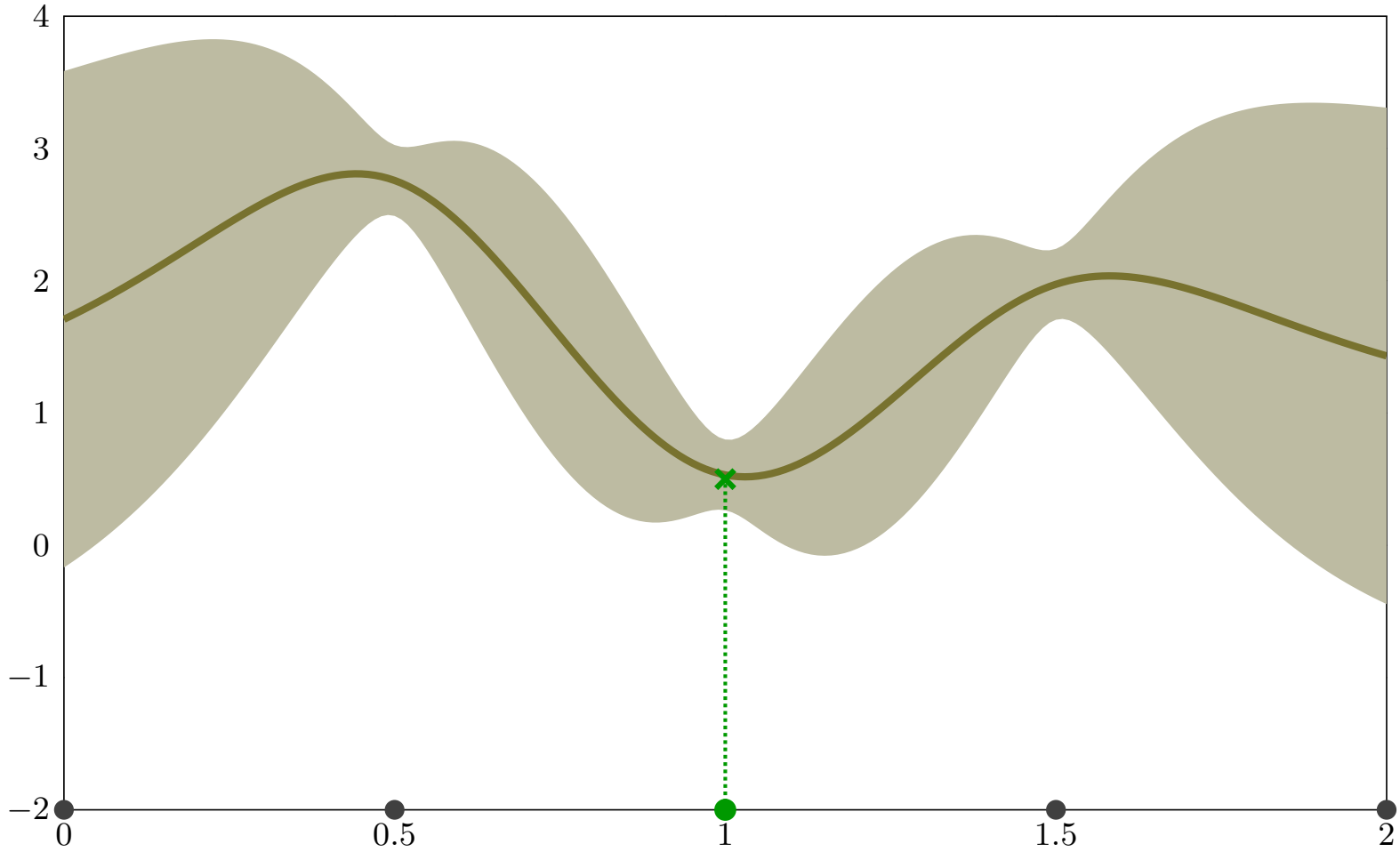

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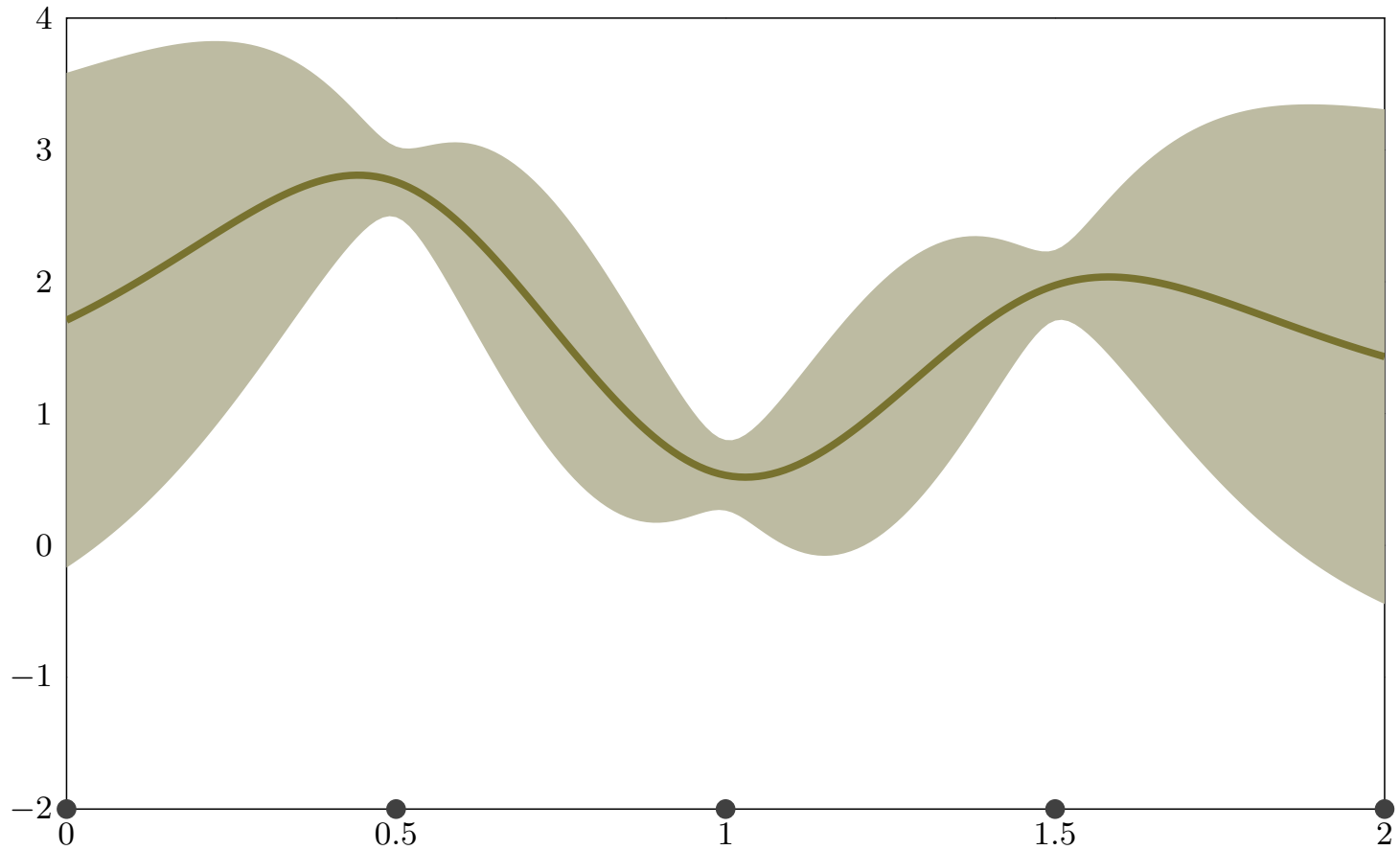

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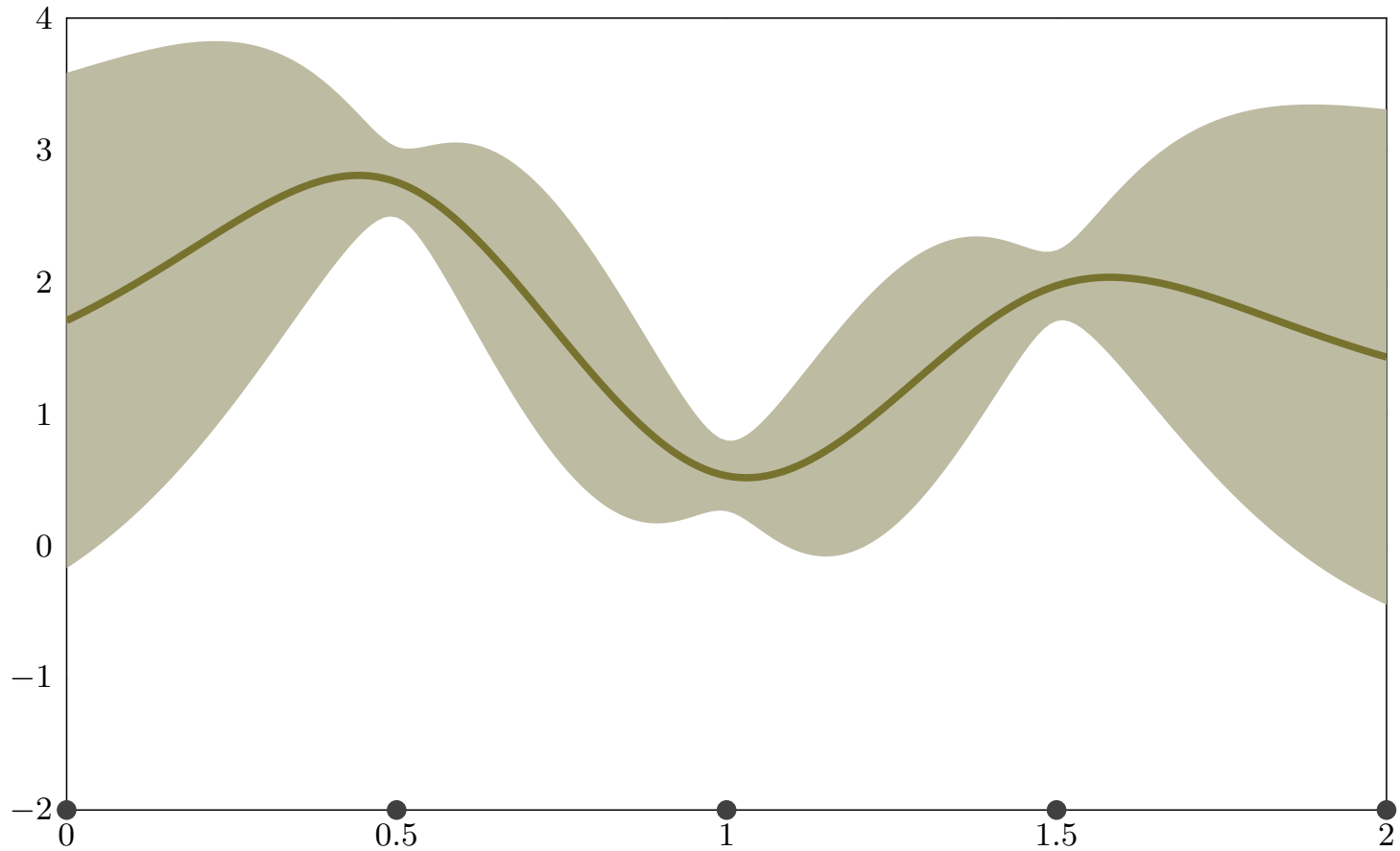

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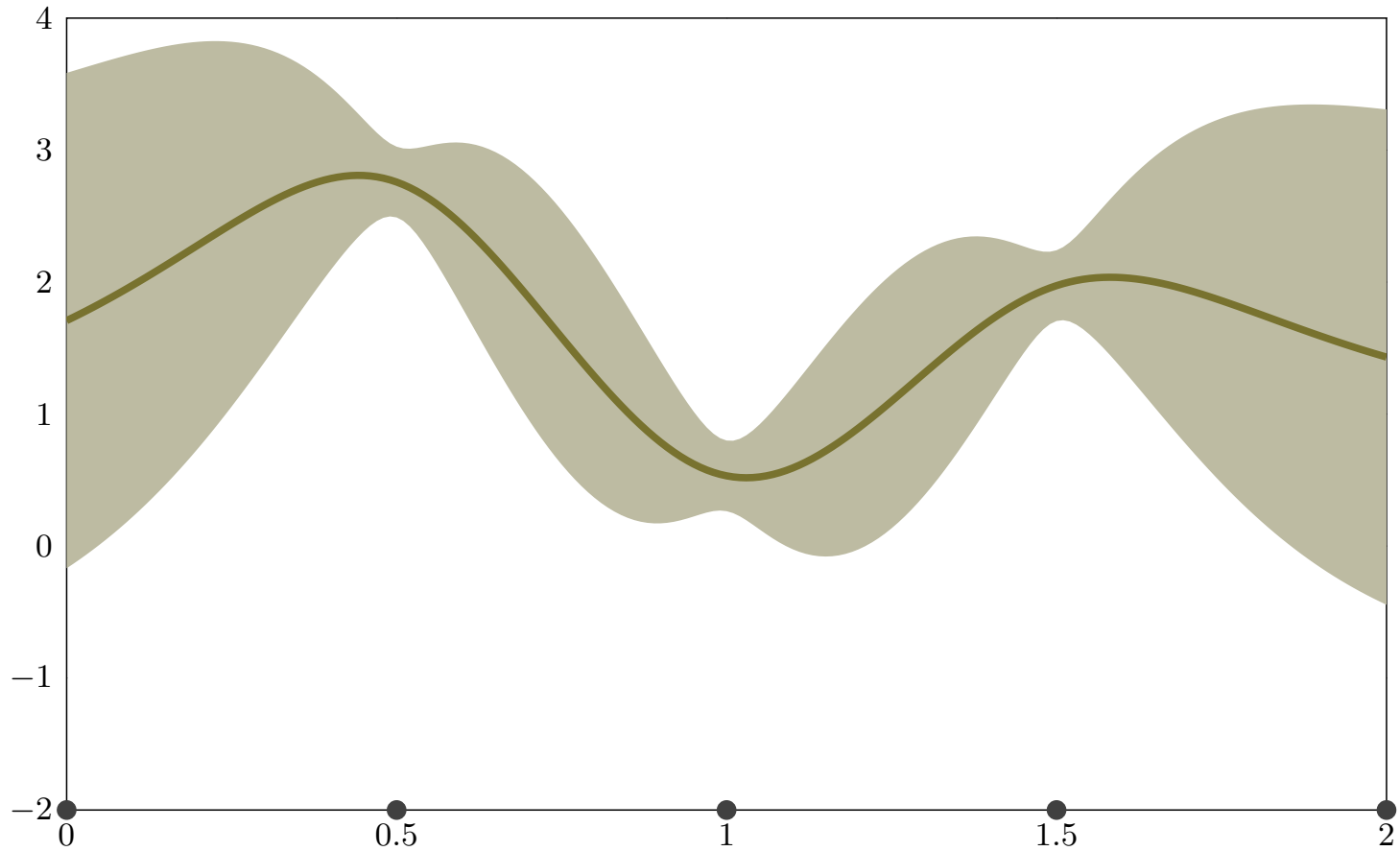

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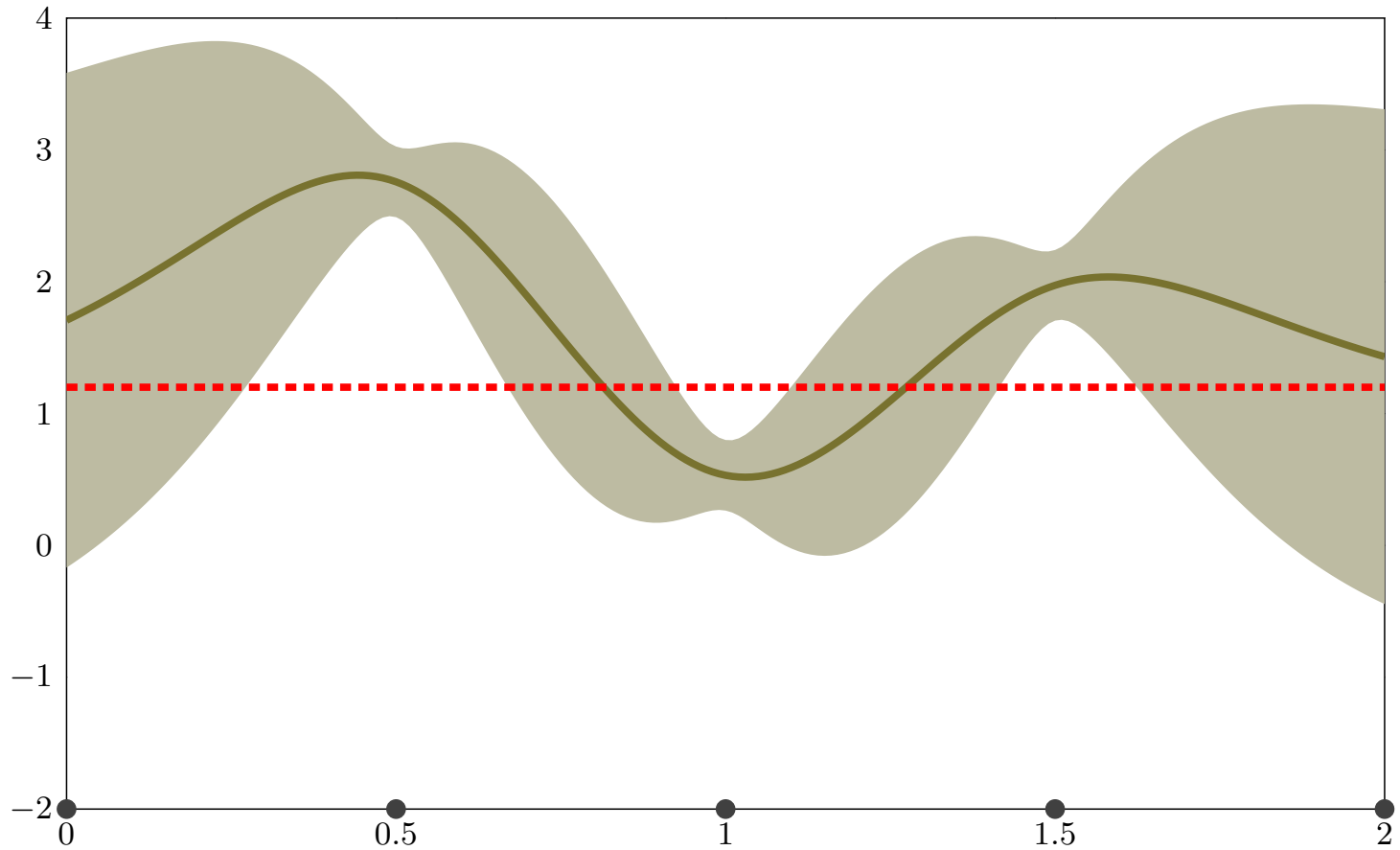

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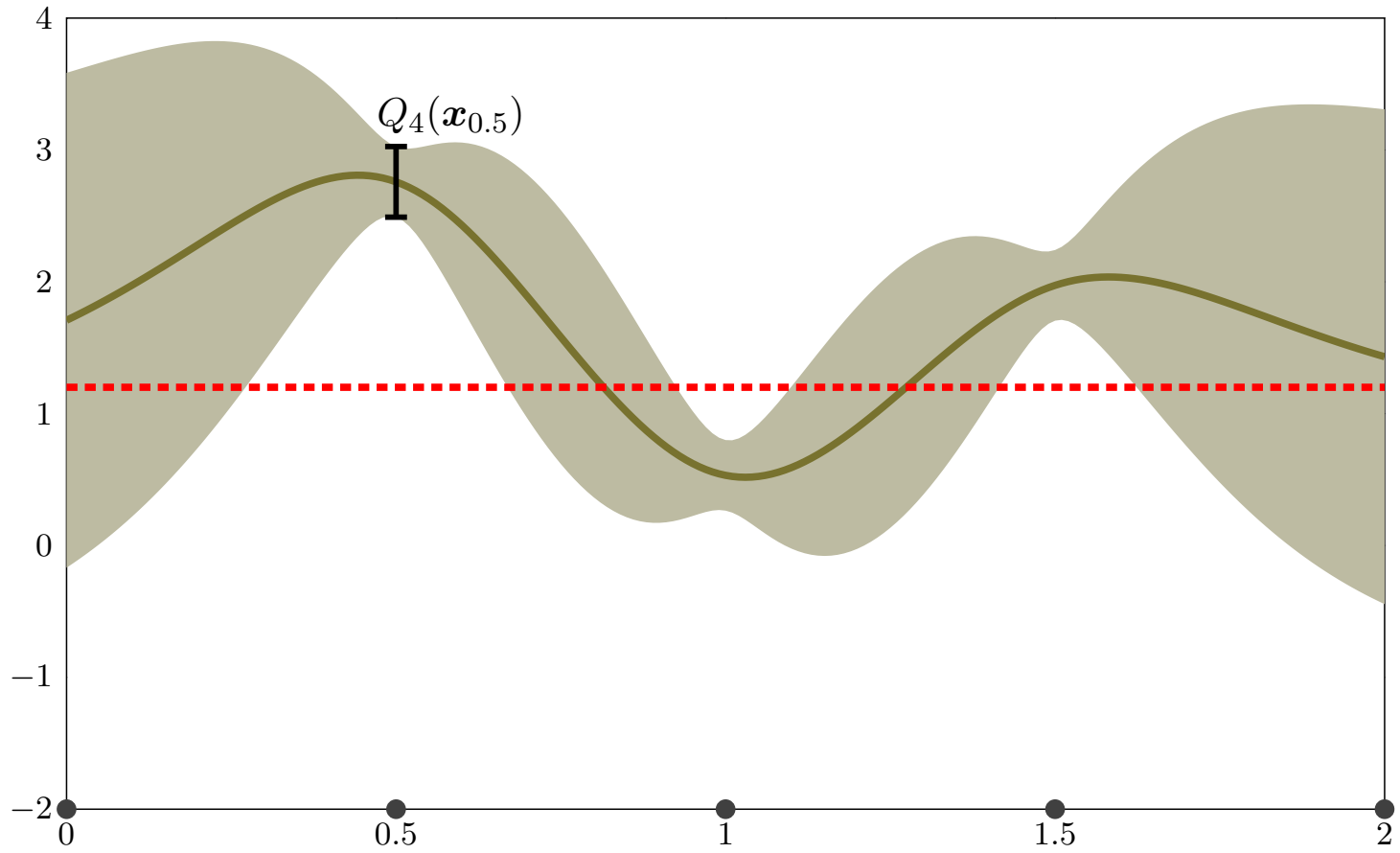

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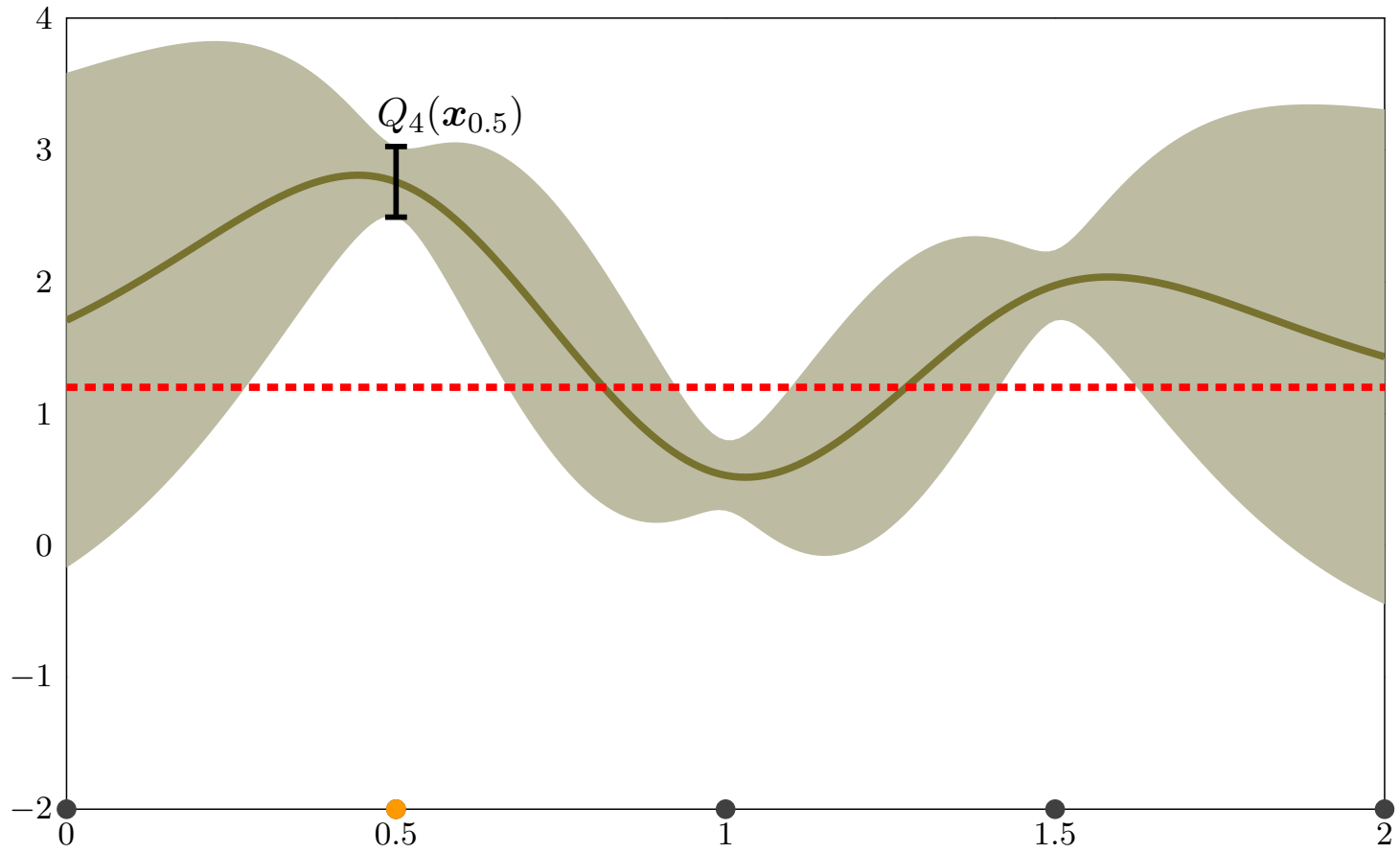

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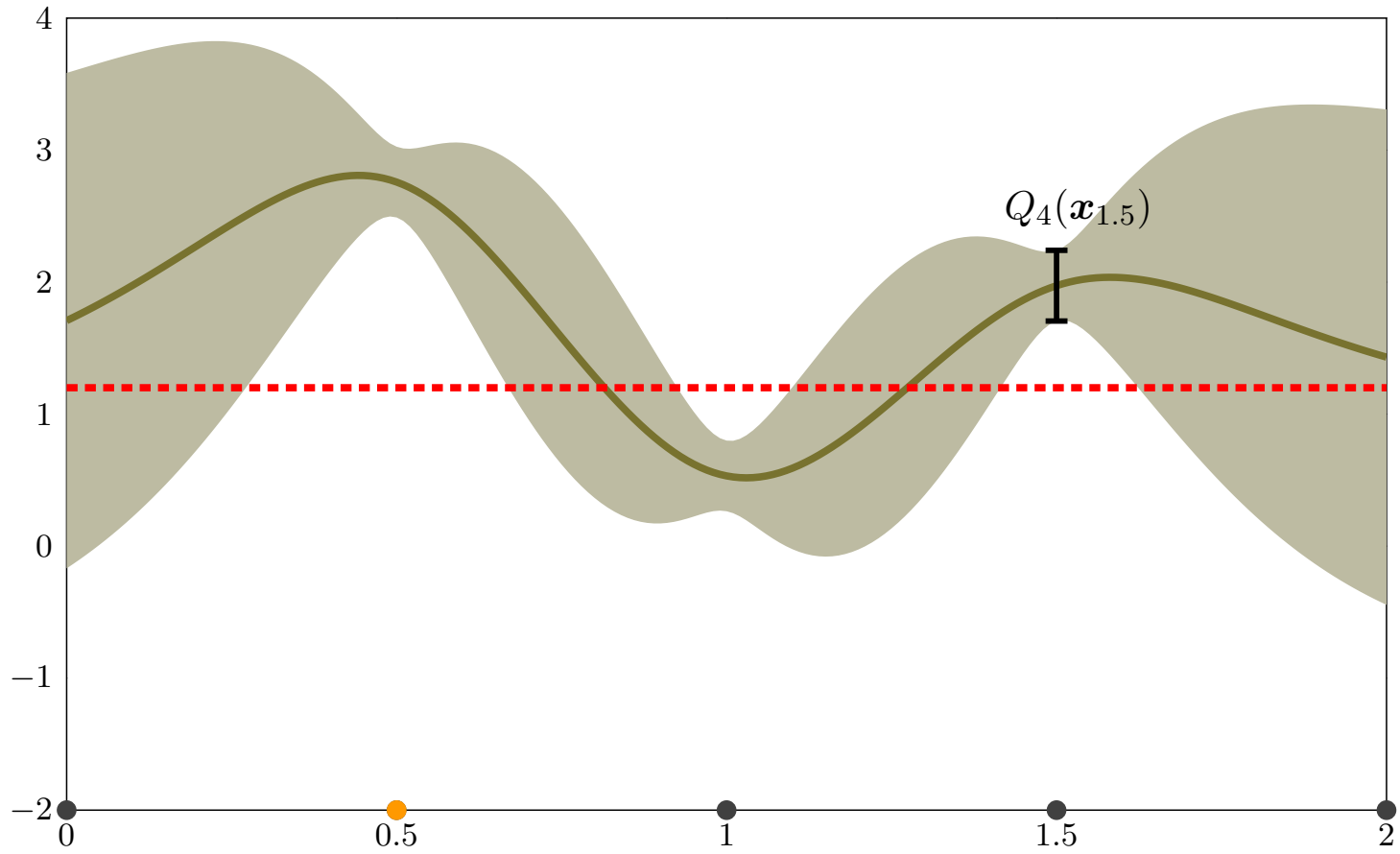

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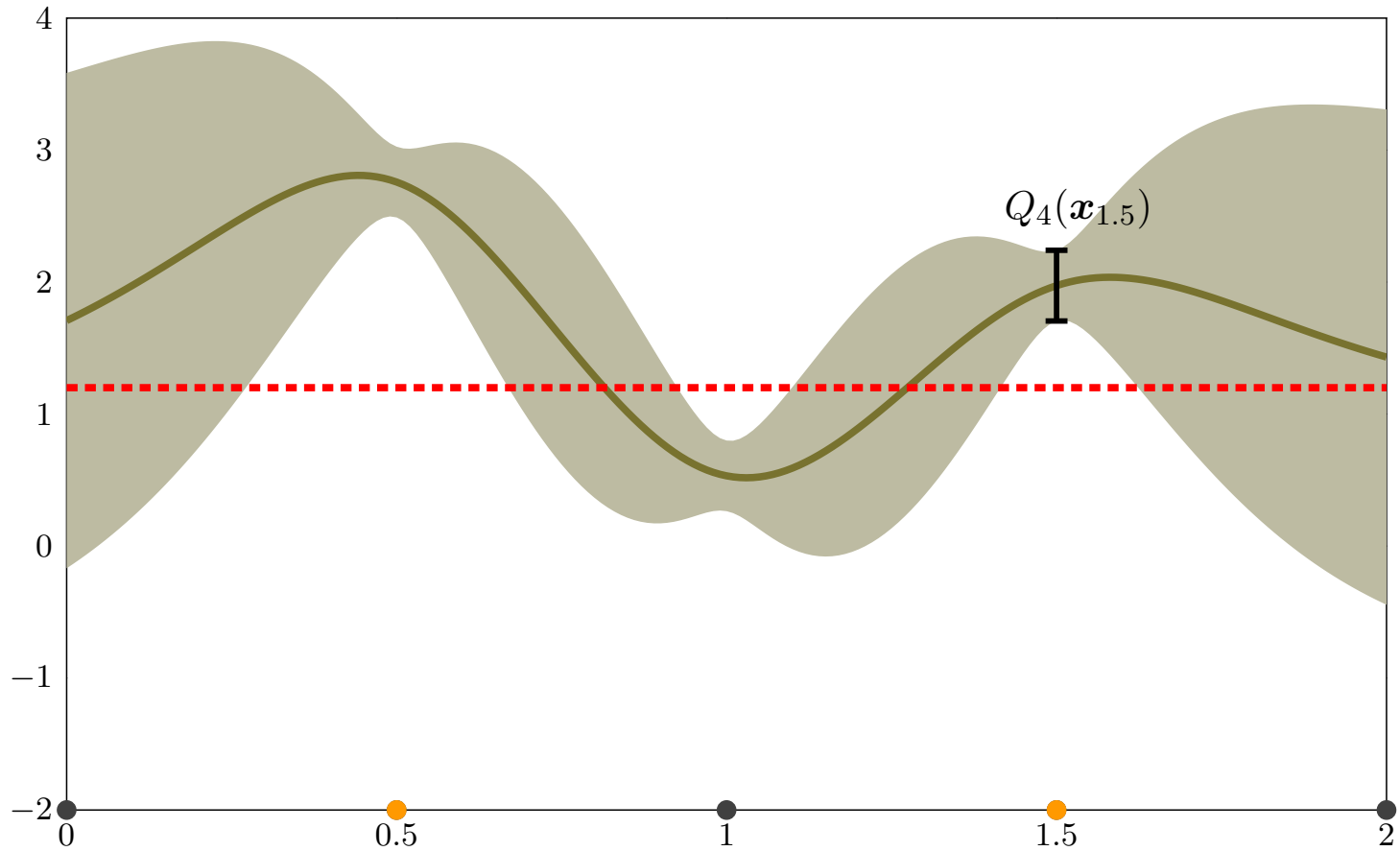

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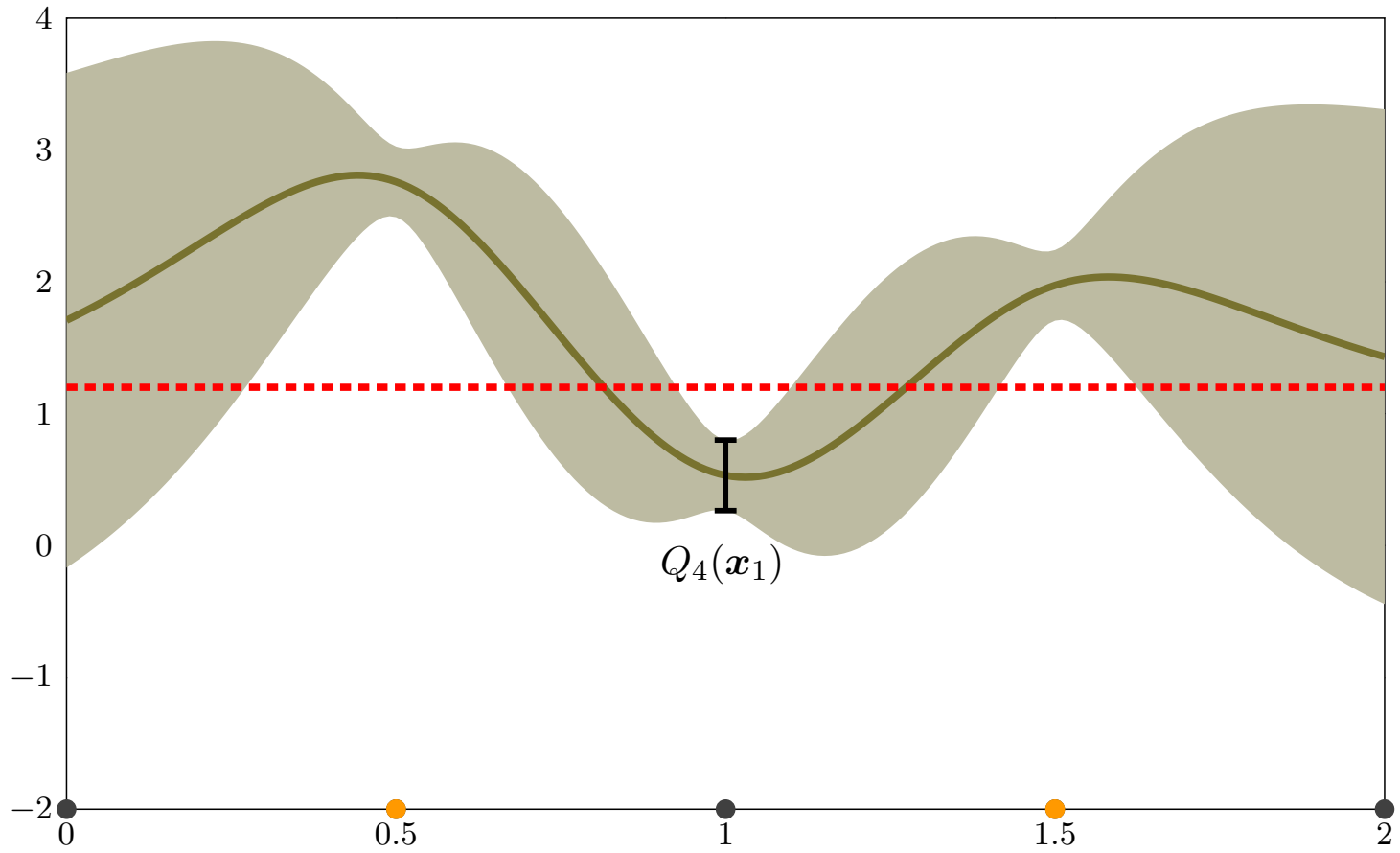

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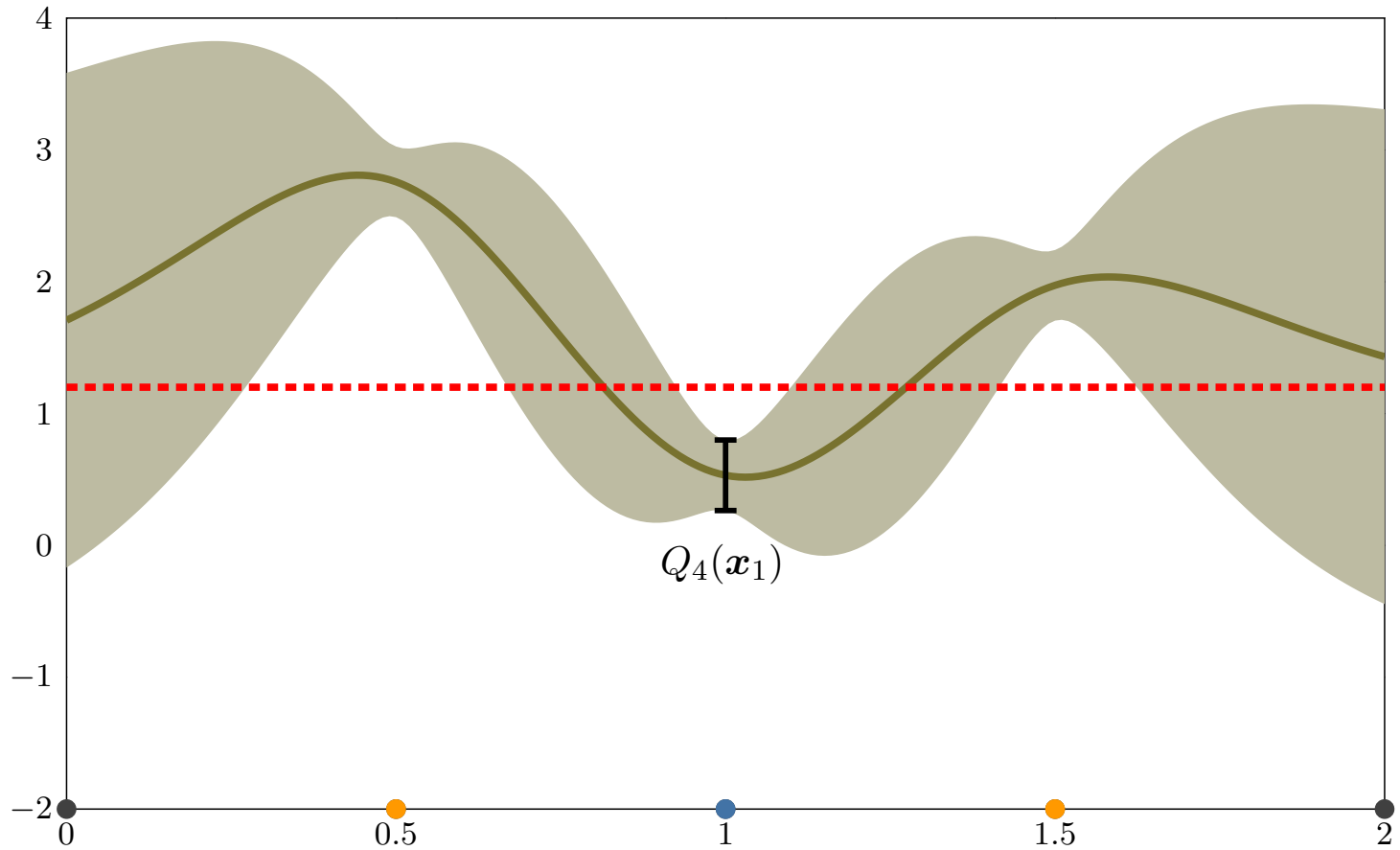

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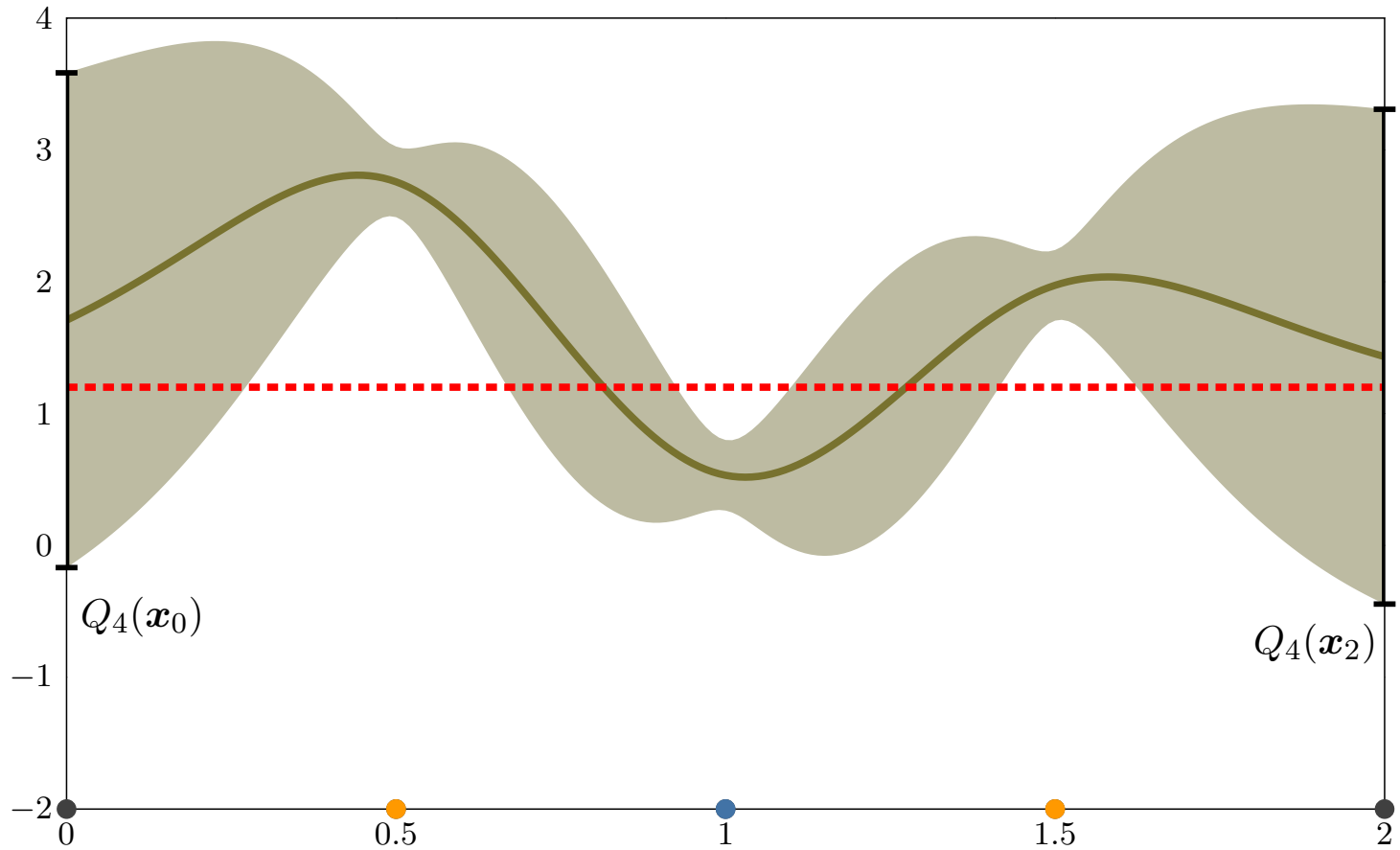

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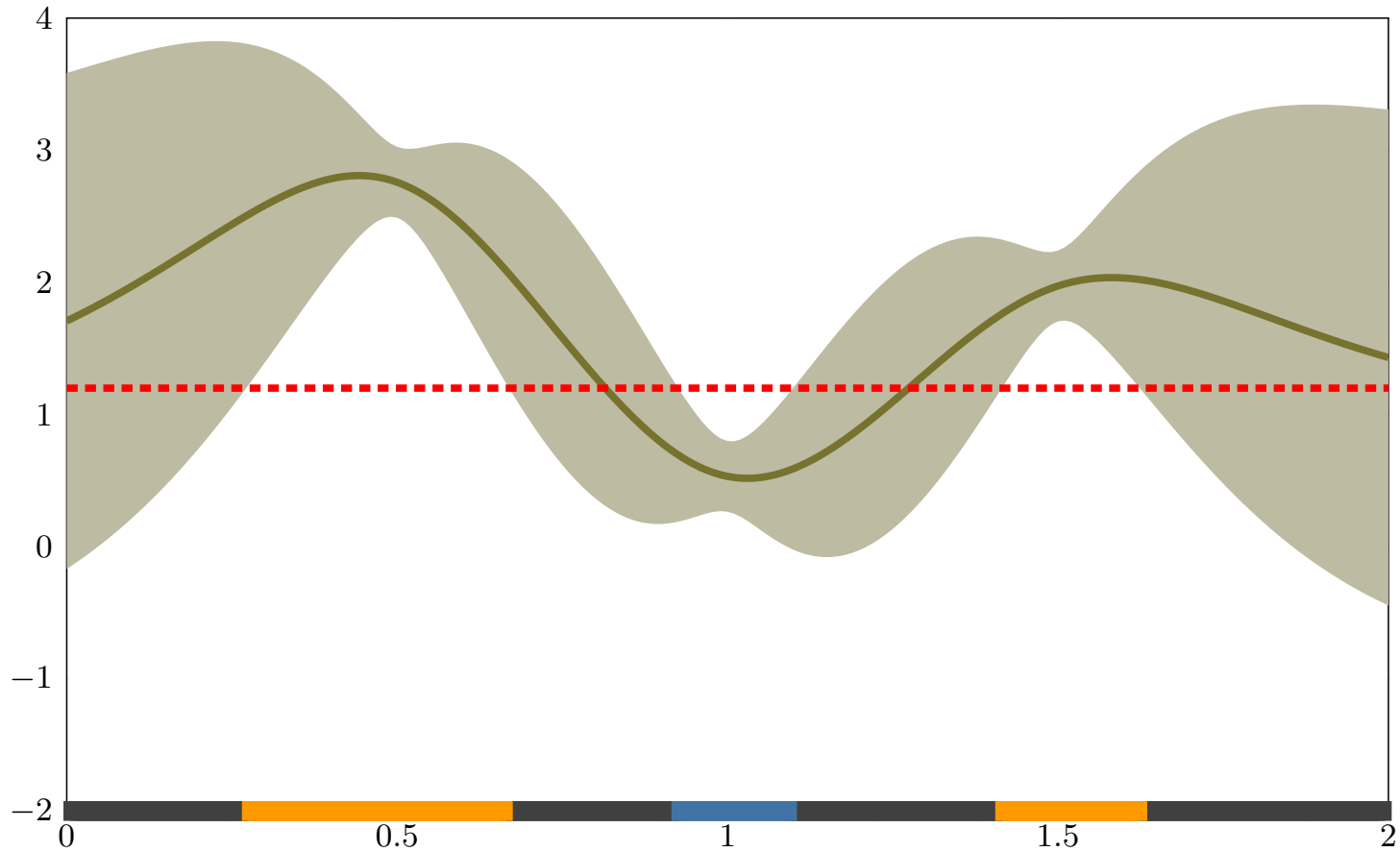

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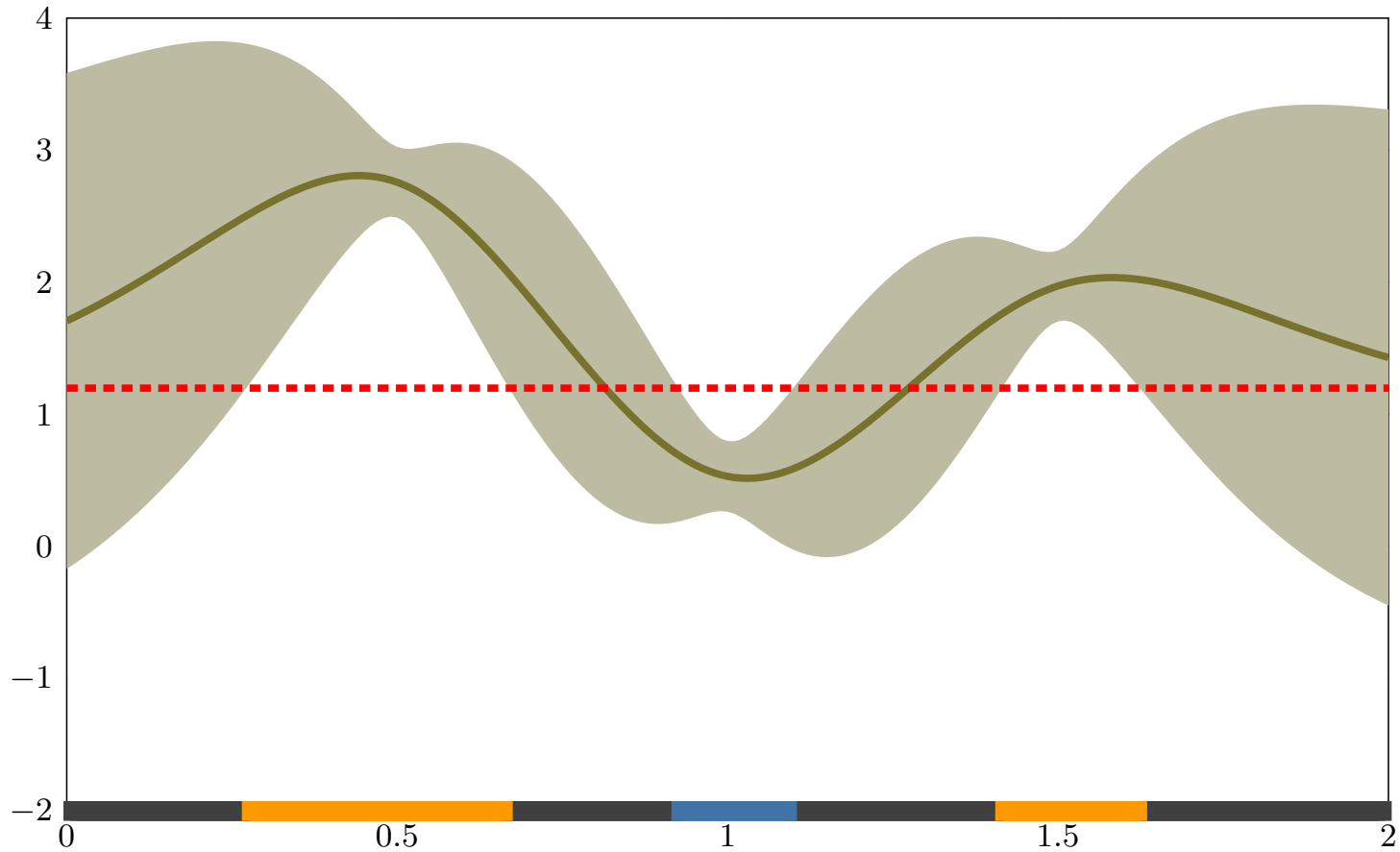
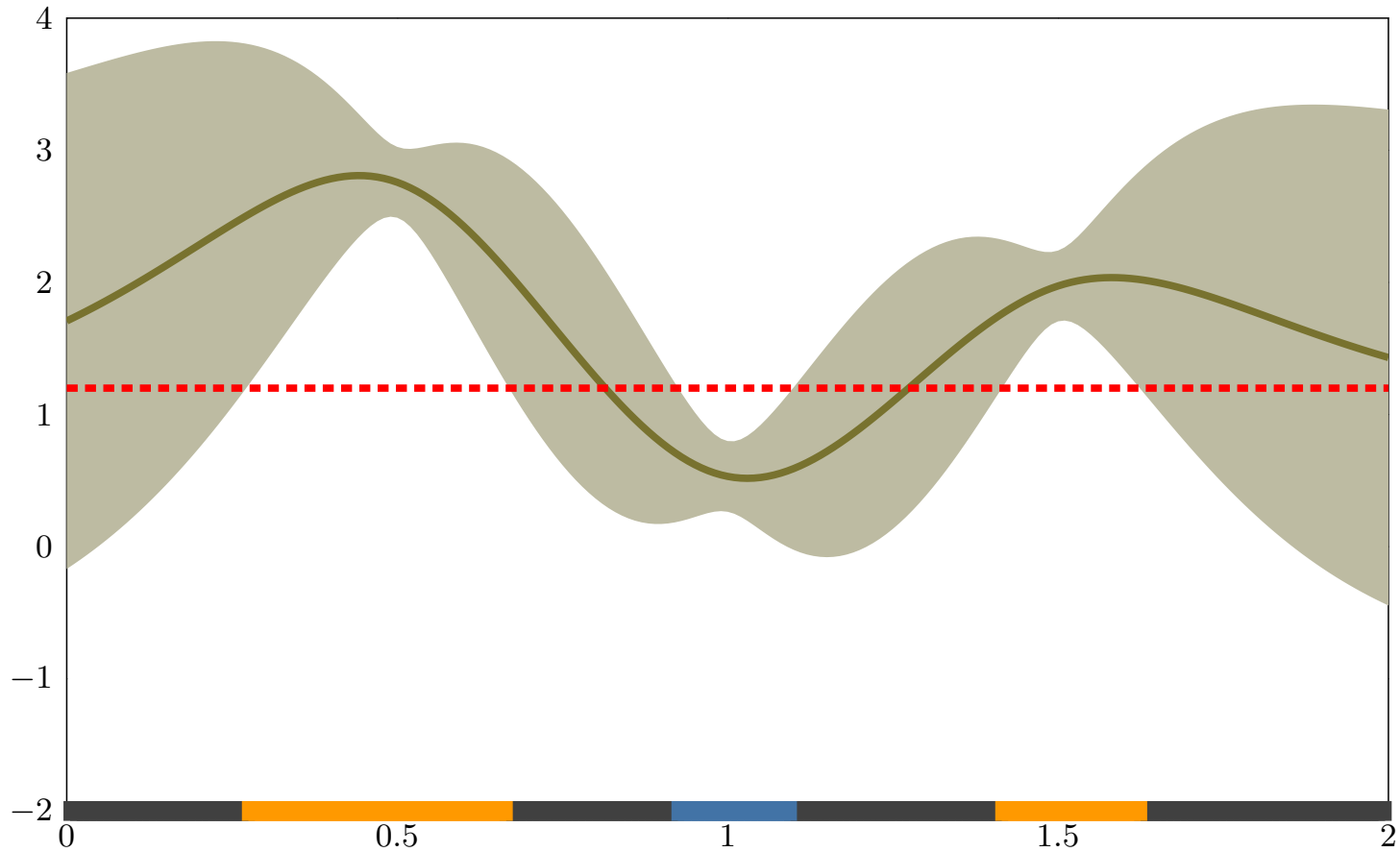
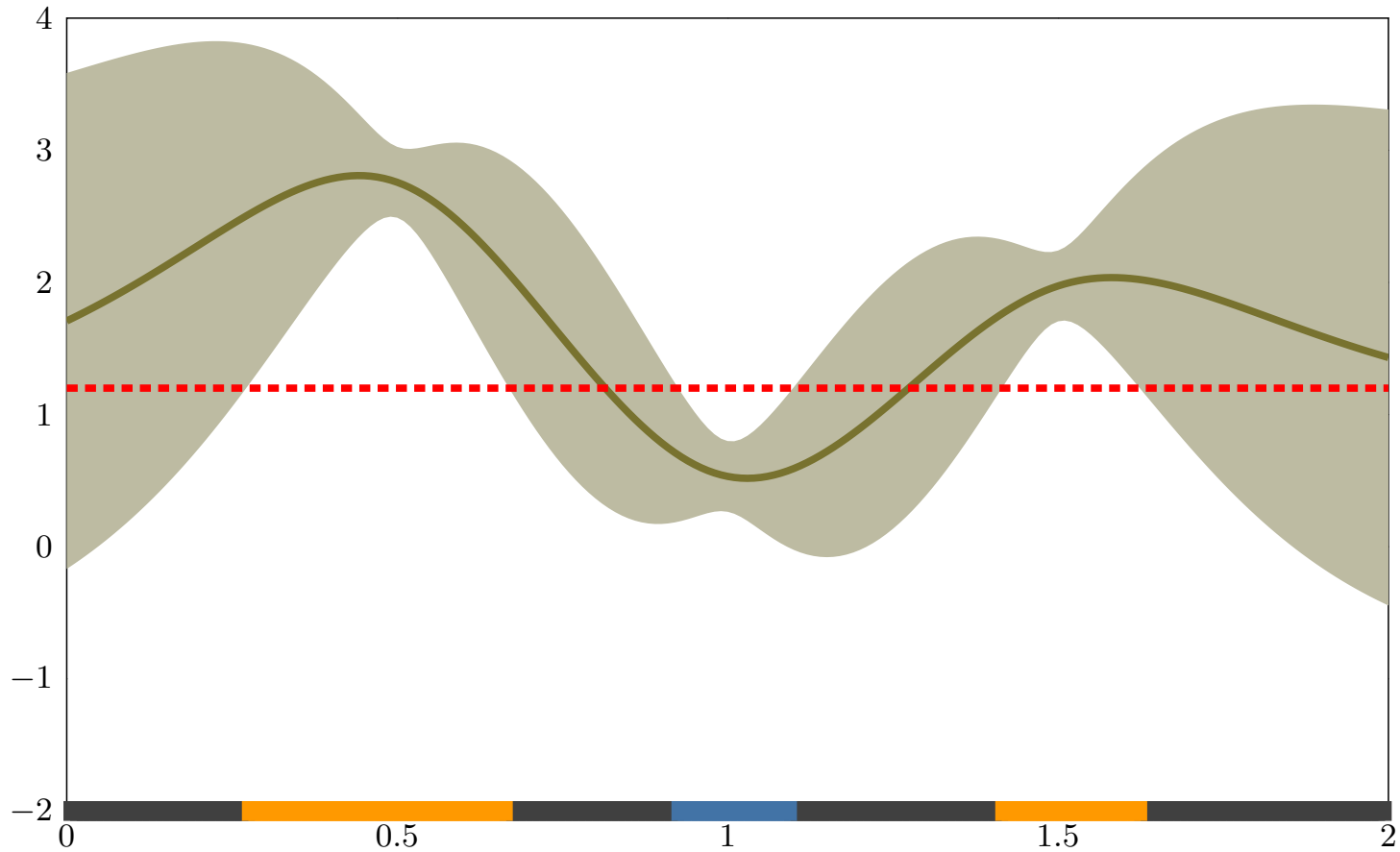


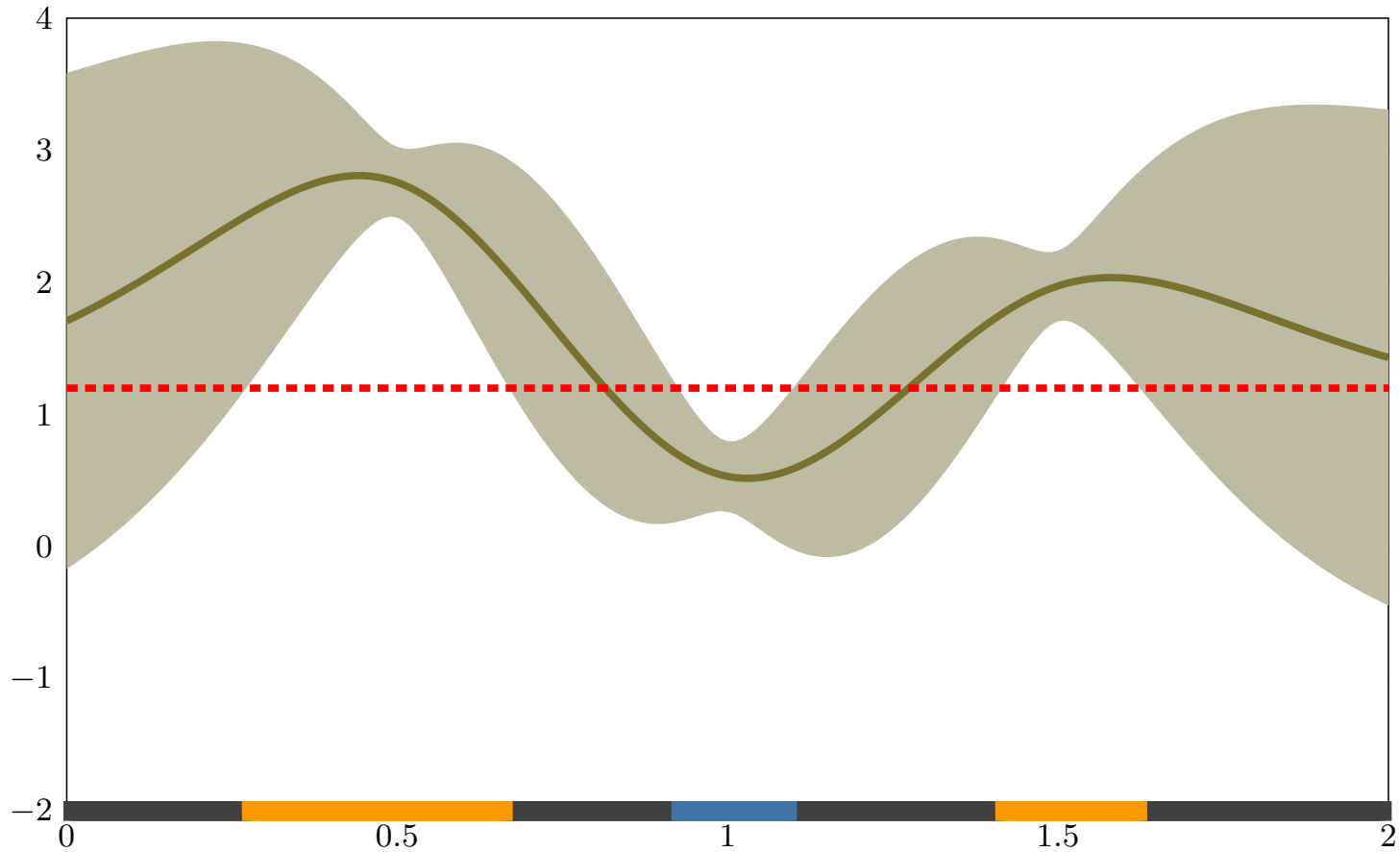
1. How do we **estimate** the function? ✓
2. How do we **classify**? ✓
3. How do we **select** "informative" measurements?



1. How do we **estimate** the function? ✓
2. How do we **classify**? ✓
3. How do we **select** "informative" measurements?
   - Pick among the yet unclassified...



1. How do we **estimate** the function? ✓
2. How do we **classify**? ✓
3. How do we **select** "informative" measurements?
   - Pick among the yet unclassified...
   - ...the most "ambiguous" point



1. How do we **estimate** the function? ✓
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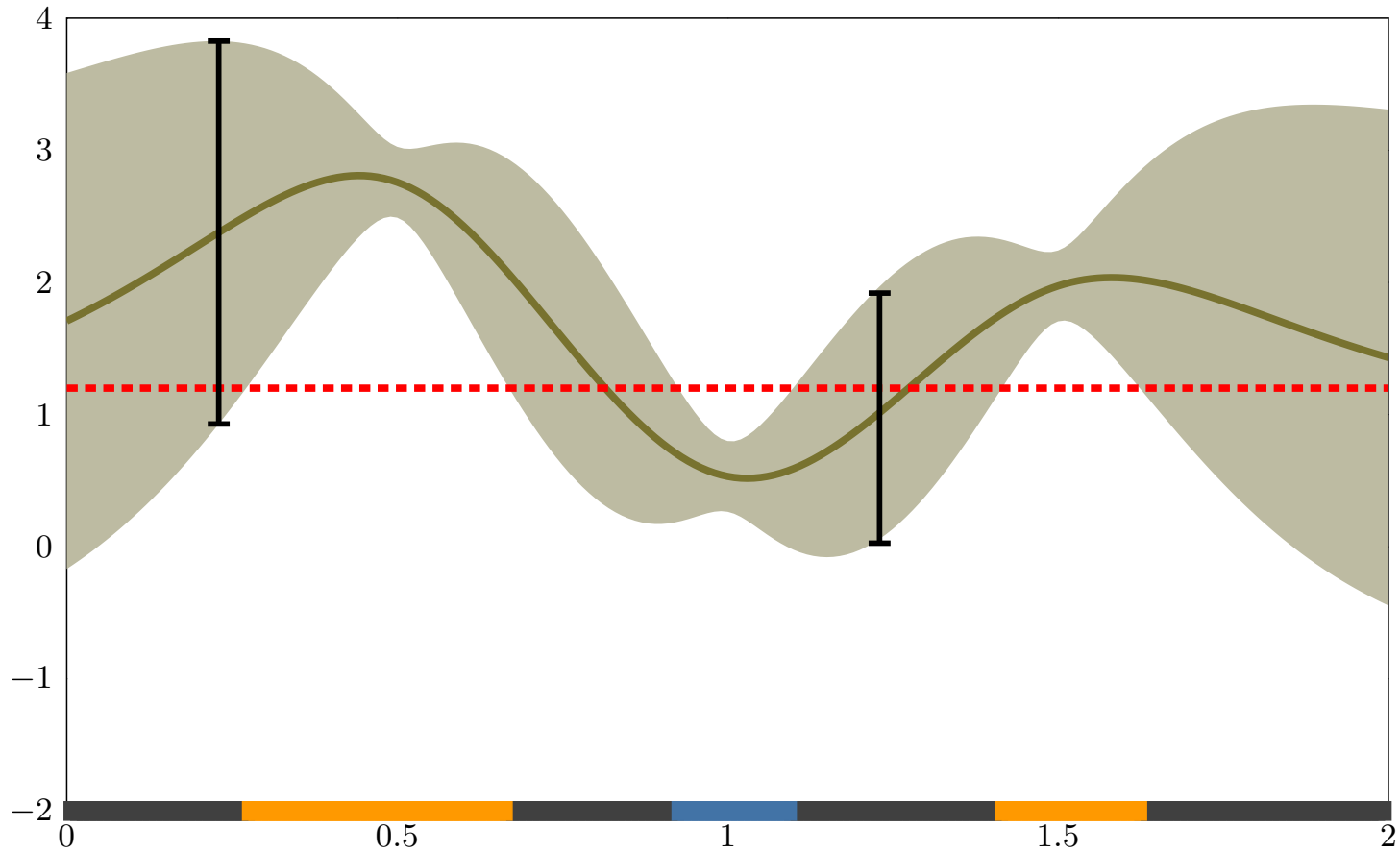
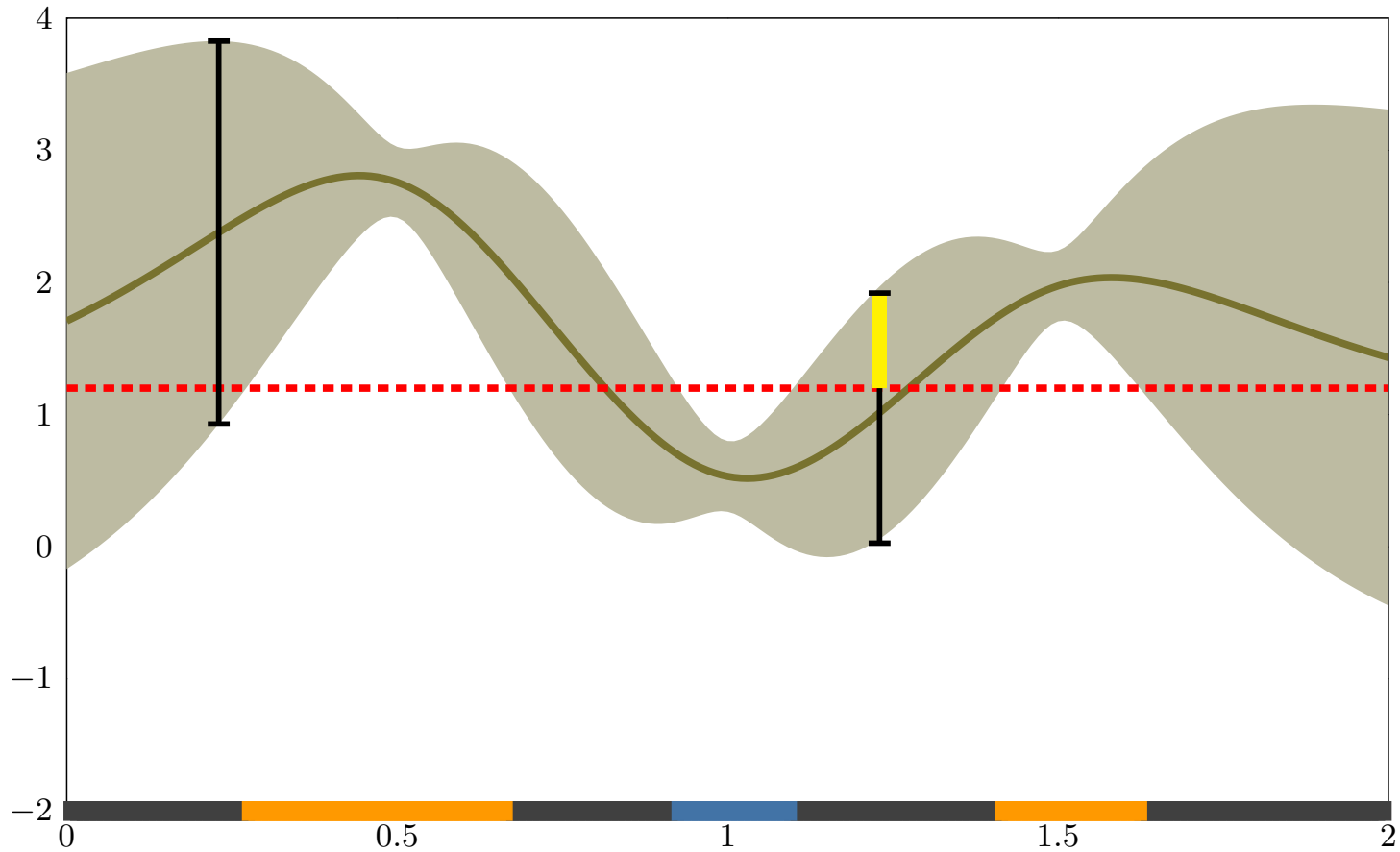
   - Pick among the yet unclassified...
   - ...the most "ambiguous" point



1. How do we **estimate** the function? ✓
2. How do we **classify**? ✓
3. How do we **select** "informative" measurements?
   - Pick among the yet unclassified...
   - ...the most "ambiguous" point



1. How do we **estimate** the function? ✓
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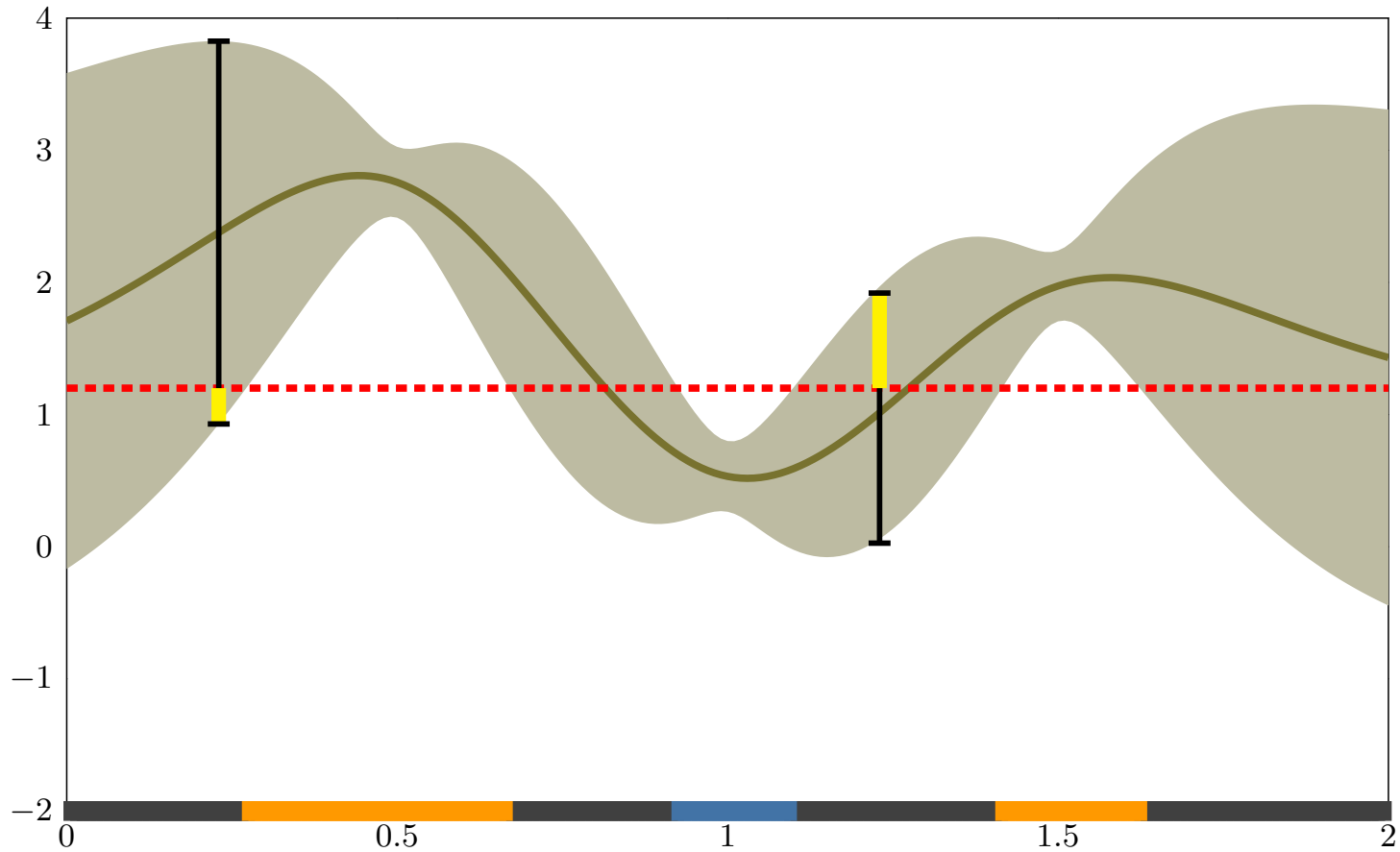
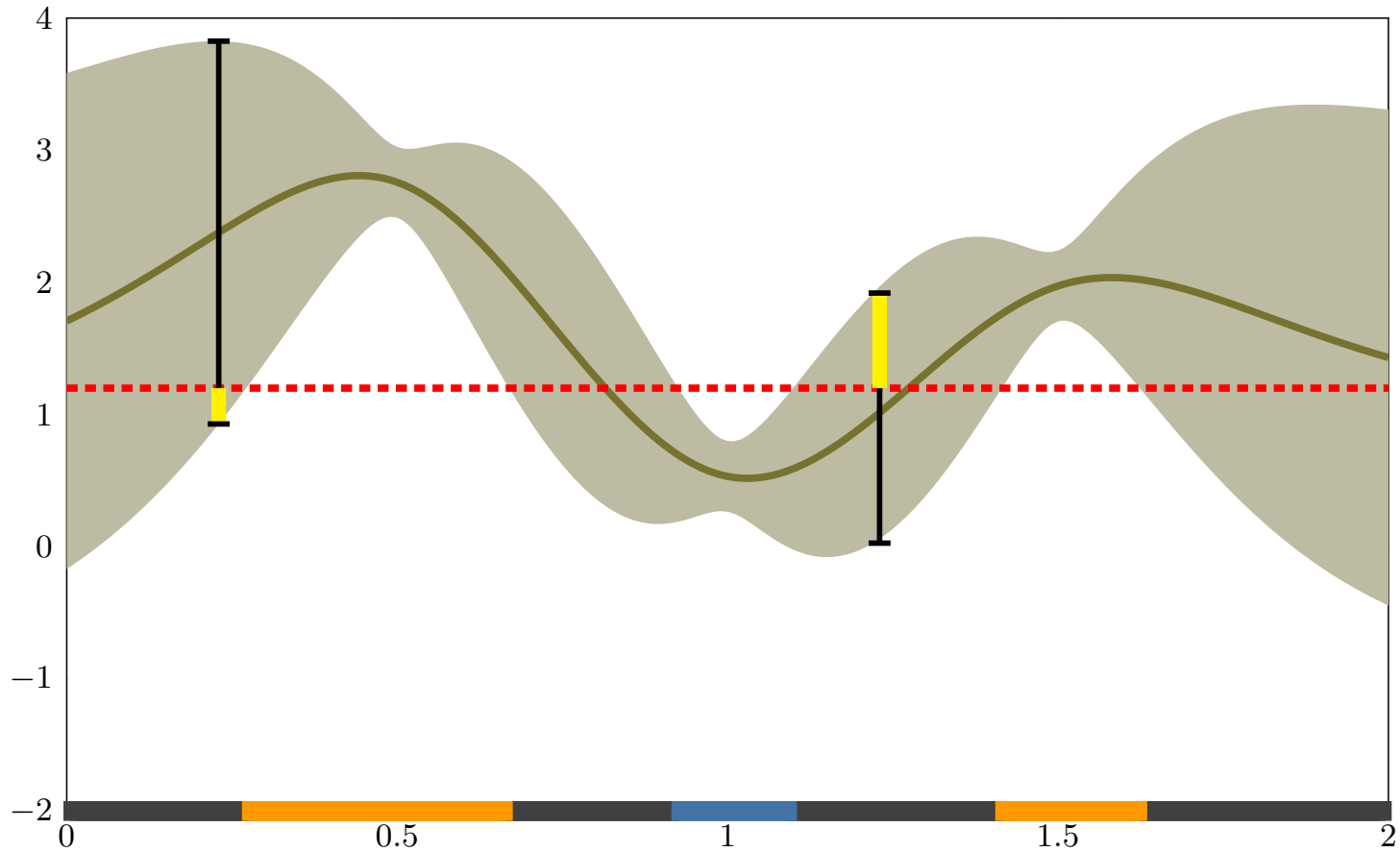
   - Pick among the yet unclassified...
   - ...the most "ambiguous" point



1. How do we **estimate** the function? ✓
2. How do we **classify**? ✓
3. How do we **select** "informative" measurements?
   - Pick among the yet unclassified...
   - ...the most "ambiguous" point (max. variance or random also work)



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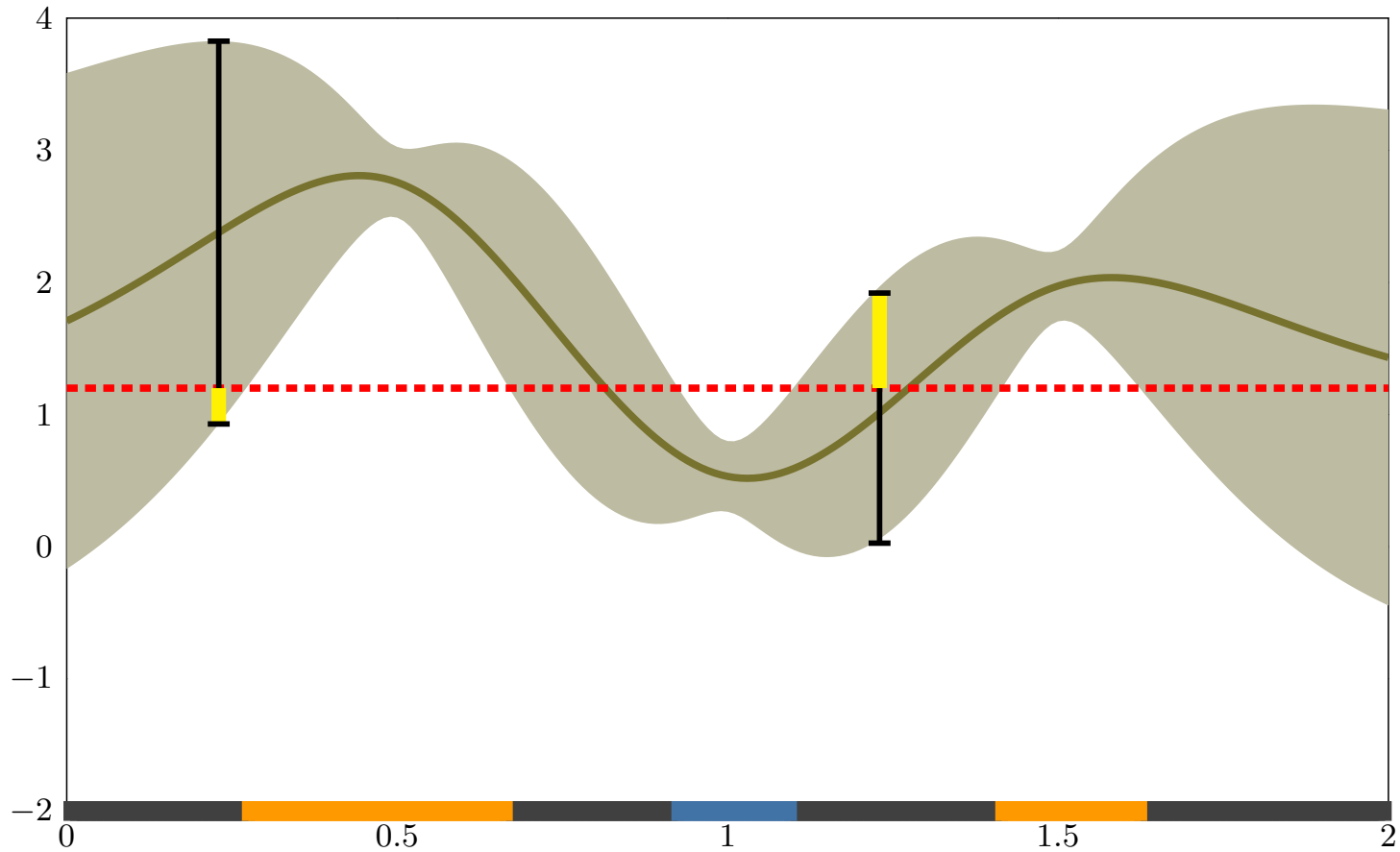
   - Pick among the yet unclassified...
   - ...the most "ambiguous" point (max. variance or random also work)



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

The Level Set Estimation (LSE) algorithm

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

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

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

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

$t \leftarrow 1$

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

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

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

$H_0 \leftarrow \varnothing,\ L_0 \leftarrow \varnothing,\ U_0 \leftarrow D$
$C_0(\boldsymbol{x}) \leftarrow \mathbb{R}$, for all $\boldsymbol{x} \in D$
$t \leftarrow 1$
while $U_{t-1} \neq \varnothing$ **do**
  $H_t \leftarrow H_{t-1},\ L_t \leftarrow L_{t-1},\ U_t \leftarrow U_{t-1}$

  $t \leftarrow t+1$
end while
$\hat{H} \leftarrow H_{t-1}$
$\hat{L} \leftarrow L_{t-1}$

The Level Set Estimation (LSE) algorithm

$\leftarrow$ loop until all points have been classified

The Level Set Estimation (LSE) algorithm

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

$H_0 \leftarrow \varnothing,\ L_0 \leftarrow \varnothing,\ U_0 \leftarrow D$
$C_0(\boldsymbol{x}) \leftarrow \mathbb{R}$, for all $\boldsymbol{x} \in D$
$t \leftarrow 1$
while $U_{t-1} \neq \varnothing$ **do** ← loop until all points have been classified
  $H_t \leftarrow H_{t-1},\ L_t \leftarrow L_{t-1},\ U_t \leftarrow U_{t-1}$
  for all $\boldsymbol{x} \in U_{t-1}$ **do**
    $C_t(\boldsymbol{x}) \leftarrow C_{t-1}(\boldsymbol{x}) \cap Q_t(\boldsymbol{x})$
    if $\min(C_t(\boldsymbol{x})) + \epsilon > h$ **then** ← classify
      $U_t \leftarrow U_t \setminus \{\boldsymbol{x}\}$
      $H_t \leftarrow H_t \cup \{\boldsymbol{x}\}$
    else if $\max(C_t(\boldsymbol{x})) - \epsilon \leq h$ **then**
      $U_t \leftarrow U_t \setminus \{\boldsymbol{x}\}$
      $L_t \leftarrow L_t \cup \{\boldsymbol{x}\}$
    end if
  end for
  $t \leftarrow t + 1$
end while
$\hat{H} \leftarrow H_{t-1}$
$\hat{L} \leftarrow L_{t-1}$

The Level Set Estimation (LSE) algorithm

Input: sample set D, GP prior $(\mu_0,\ k,\ \sigma_0)$, thr. value h, accuracy parameter ϵ
Output: predicted sets $\hat{H},\ \hat{L}$

$H_0 \leftarrow \varnothing,\ L_0 \leftarrow \varnothing,\ U_0 \leftarrow D$
$C_0(\boldsymbol{x}) \leftarrow \mathbb{R}$, for all $\boldsymbol{x} \in D$
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  $H_t \leftarrow H_{t-1},\ L_t \leftarrow L_{t-1},\ U_t \leftarrow U_{t-1}$
  for all $\boldsymbol{x} \in U_{t-1}$ **do**
    $C_t(\boldsymbol{x}) \leftarrow C_{t-1}(\boldsymbol{x}) \cap Q_t(\boldsymbol{x})$
    if $\min(C_t(\boldsymbol{x})) + \epsilon > h$ **then** ← classify
      $U_t \leftarrow U_t \setminus \{\boldsymbol{x}\}$
      $H_t \leftarrow H_t \cup \{\boldsymbol{x}\}$
    else if $\max(C_t(\boldsymbol{x})) - \epsilon \leq h$ **then**
      $U_t \leftarrow U_t \setminus \{\boldsymbol{x}\}$
      $L_t \leftarrow L_t \cup \{\boldsymbol{x}\}$
    end if
  end for
  $\boldsymbol{x}_t \leftarrow \operatorname{argmax}\{a_t(\boldsymbol{x}) \mid \boldsymbol{x} \in U_t\}$ ← select max. ambiguity point
  $y_t \leftarrow f(\boldsymbol{x}_t) + n_t$
  $t \leftarrow t + 1$
end while
$\hat{H} \leftarrow H_{t-1}$
$\hat{L} \leftarrow L_{t-1}$

The Level Set Estimation (LSE) algorithm

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

$H_0 \leftarrow \varnothing,\ L_0 \leftarrow \varnothing,\ U_0 \leftarrow D$
$C_0(\boldsymbol{x}) \leftarrow \mathbb{R}$, for all $\boldsymbol{x} \in D$
$t \leftarrow 1$
while $U_{t-1} \neq \varnothing$ **do** ← loop until all points have been classified
  $H_t \leftarrow H_{t-1},\ L_t \leftarrow L_{t-1},\ U_t \leftarrow U_{t-1}$
  for all $\boldsymbol{x} \in U_{t-1}$ **do**
    $C_t(\boldsymbol{x}) \leftarrow C_{t-1}(\boldsymbol{x}) \cap Q_t(\boldsymbol{x})$
    if $\min(C_t(\boldsymbol{x})) + \epsilon > h$ **then** ← classify
      $U_t \leftarrow U_t \setminus \{\boldsymbol{x}\}$
      $H_t \leftarrow H_t \cup \{\boldsymbol{x}\}$
    else if $\max(C_t(\boldsymbol{x})) - \epsilon \leq h$ **then**
      $U_t \leftarrow U_t \setminus \{\boldsymbol{x}\}$
      $L_t \leftarrow L_t \cup \{\boldsymbol{x}\}$
    end if
  end for
  $\boldsymbol{x}_t \leftarrow \operatorname{argmax}\{a_t(\boldsymbol{x}) \mid \boldsymbol{x} \in U_t\}$ ← select max. ambiguity point
  $y_t \leftarrow f(\boldsymbol{x}_t) + n_t$
  Compute $\mu_t(\boldsymbol{x})$ and $\sigma_t(\boldsymbol{x})$, $\forall \boldsymbol{x} \in U_t$ ← update GP estimate
  $t \leftarrow t + 1$
end while
$\hat{H} \leftarrow H_{t-1}$
$\hat{L} \leftarrow L_{t-1}$

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

$H_0 \leftarrow \varnothing,\ L_0 \leftarrow \varnothing,\ U_0 \leftarrow D$
$C_0(\boldsymbol{x}) \leftarrow \mathbb{R}$, for all $\boldsymbol{x} \in D$
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    if $\min(C_t(\boldsymbol{x})) + \epsilon > h$ **then**
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      $H_t \leftarrow H_t \cup \{\boldsymbol{x}\}$
    else if $\max(C_t(\boldsymbol{x})) - \epsilon \leq h$ **then**
      $U_t \leftarrow U_t \setminus \{\boldsymbol{x}\}$
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    end if
  end for
  $\boldsymbol{x}_t \leftarrow \operatorname{argmax}\{a_t(\boldsymbol{x}) \mid \boldsymbol{x} \in U_t\}$
  $y_t \leftarrow f(\boldsymbol{x}_t) + n_t$
  Compute $\mu_t(\boldsymbol{x})$ and $\sigma_t(\boldsymbol{x})$, $\forall \boldsymbol{x} \in U_t$
  $t \leftarrow t + 1$
end while
$\hat{H} \leftarrow H_{t-1}$
$\hat{L} \leftarrow L_{t-1}$

The Level Set Estimation (LSE) algorithm

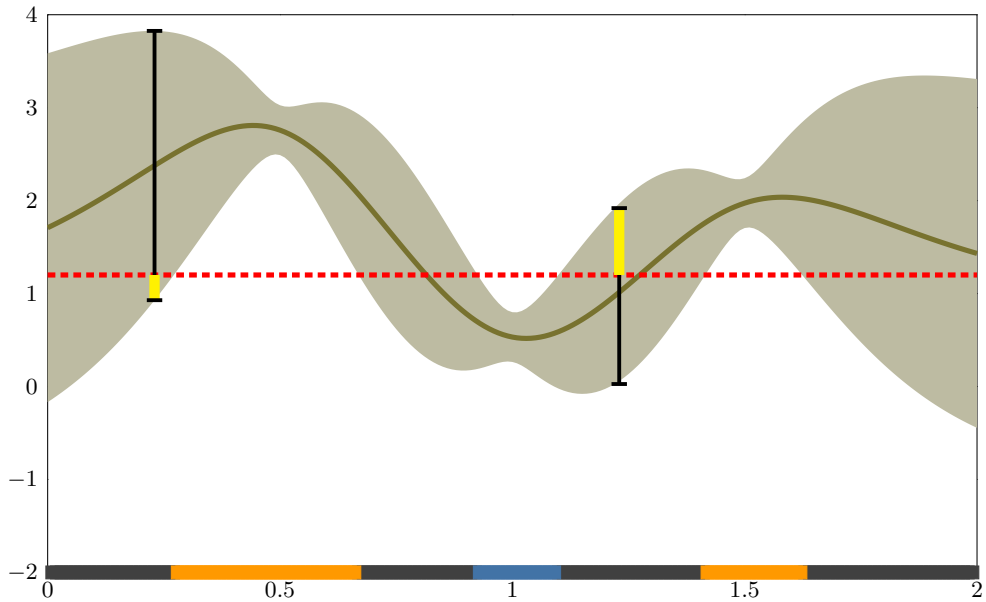
- Monotonicity of
  1. confidence intervals
  2. classification

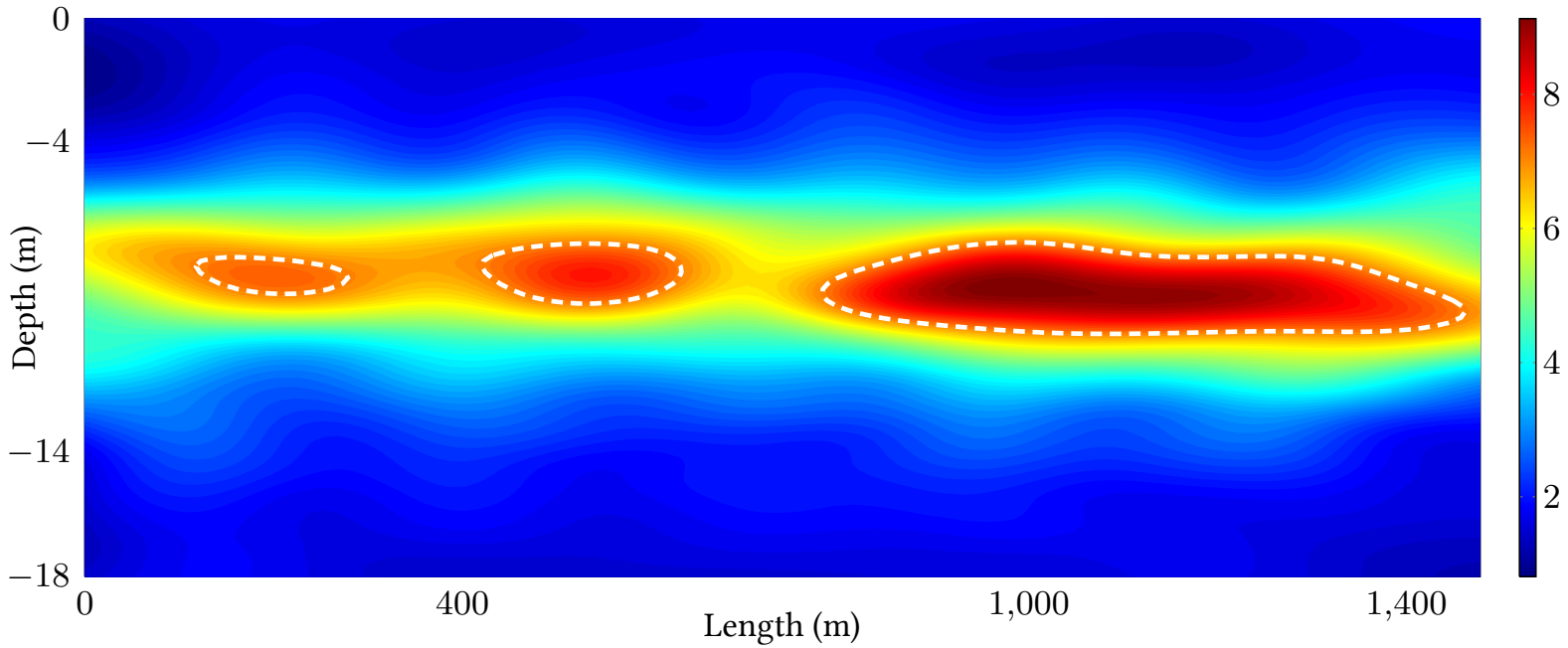
Input: sample set D, GP prior (μ_0, k, σ_0), thr. value h, accuracy parameter ϵ
Output: predicted sets $\hat{H}$, $\hat{L}$

$H_0 \leftarrow \varnothing,\ L_0 \leftarrow \varnothing,\ U_0 \leftarrow D$
$C_0(\boldsymbol{x}) \leftarrow \mathbb{R}$, for all $\boldsymbol{x} \in D$
$t \leftarrow 1$
while $U_{t-1} \neq \varnothing$ **do**
  $H_t \leftarrow H_{t-1},\ L_t \leftarrow L_{t-1},\ U_t \leftarrow U_{t-1}$
  for all $\boldsymbol{x} \in U_{t-1}$ **do**
    $C_t(\boldsymbol{x}) \leftarrow C_{t-1}(\boldsymbol{x}) \cap Q_t(\boldsymbol{x})$
    if $\min(C_t(\boldsymbol{x})) + \epsilon > h$ **then**
      $U_t \leftarrow U_t \setminus \{\boldsymbol{x}\}$
      $H_t \leftarrow H_t \cup \{\boldsymbol{x}\}$
    else if $\max(C_t(\boldsymbol{x})) - \epsilon \leq h$ **then**
      $U_t \leftarrow U_t \setminus \{\boldsymbol{x}\}$
      $L_t \leftarrow L_t \cup \{\boldsymbol{x}\}$
    end if
  end for
  $\boldsymbol{x}_t \leftarrow \operatorname{argmax}\{a_t(\boldsymbol{x}) \mid \boldsymbol{x} \in U_t\}$
  $y_t \leftarrow f(\boldsymbol{x}_t) + n_t$
  Compute $\mu_t(\boldsymbol{x})$ and $\sigma_t(\boldsymbol{x})$, $\forall \boldsymbol{x} \in U_t$
  $t \leftarrow t + 1$
end while
$\hat{H} \leftarrow H_{t-1}$
$\hat{L} \leftarrow L_{t-1}$

The Level Set Estimation (LSE) algorithm

- Monotonicity of
  1. confidence intervals
  2. classification
- Relaxed classification rules by an accuracy parameter ϵ
  (trades off sampling cost for accuracy)

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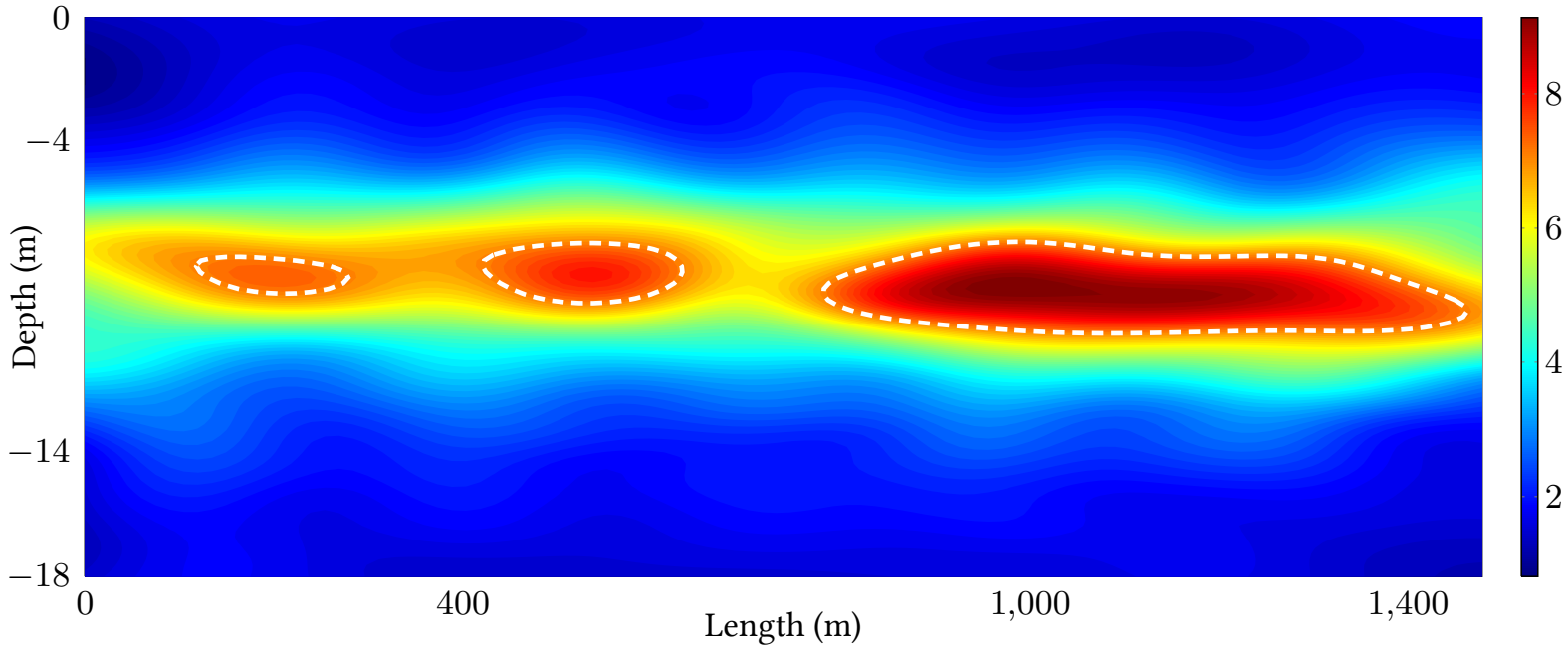
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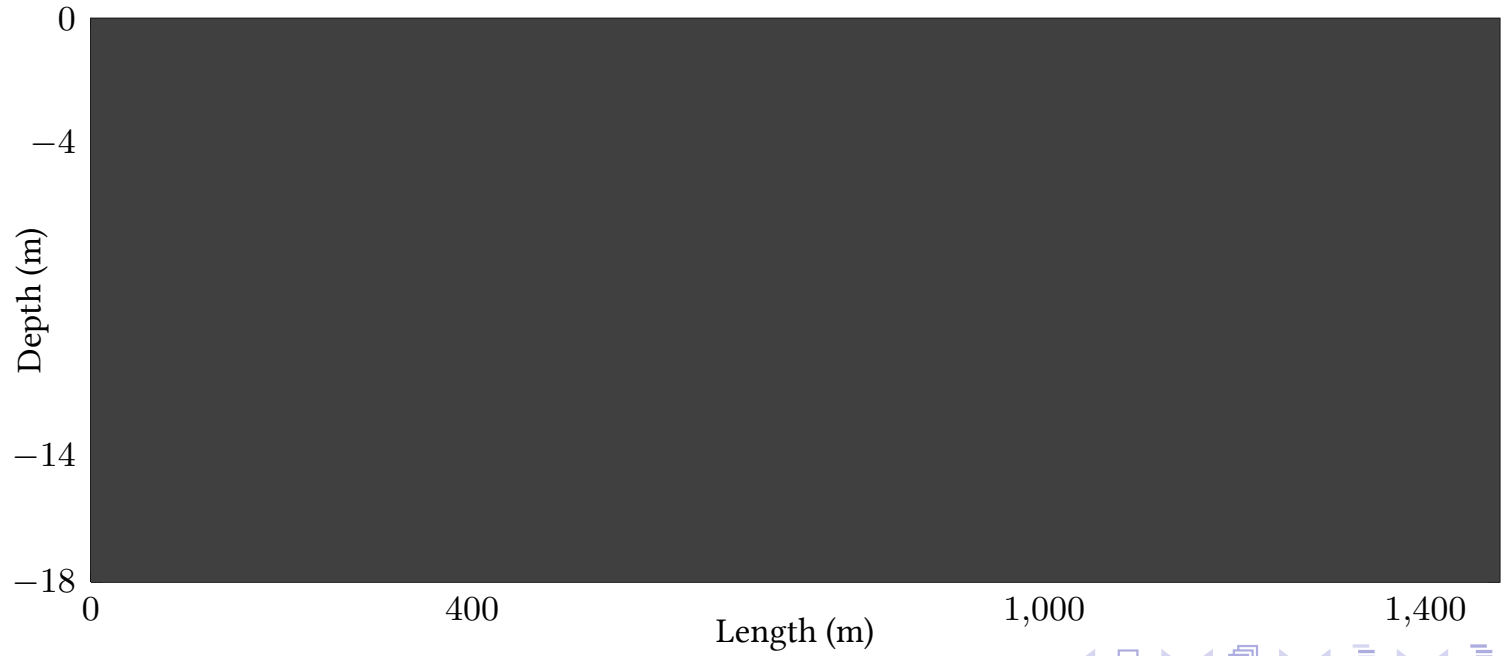
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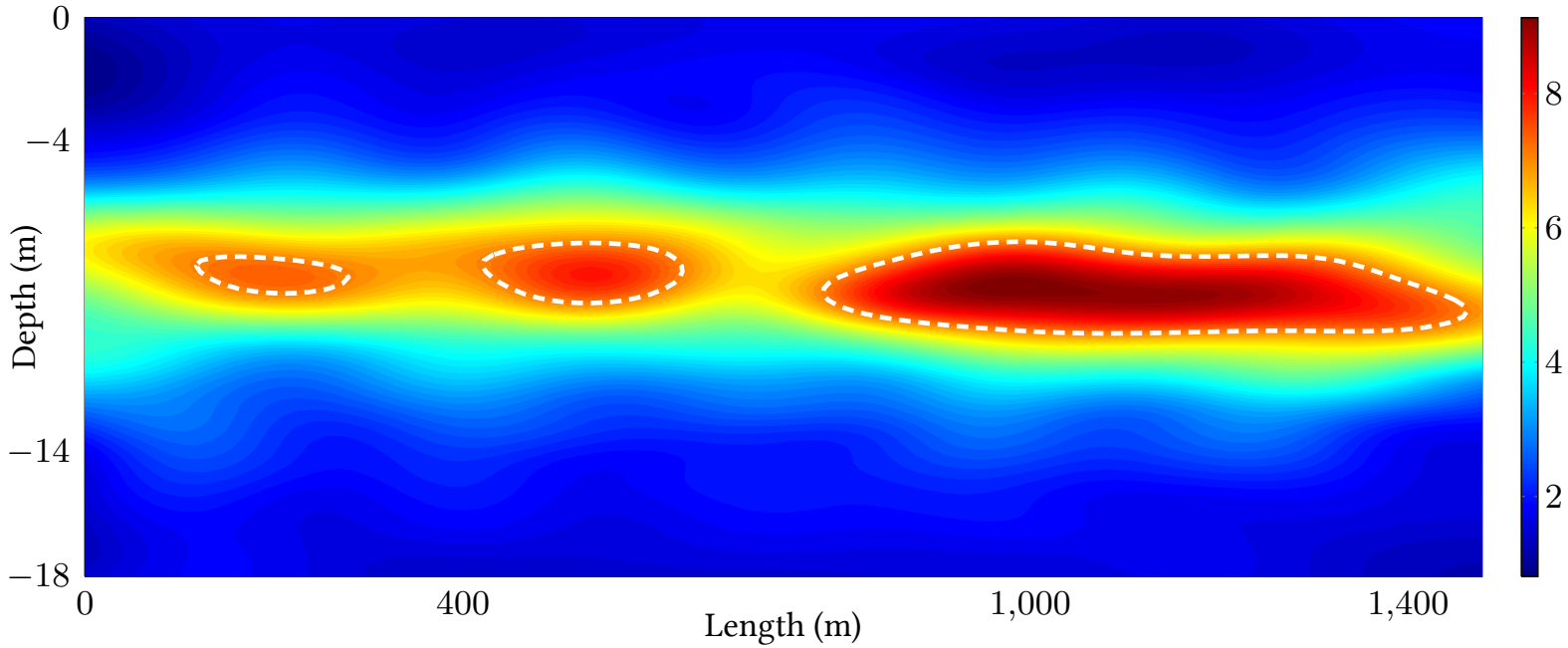
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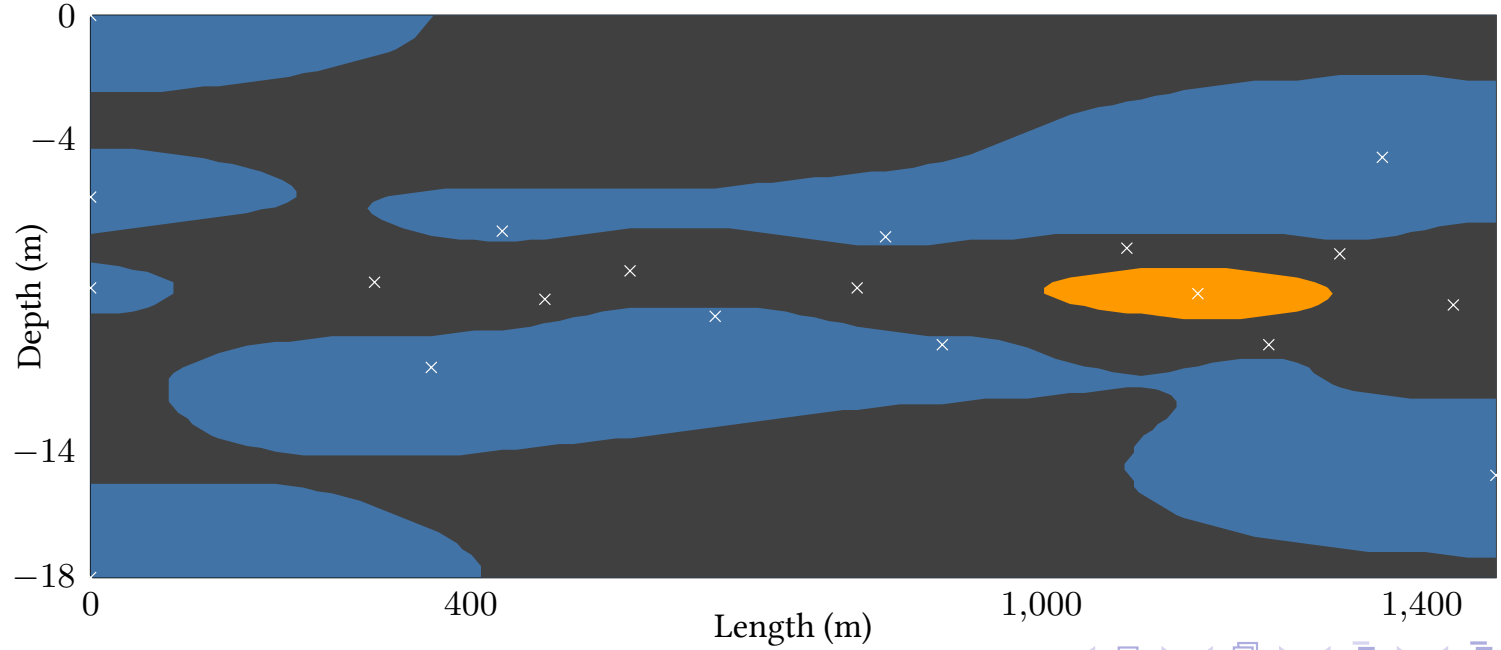
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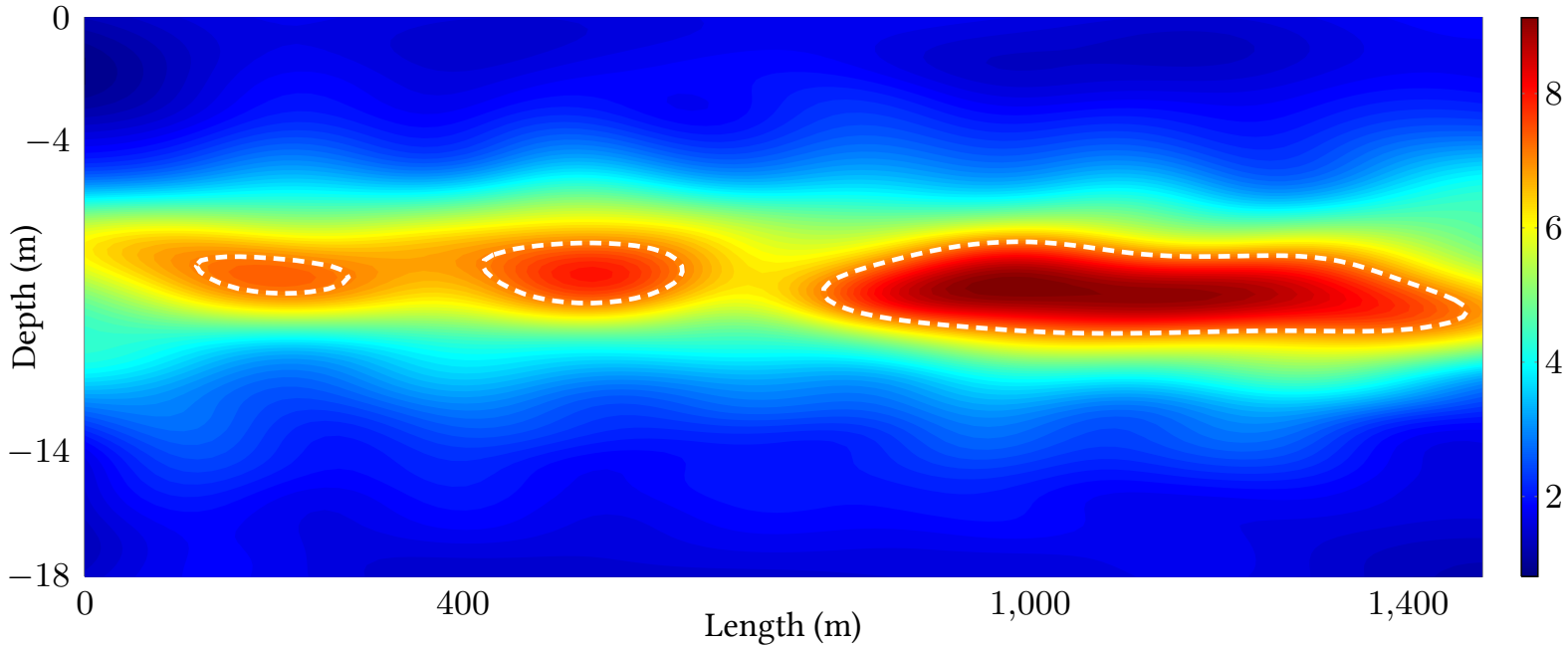
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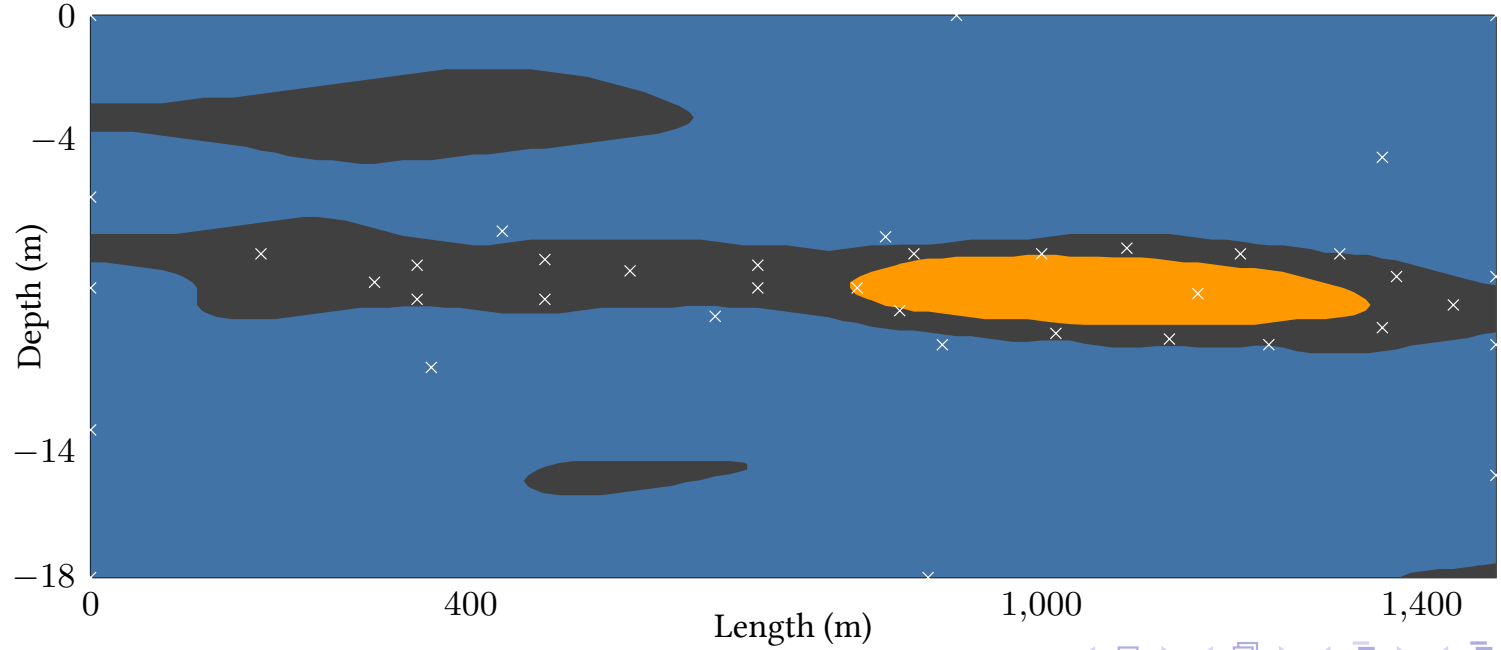
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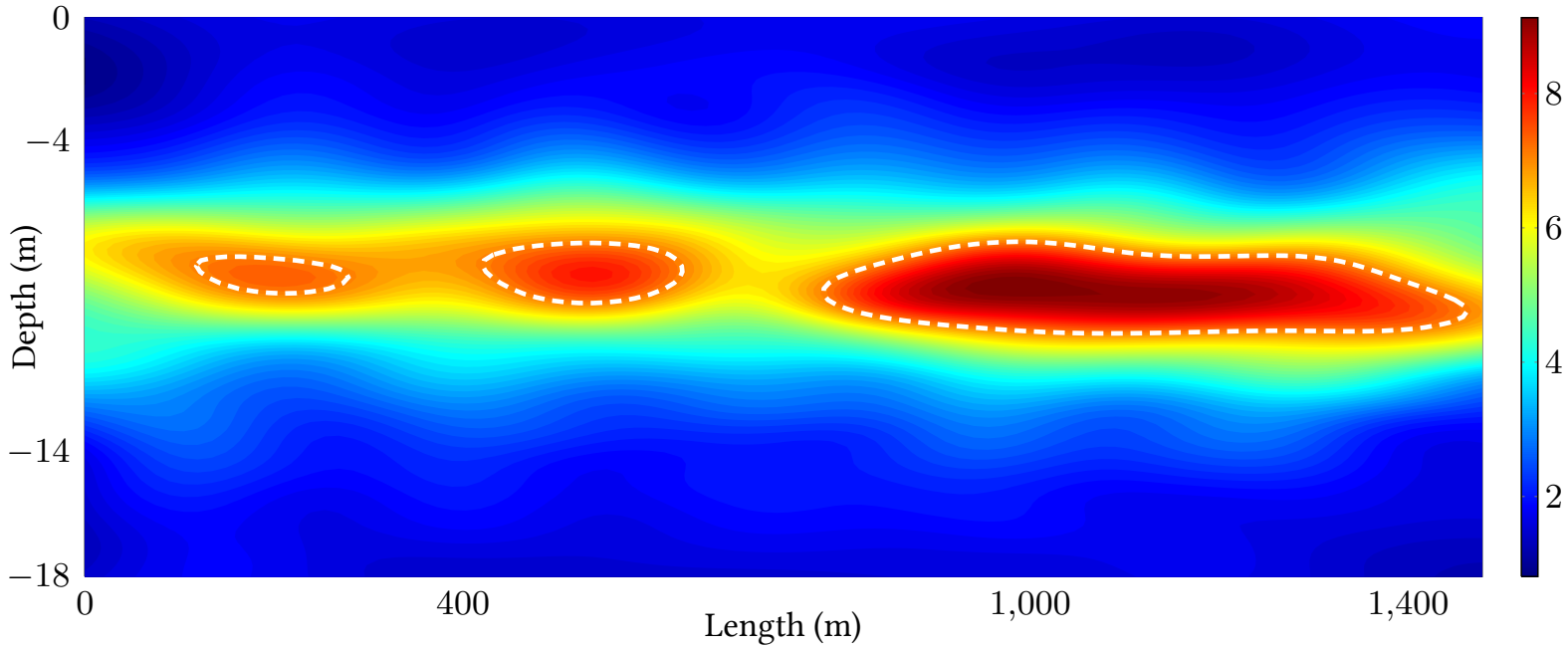
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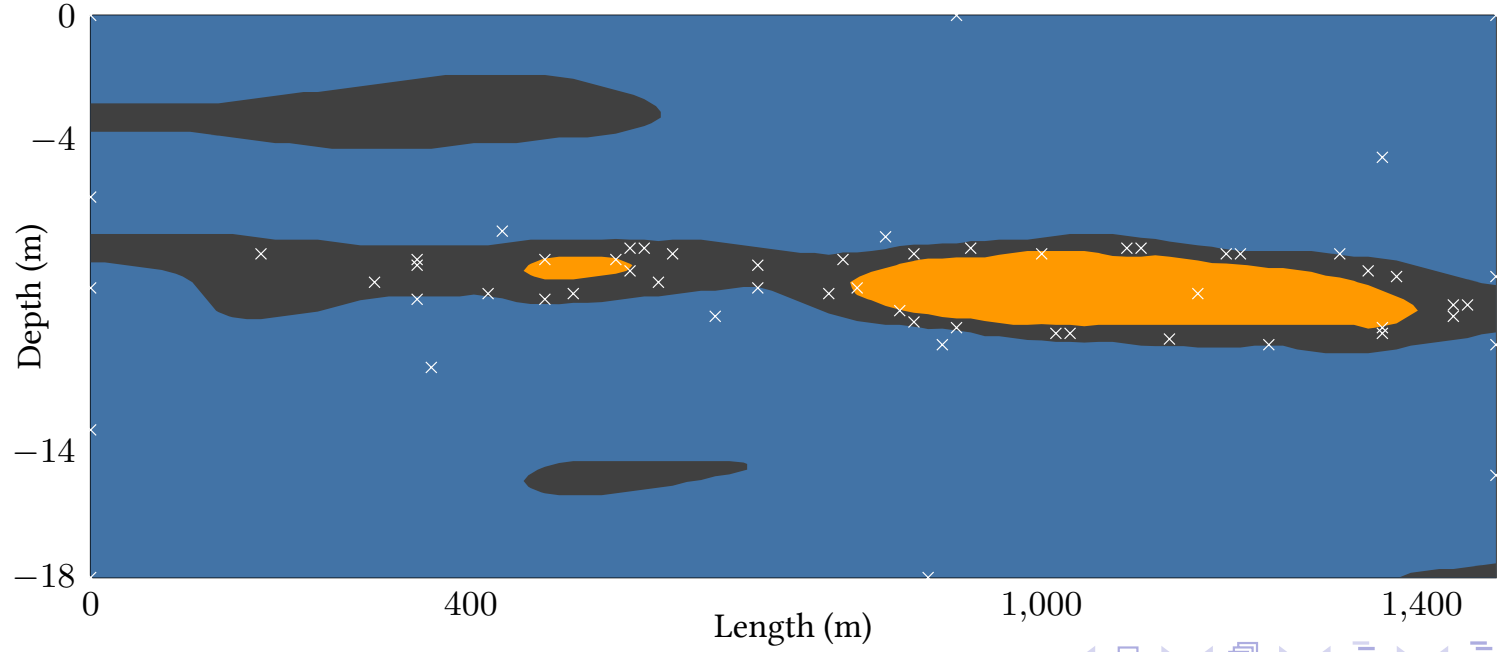
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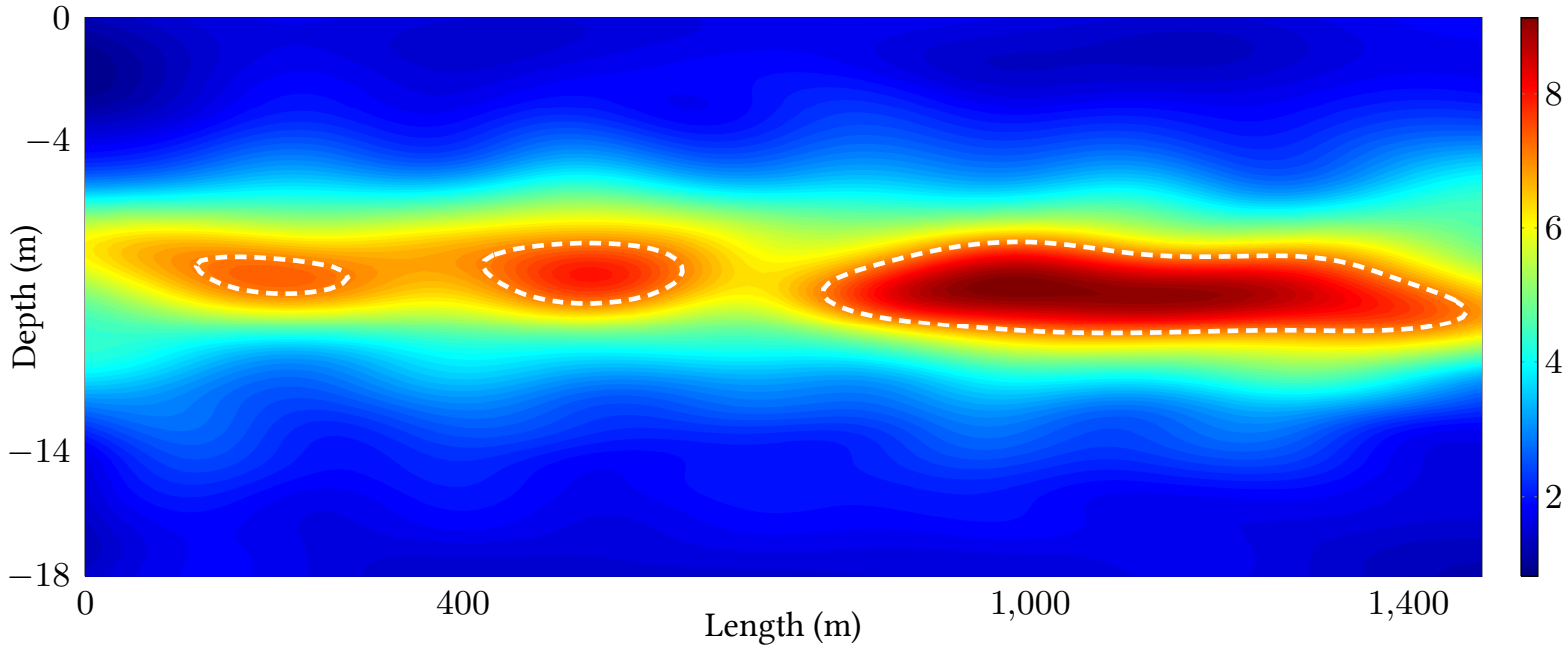
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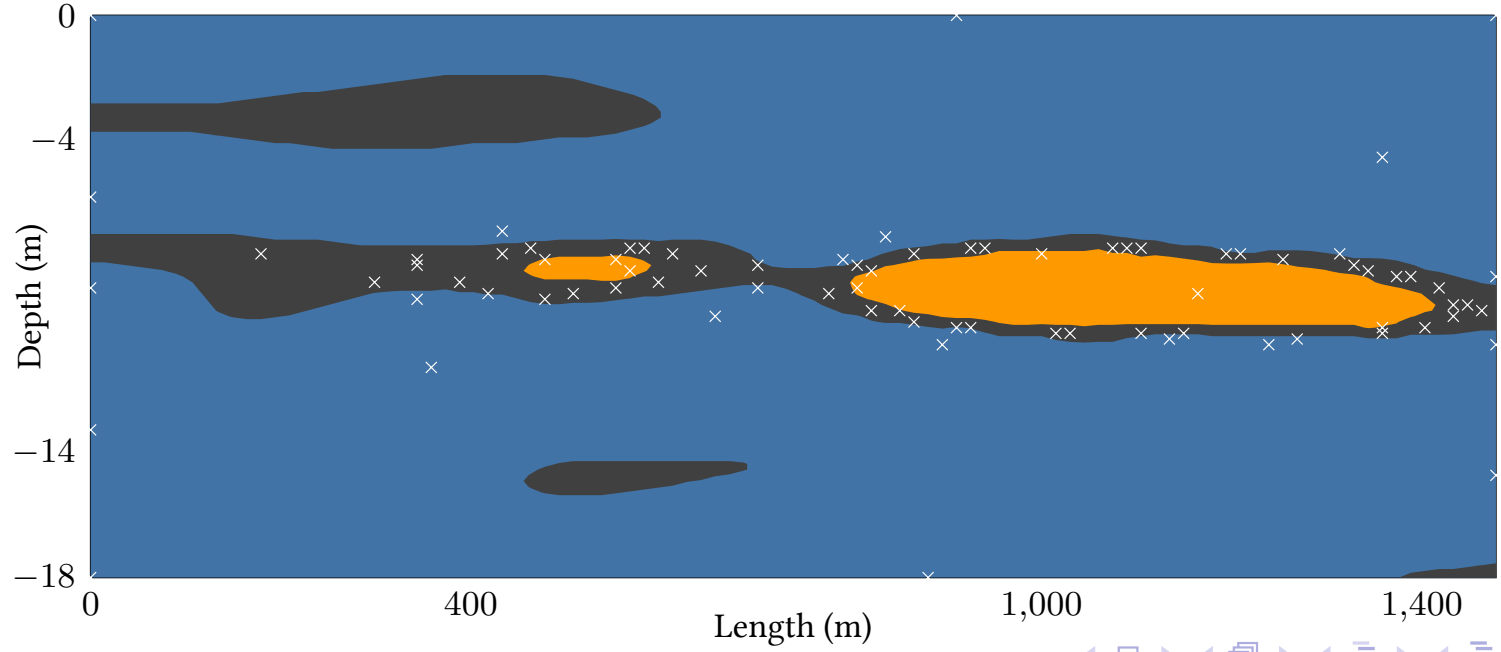
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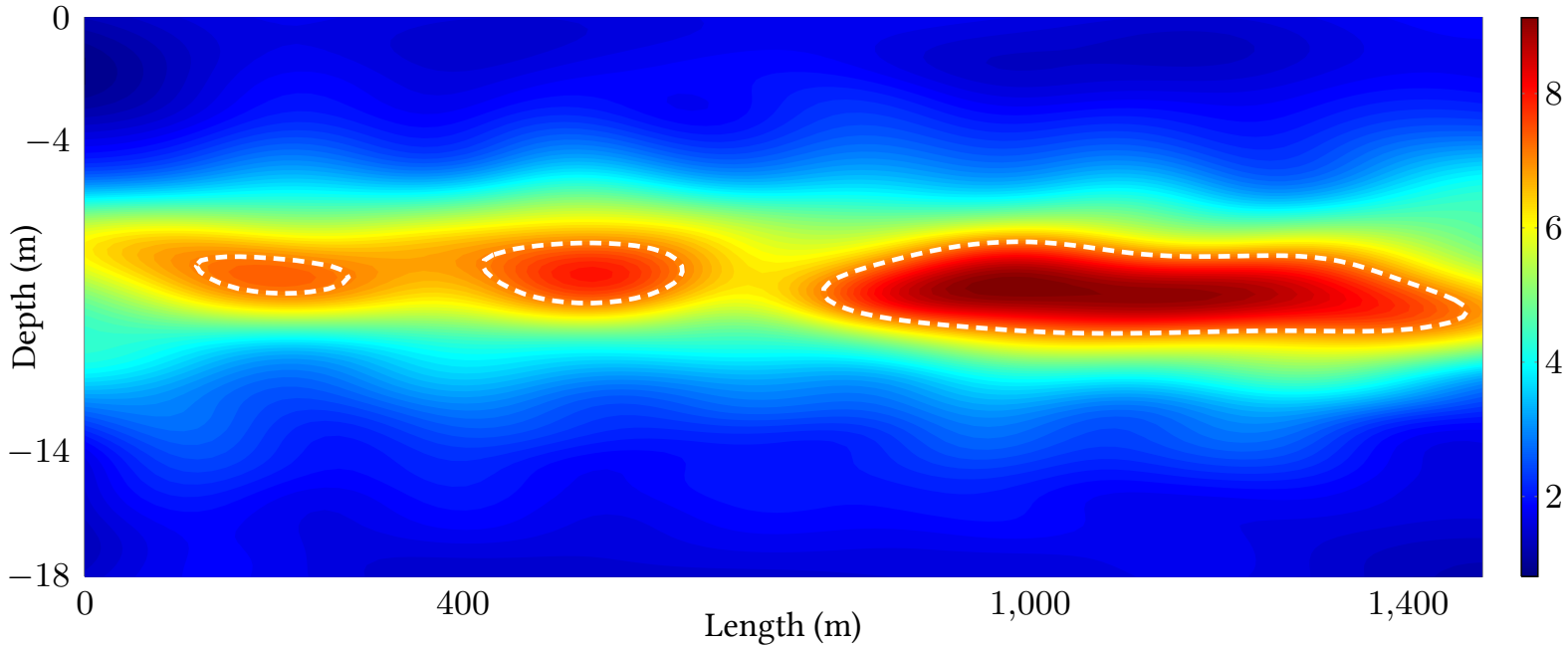
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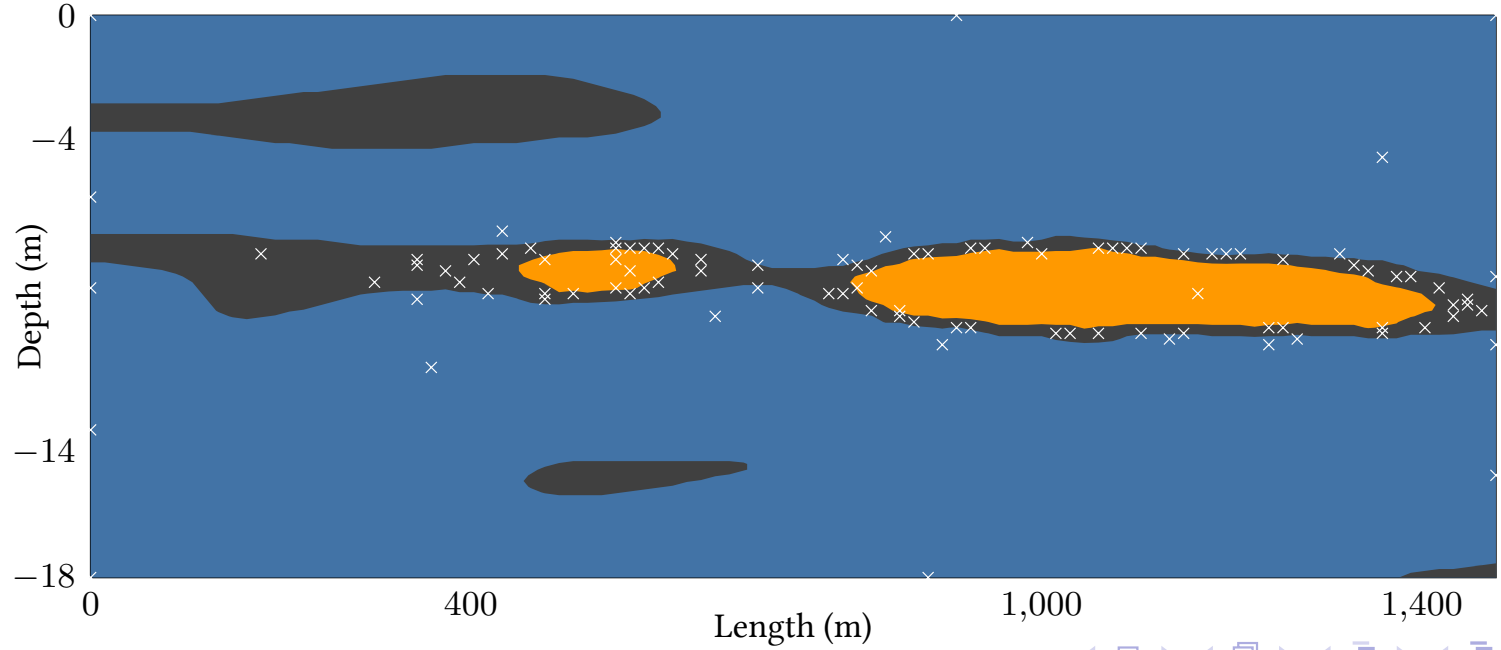
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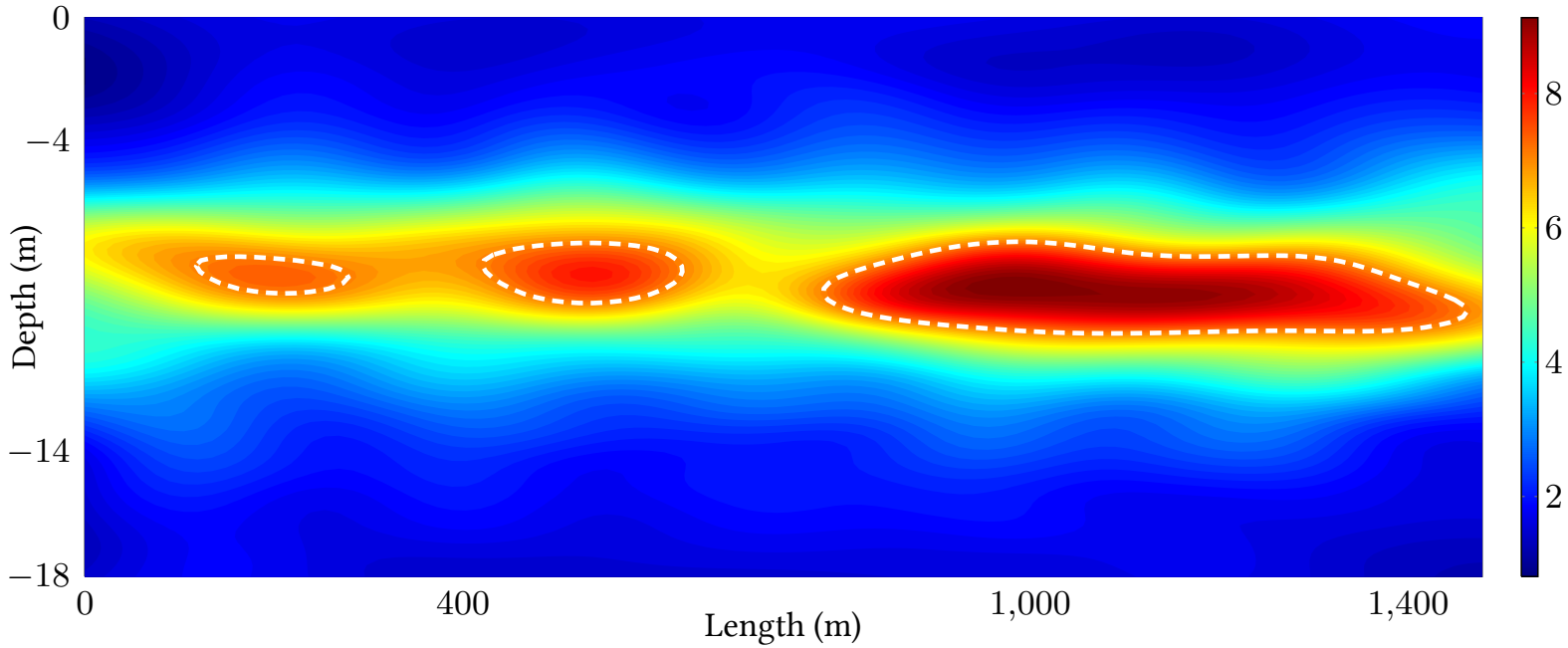
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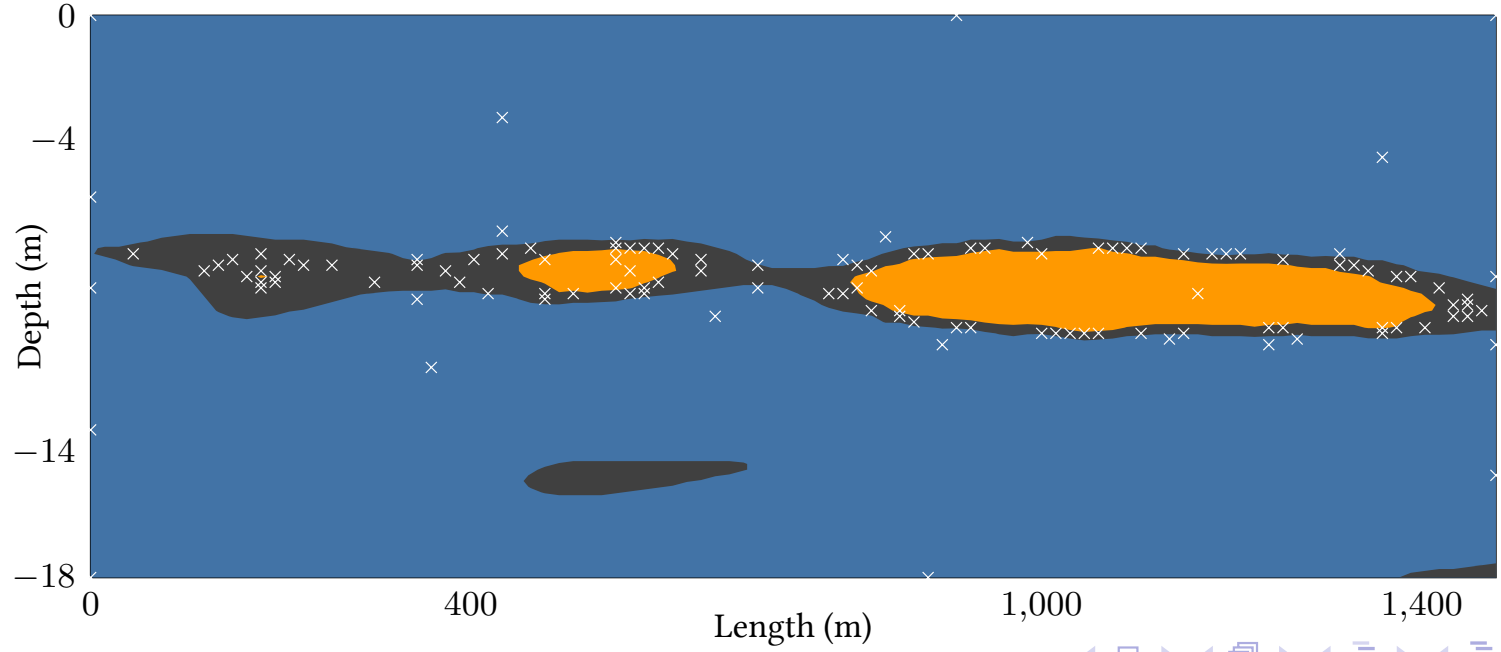
$t = 120$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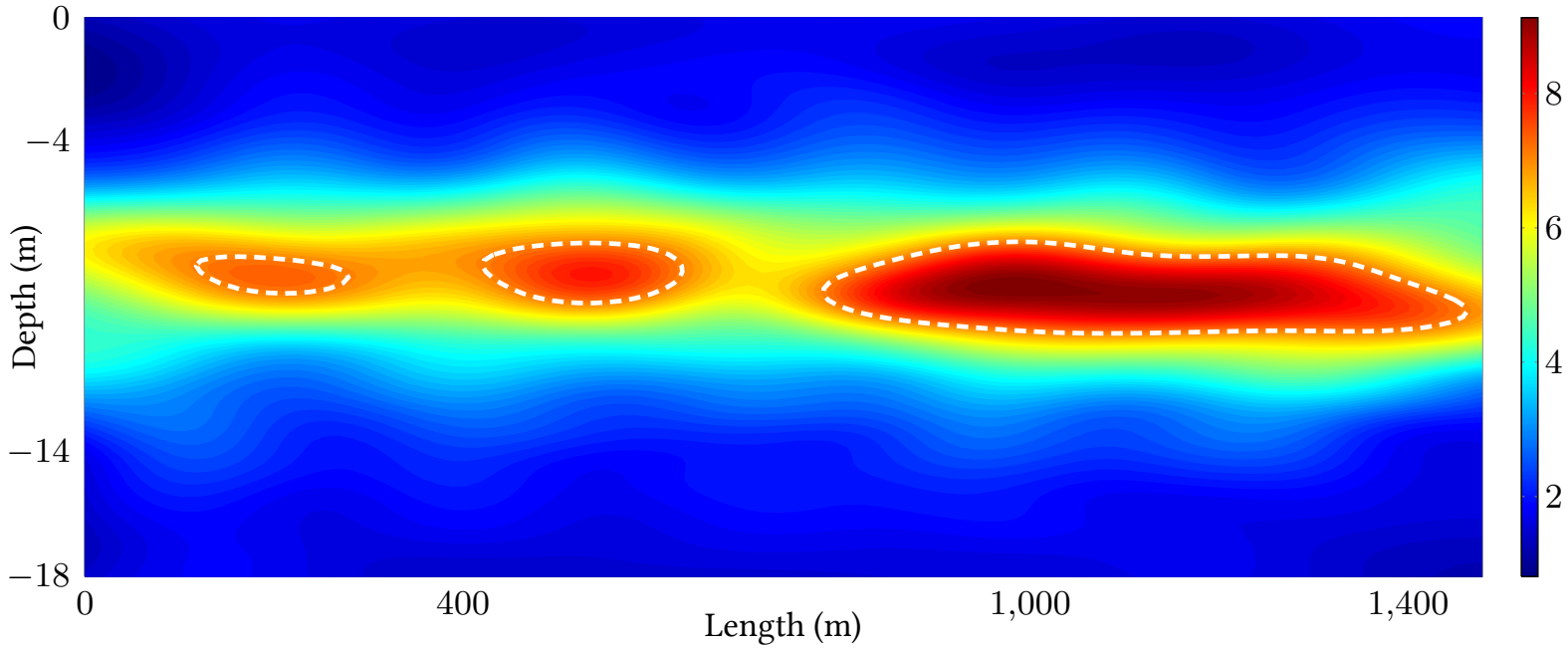
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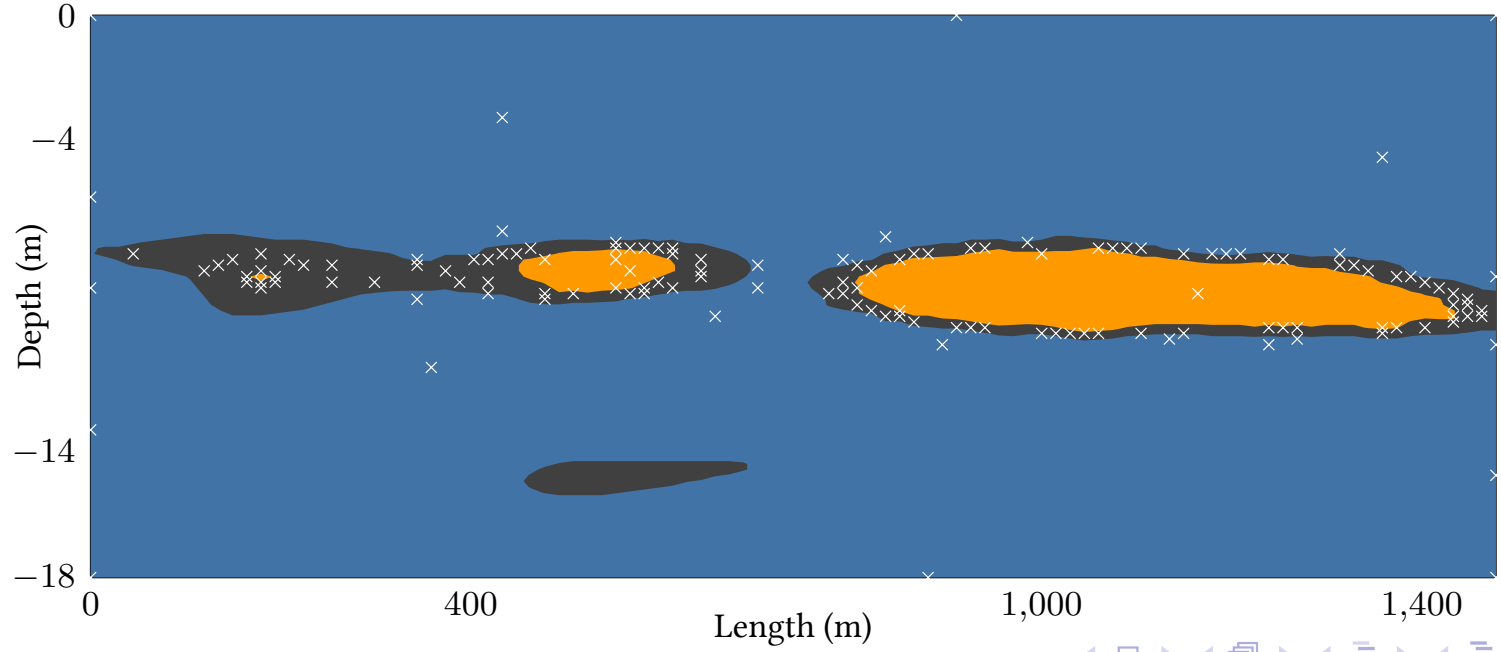
1,400
Length (m)
8
6
4
2

$t = 140$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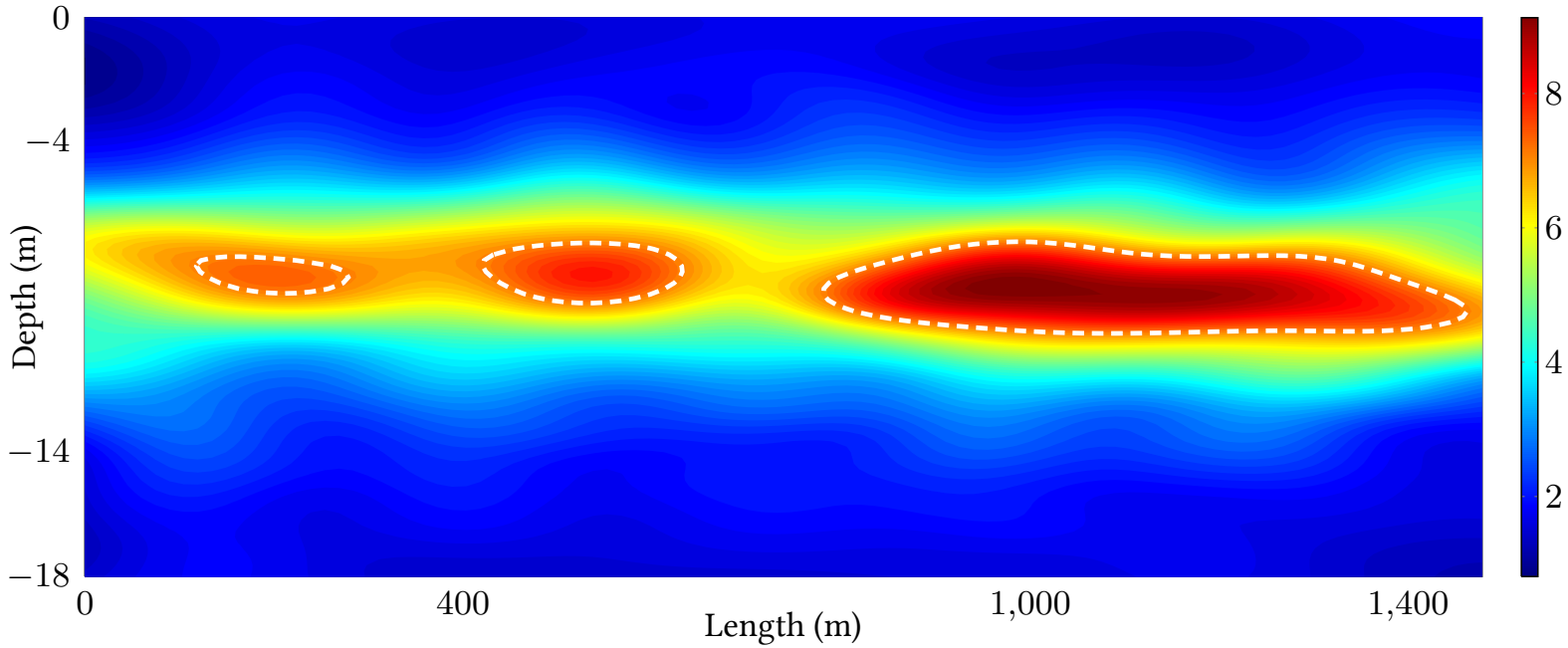
Length (m)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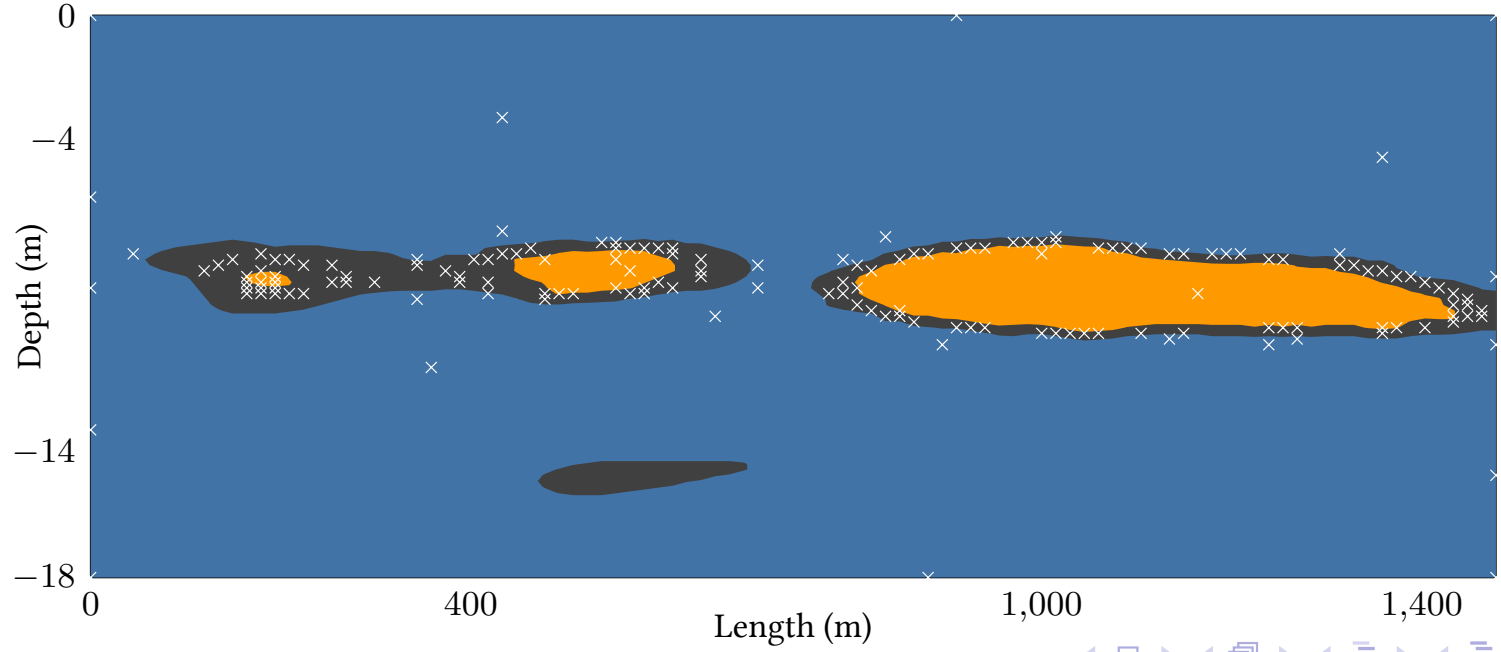
Length (m)
8
6
4
2

$t = 160$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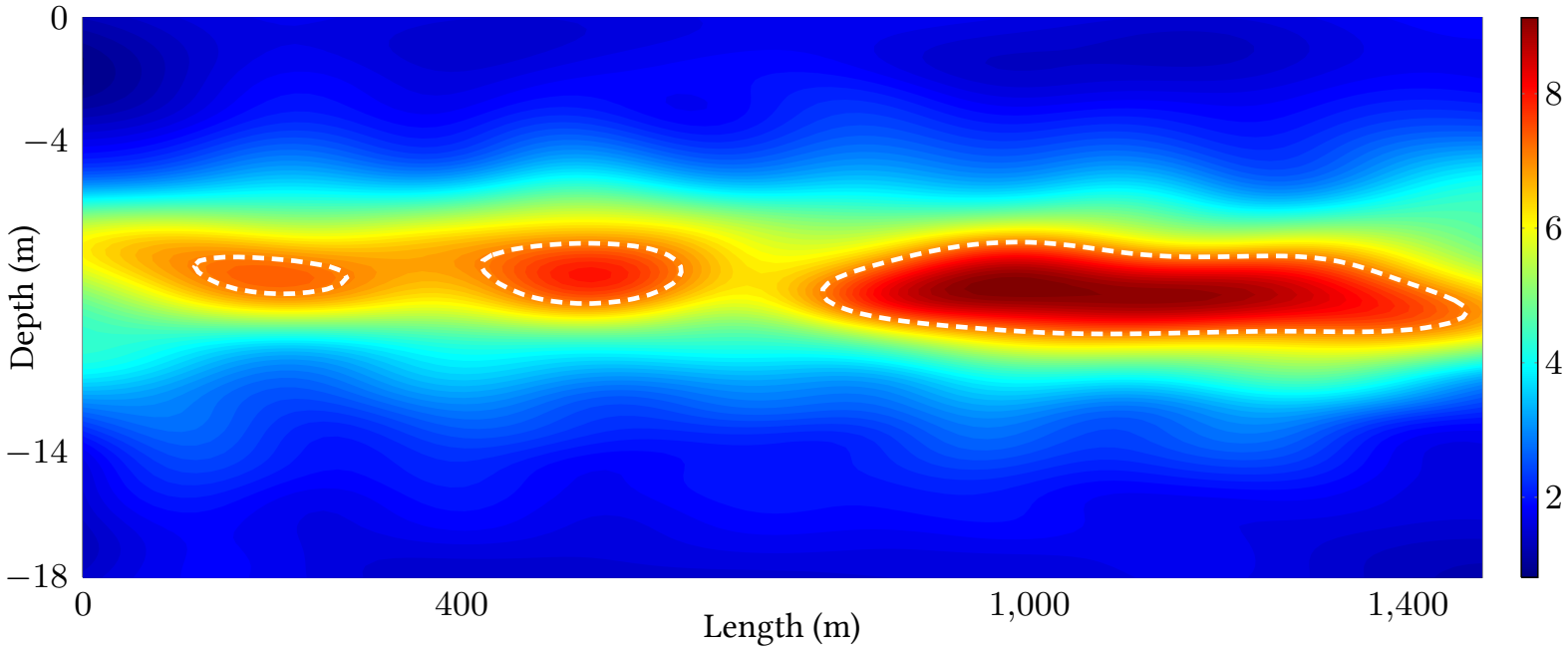
Length (m)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Length (m)
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6
4
2

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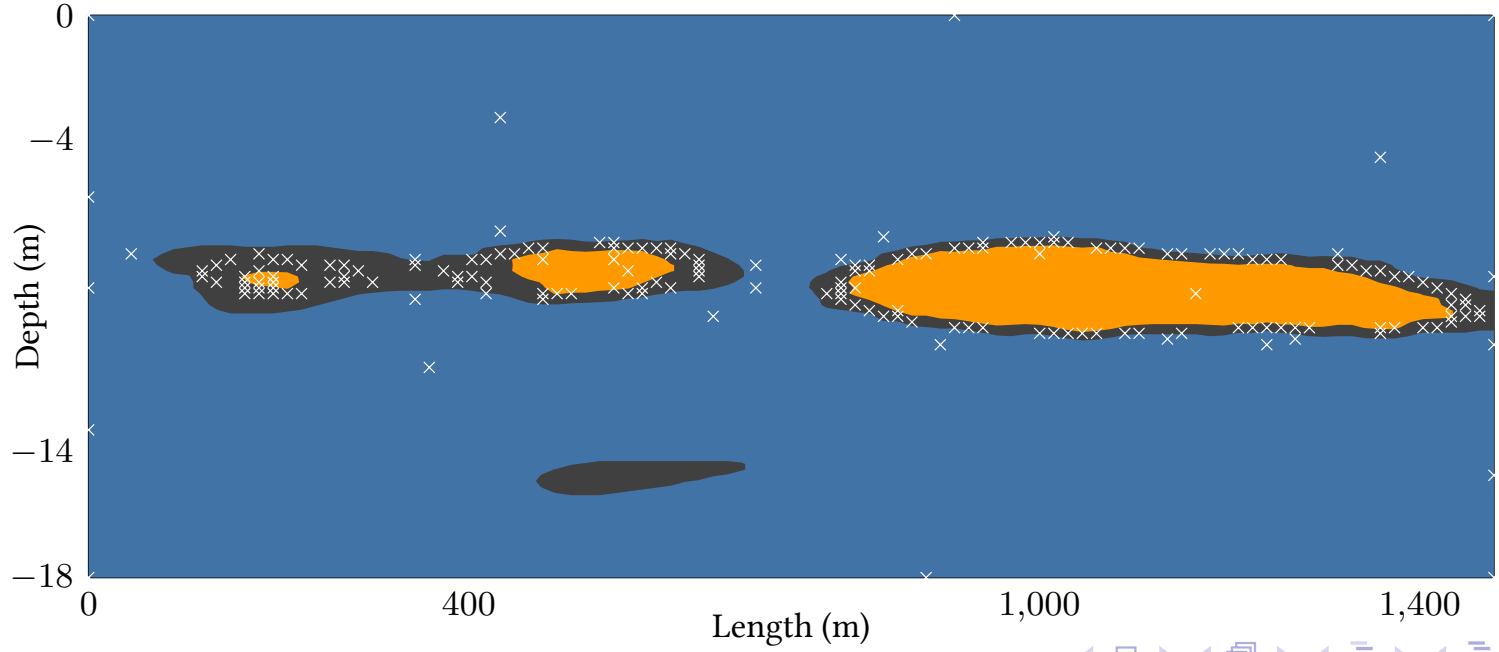
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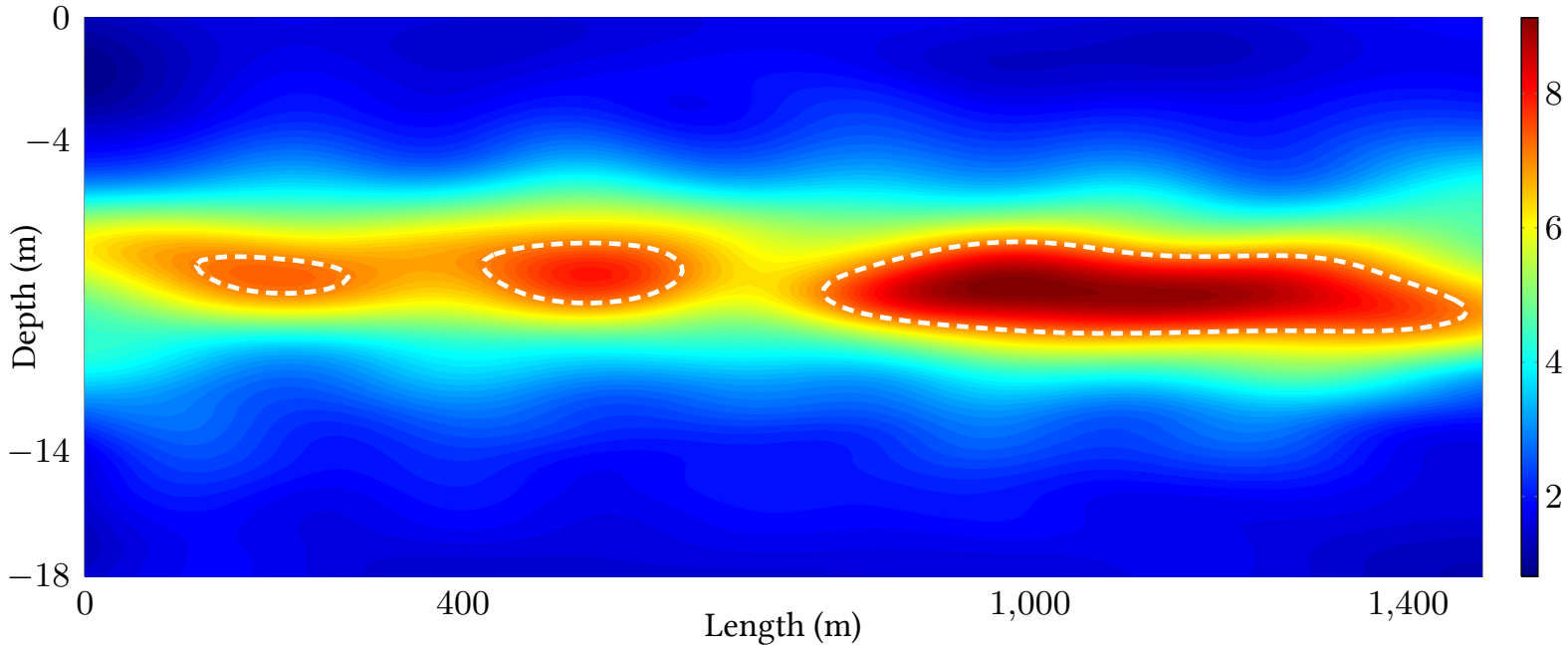
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400
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Length (m)
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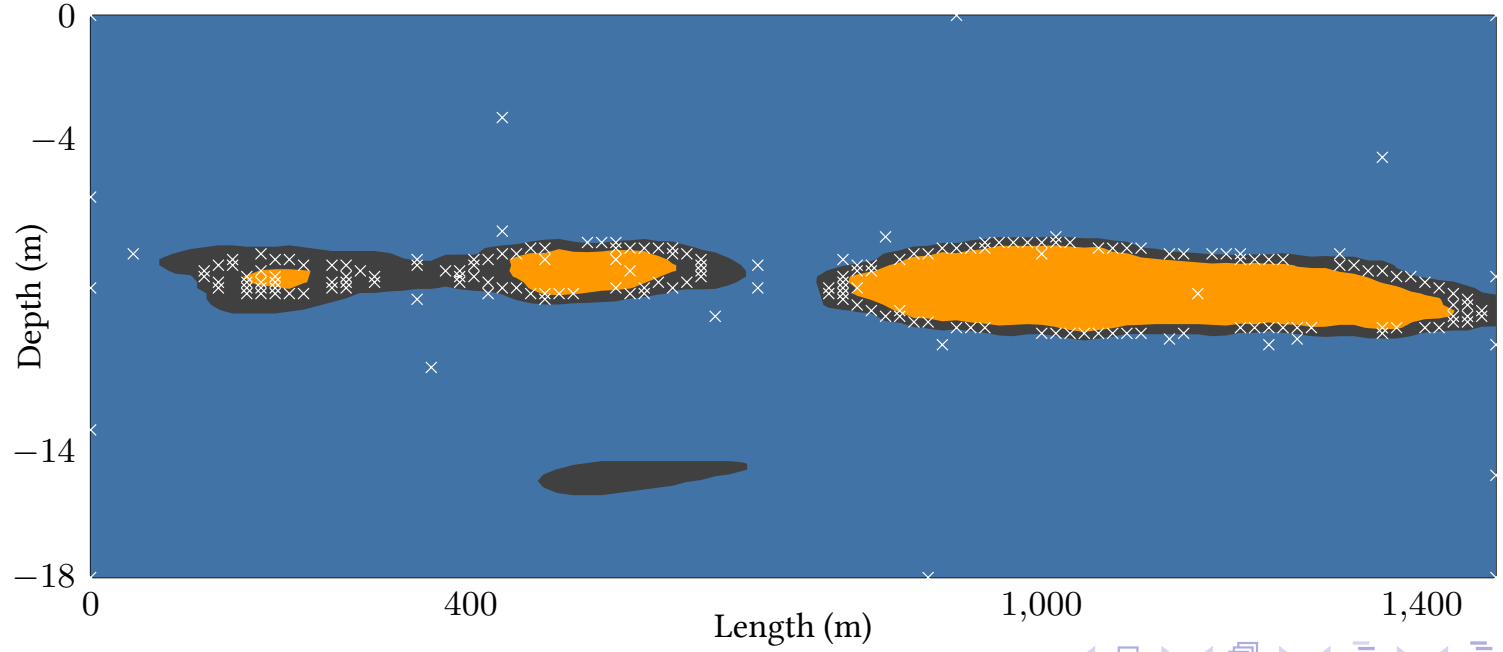
6
4
2

$t = 200$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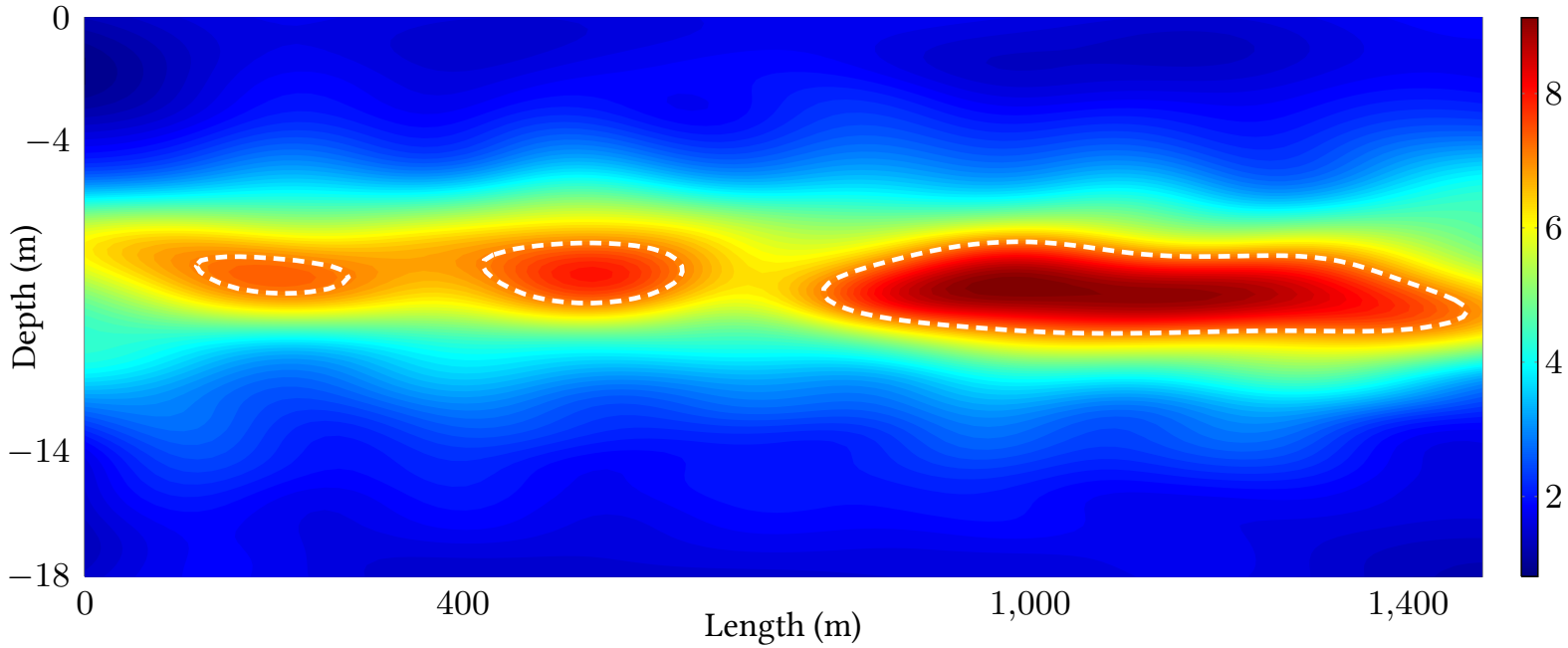
Length (m)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Depth (m)
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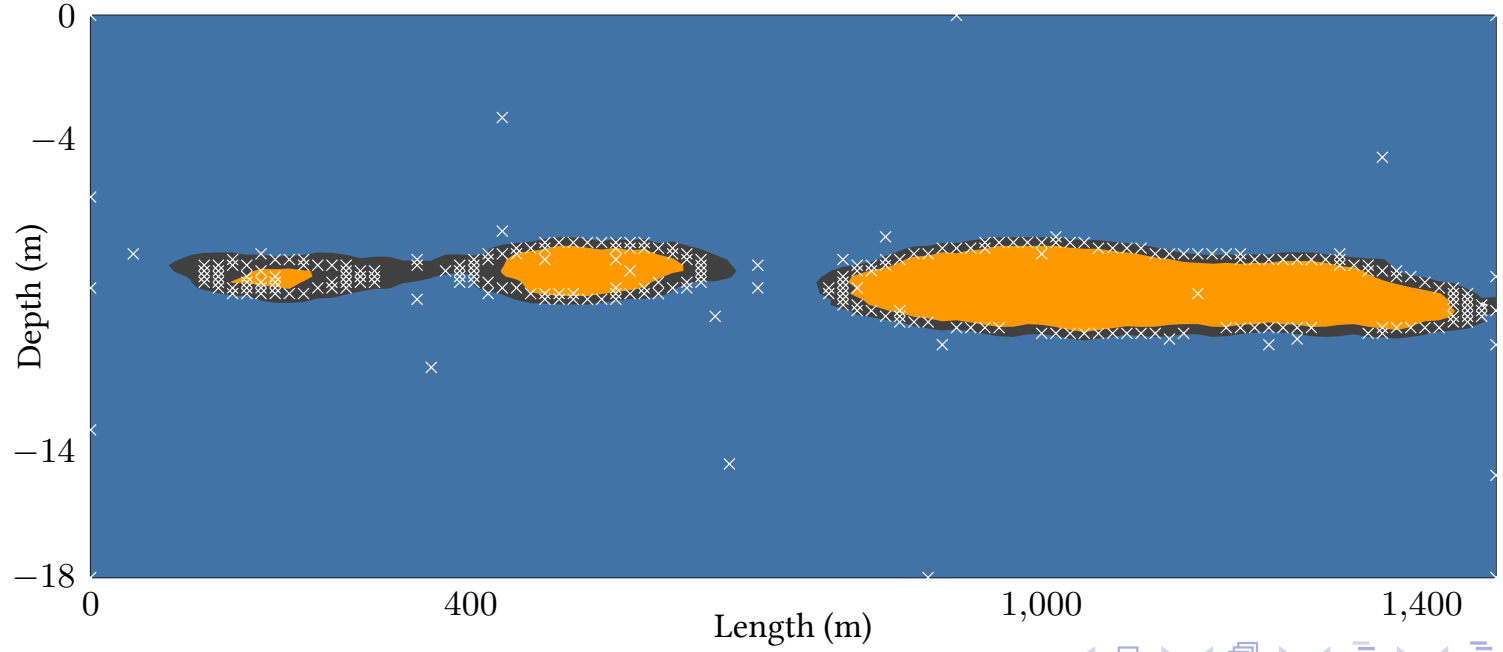
1,400
Length (m)
8
6
4
2

$t = 260$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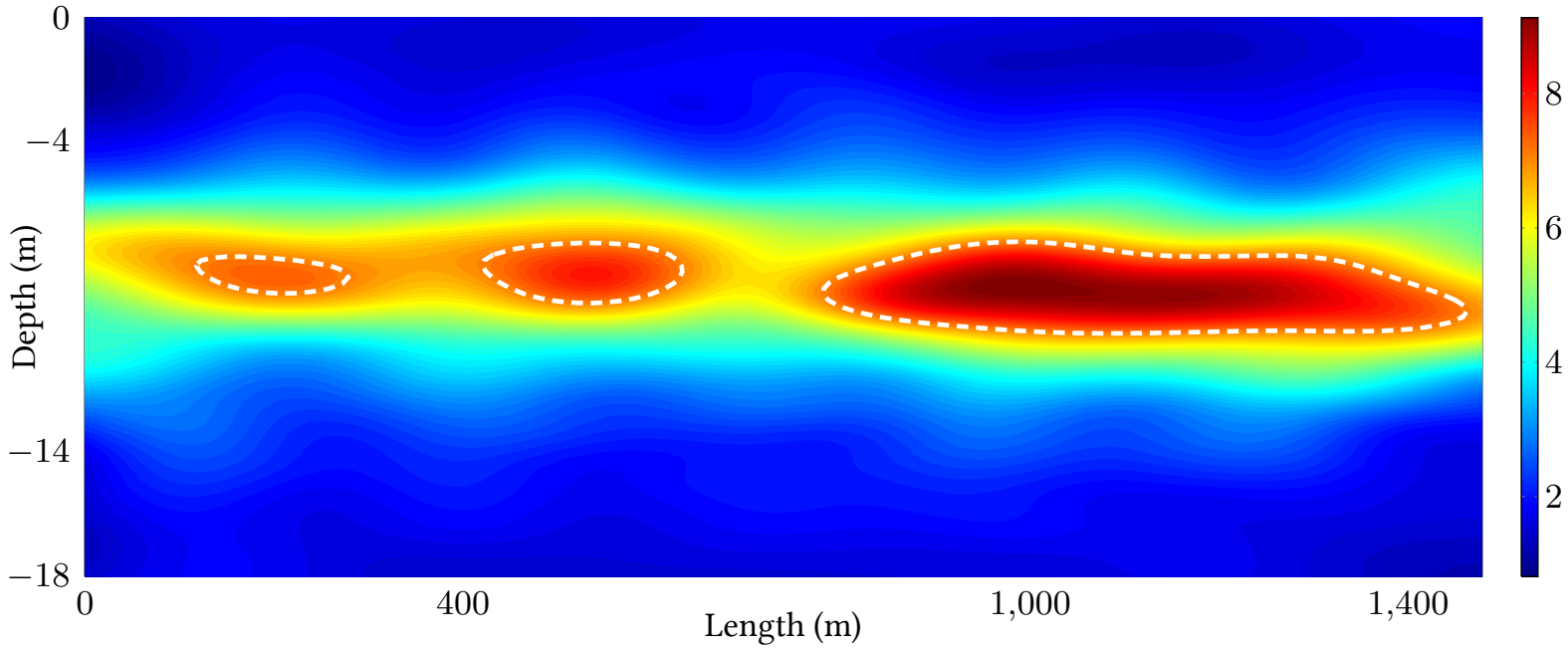
Length (m)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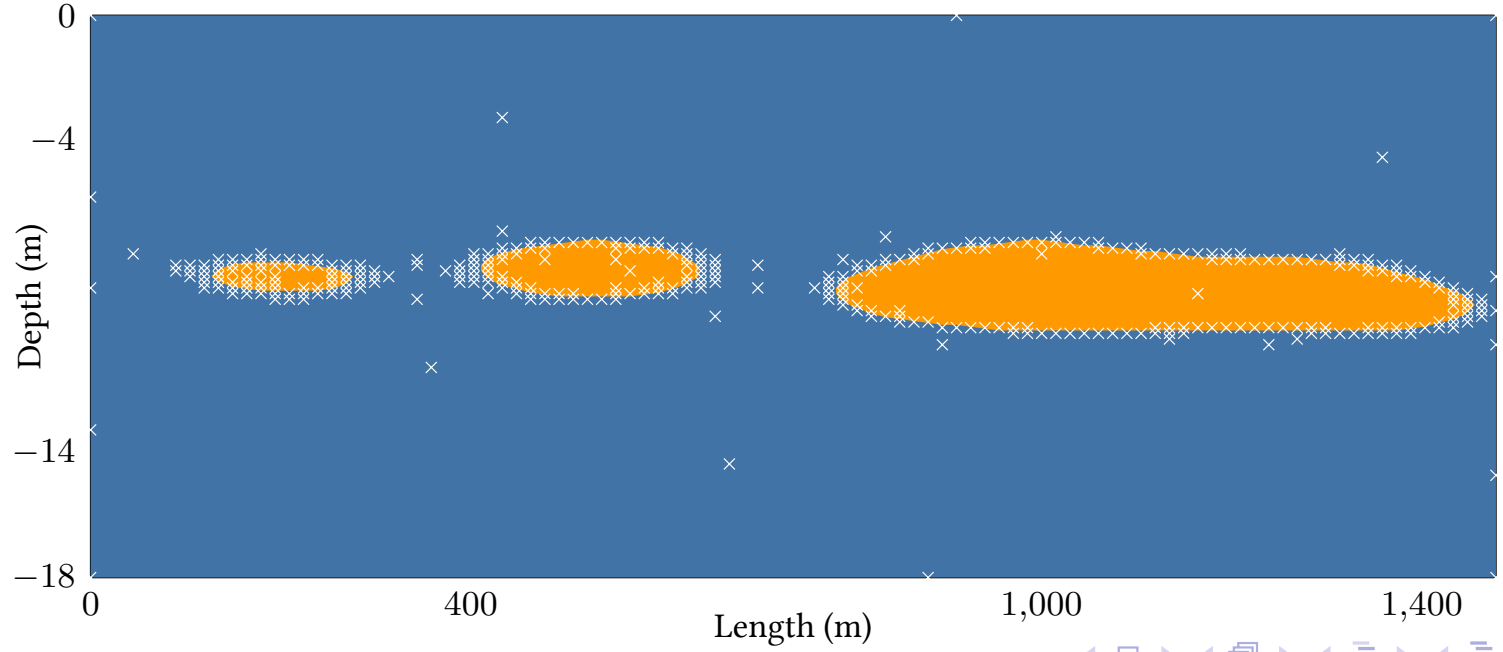
1,400
Length (m)
8
6
4
2

$t = 354$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−18
Depth (m)
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400
1,000
1,400
Length (m)

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

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

Theorem (Simplified)

If we choose β_t large enough, then:

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If we choose β_t large enough, then:

- *LSE terminates after a number of iterations T*
  1. *smoother kernel* $\Rightarrow T\downarrow$
  2. $\sigma\uparrow \Rightarrow T\uparrow$
  3. $\epsilon\uparrow \Rightarrow T\downarrow$

Theorem (Simplified)

If we choose β_t large enough, then:

- *LSE terminates after a number of iterations T*
  1. *smoother kernel* $\Rightarrow T\downarrow$
  2. $\sigma\uparrow \Rightarrow T\uparrow$
  3. $\epsilon\uparrow \Rightarrow T\downarrow$
- *The solution returned is ϵ-accurate with high probability*

Theorem (Simplified)

If we choose β_t large enough, then:

- *LSE terminates after a number of iterations T*
  1. *smoother kernel* $\Rightarrow T\downarrow$
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  3. $\epsilon\uparrow \Rightarrow T\downarrow$
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Experiments

1. LSE

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2. Maximum variance sampling:

$$\boldsymbol{x}_t = \underset{\boldsymbol{x} \in D}{\operatorname{argmax}}\, \sigma_{t-1}(\boldsymbol{x})$$

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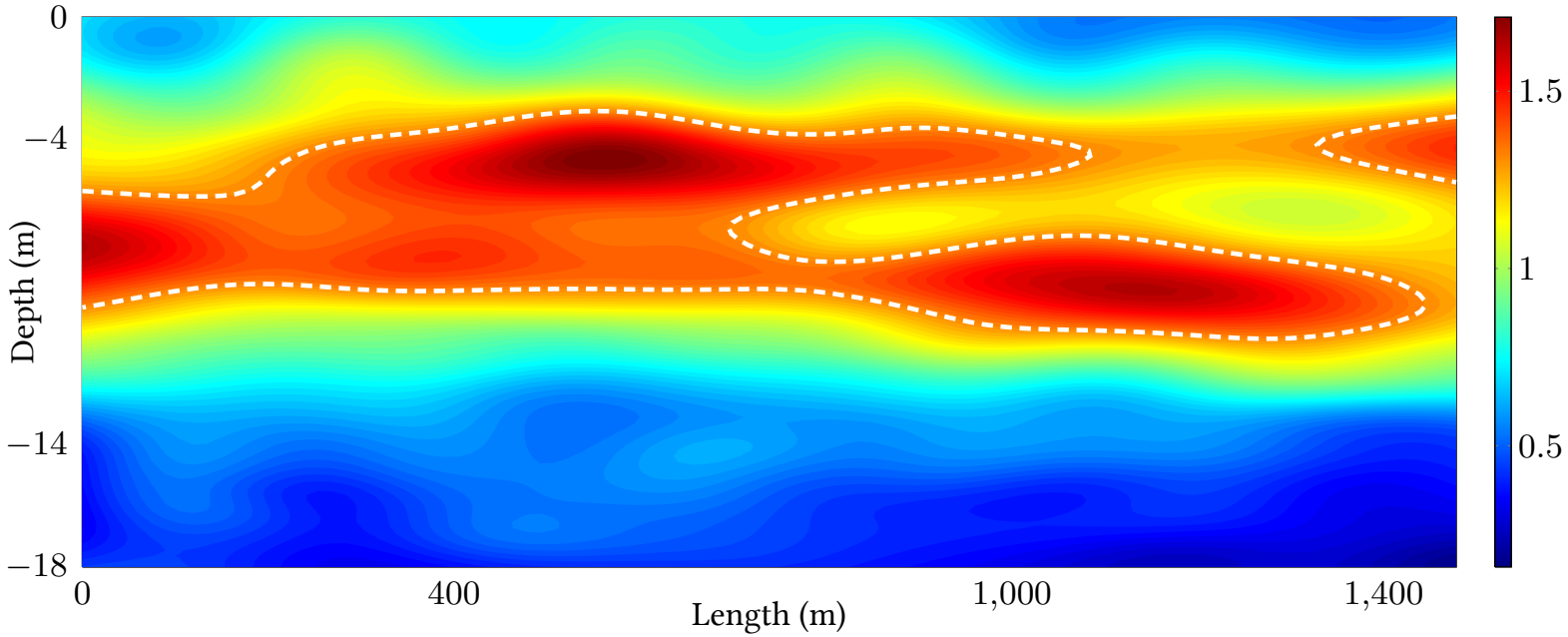
2. Maximum variance sampling:

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

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

$$\boldsymbol{x}_t \approx \operatorname*{argmax}_{\boldsymbol{x} \in D} a_{t-1}(\boldsymbol{x}) \qquad \text{(for } \beta_t^{1/2} = 1.96\text{)}$$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Length (m)
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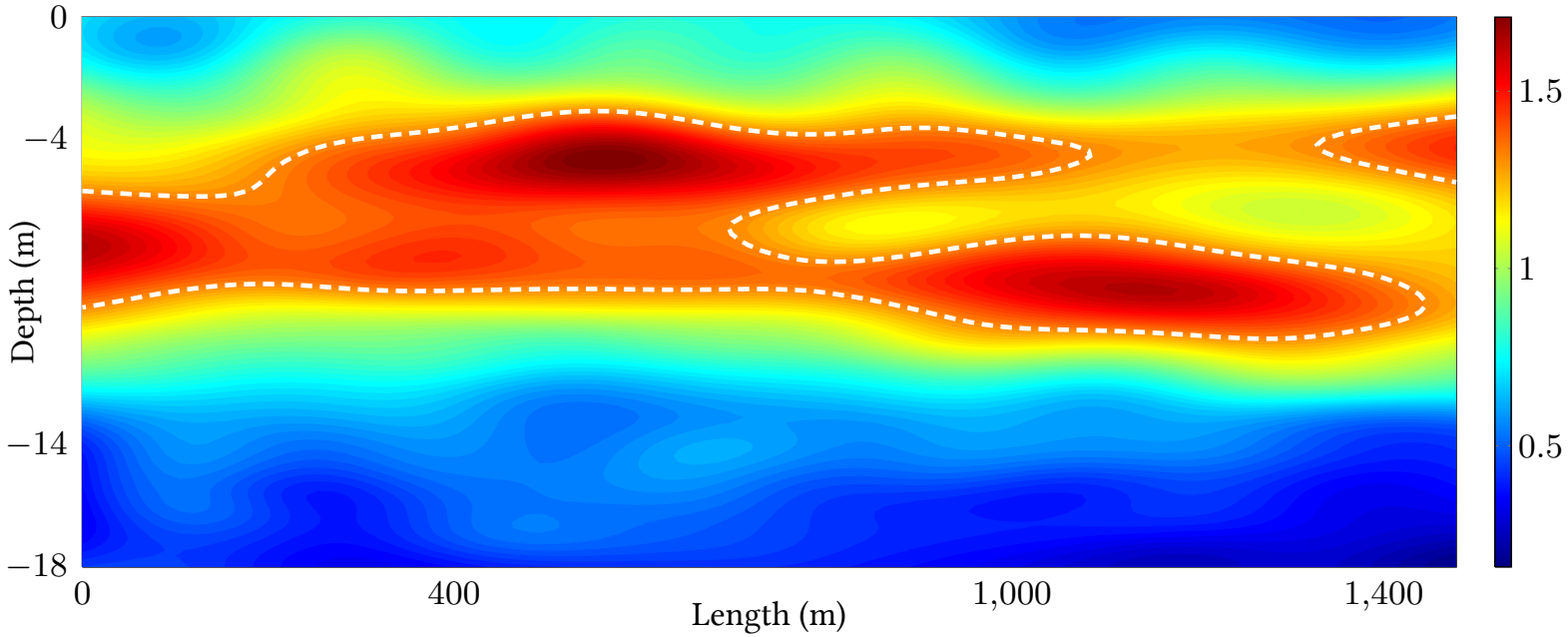
0.5


0
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Depth (m)
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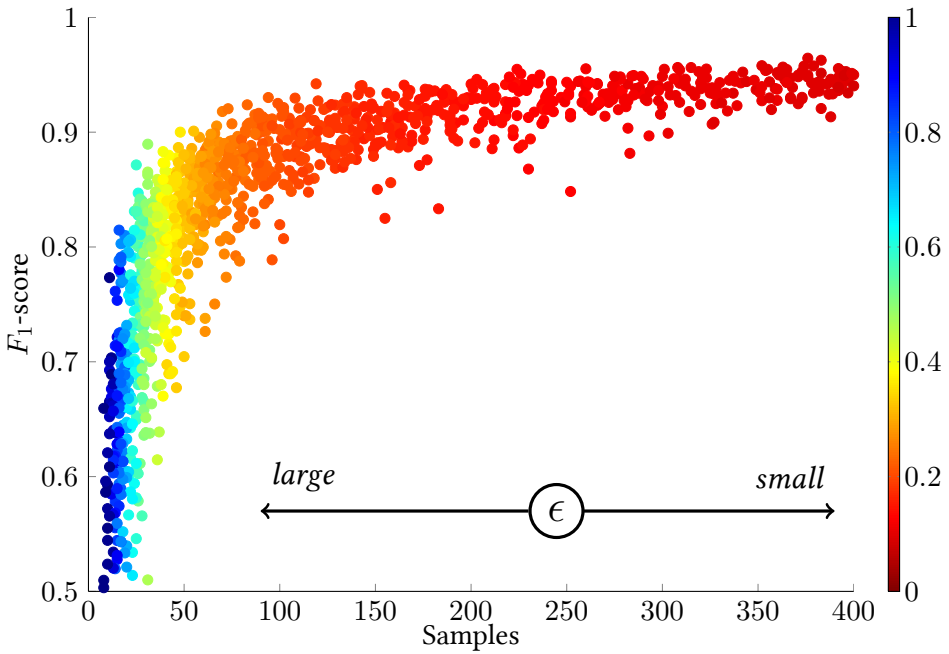
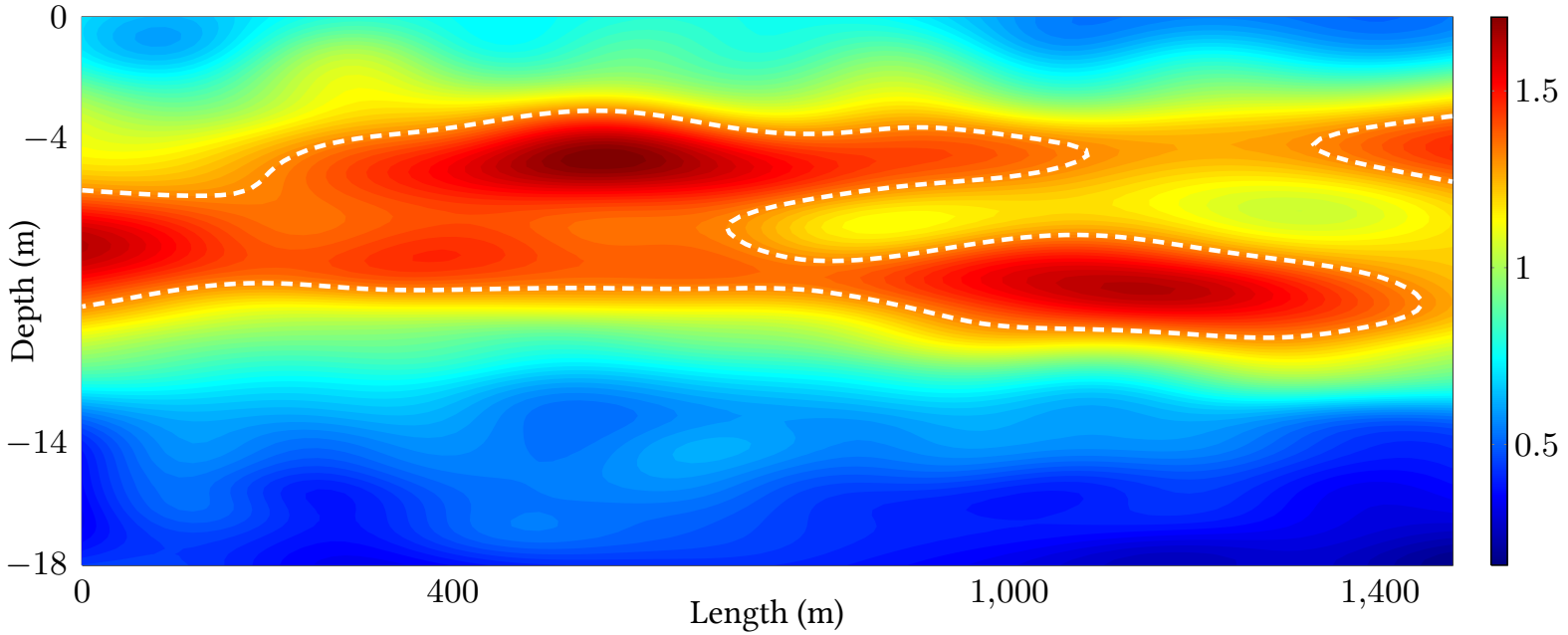
Length (m)
1.5
1
0.5


1
0.9
0.8
0.7
0.6
0.5
F_1-score
0
50
100
150
200
250
300
350
400
Samples
large
small
ϵ
1
0.8
0.6
0.4
0.2
0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Depth (m)
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400
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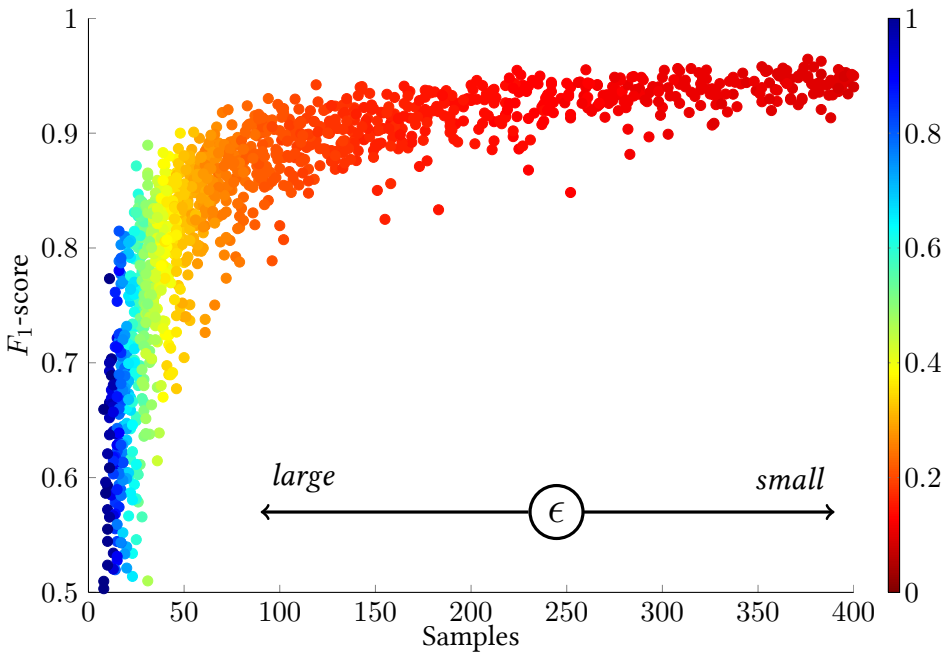
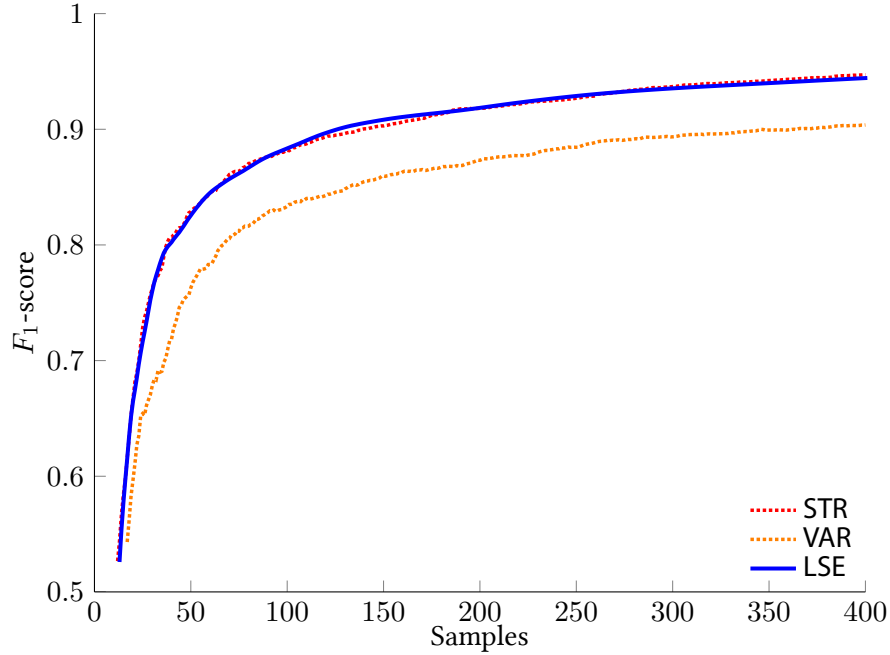
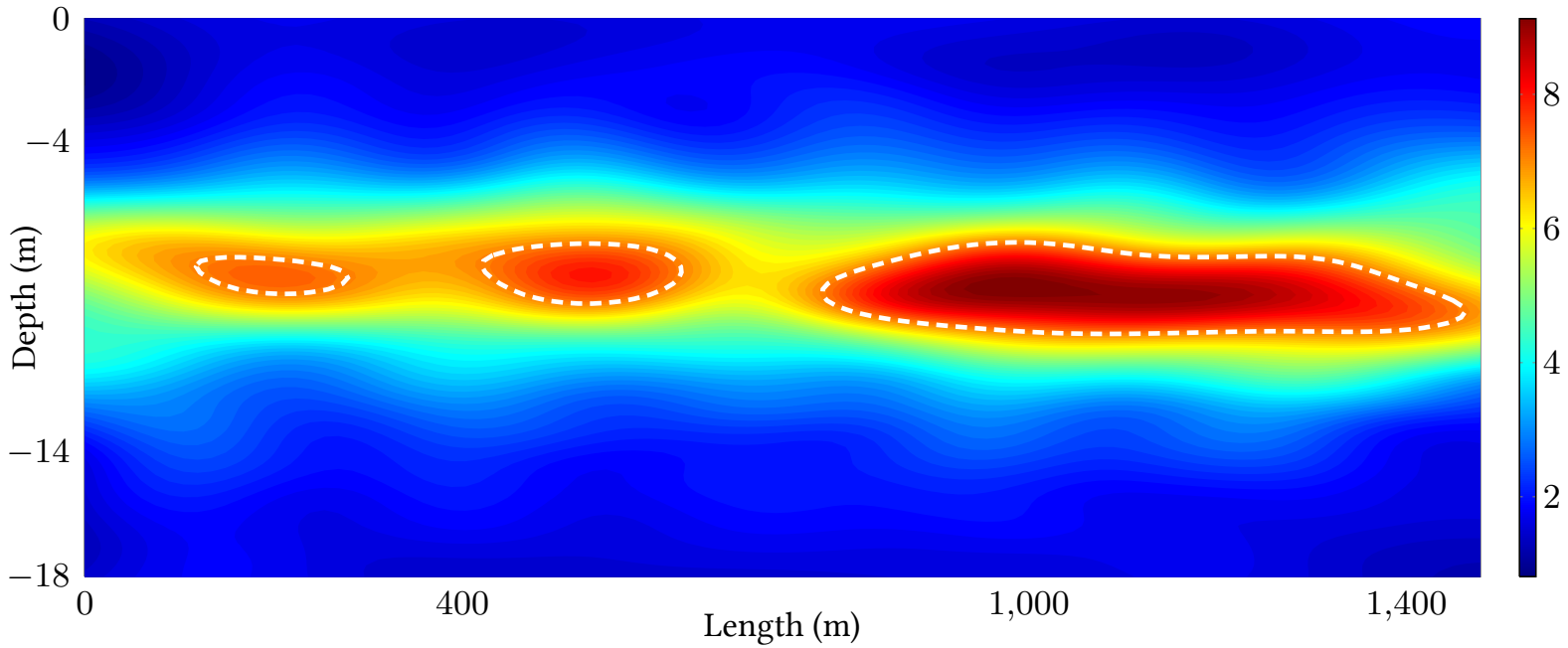
1,400
Length (m)
1.5
1
0.5


1
0.9
0.8
0.7
0.6
0.5
F_1-score
0
50
100
150
200
250
300
350
400
Samples
large
small
ϵ
1
0.8
0.6
0.4
0.2
0


1
0.9
0.8
0.7
0.6
0.5
F_1-score
0
50
100
150
200
250
300
350
400
Samples
STR
VAR
LSE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−14
−18
Depth (m)
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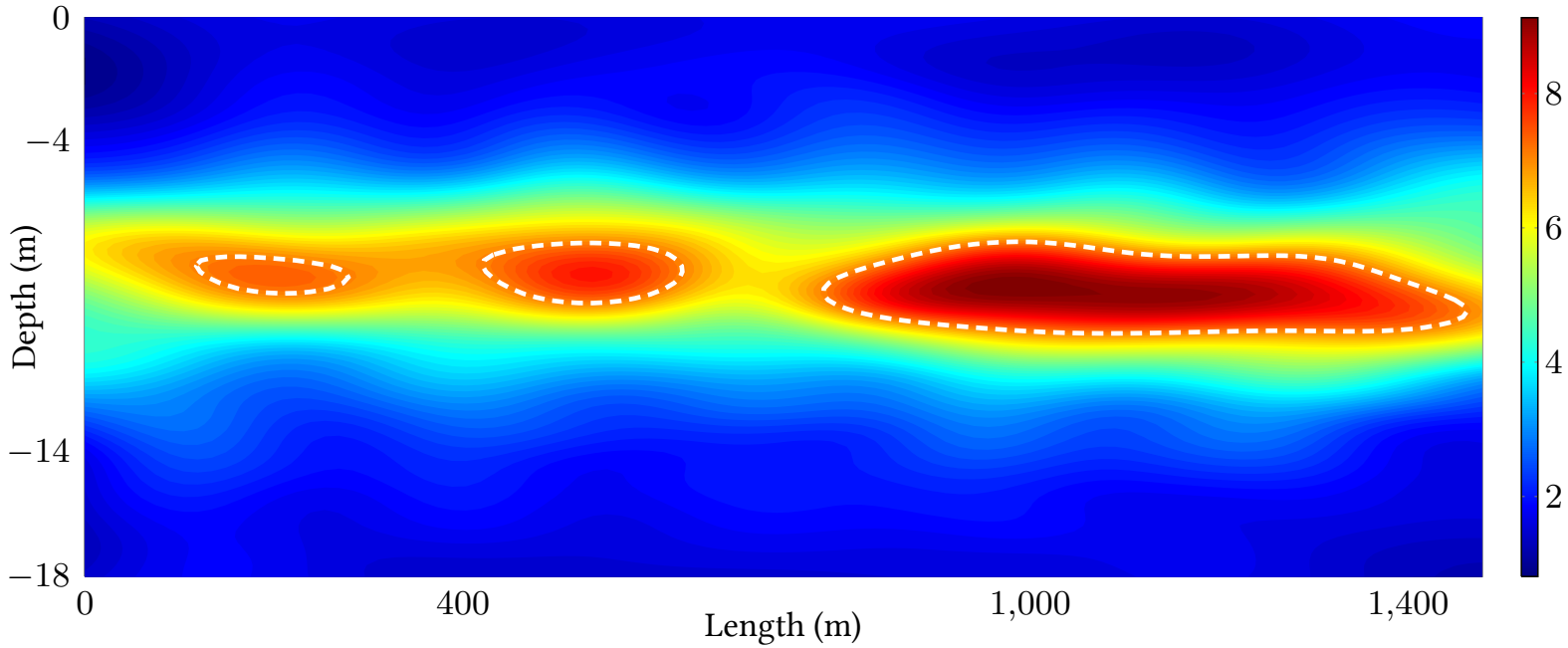
1,000
1,400
Length (m)
8
6
4
2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Depth (m)
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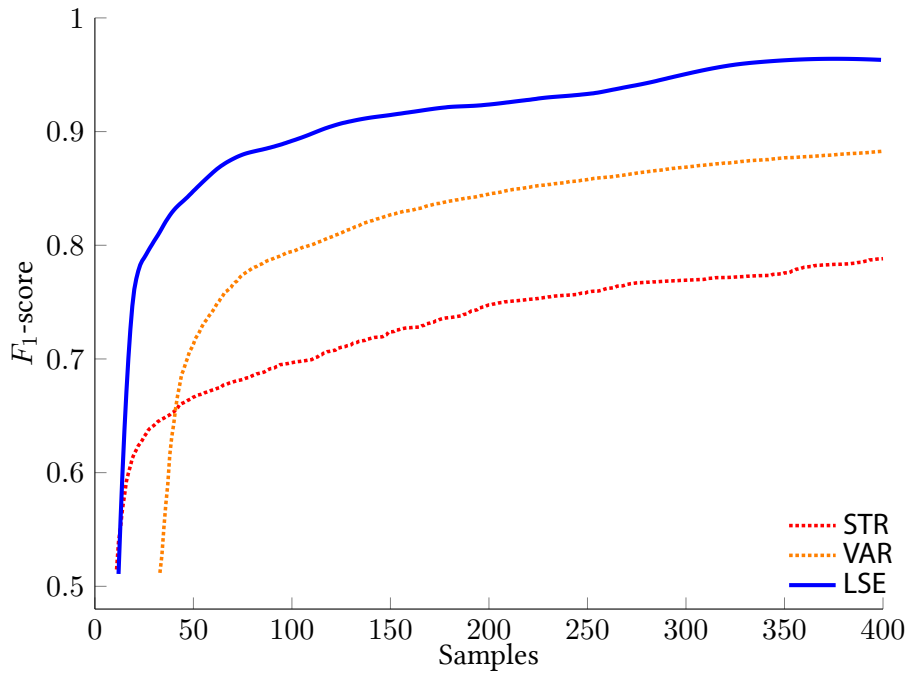
Length (m)
8
6
4
2


1
0.9
0.8
0.7
0.6
0.5
F_1-score
0
50
100
150
200
250
300
350
400
Samples
STR
VAR
LSE

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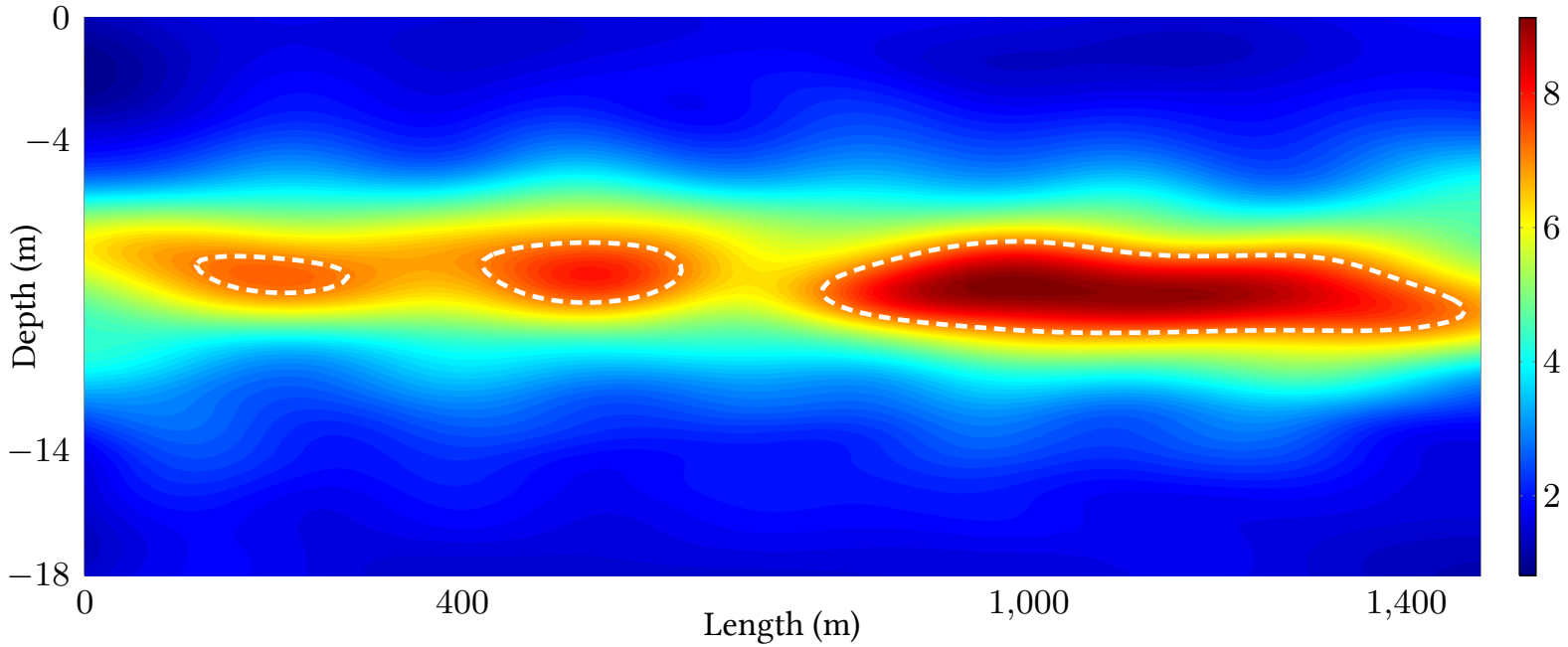
- LSE_{imp} algorithm:
  - Need to accurately estimate the maximum $\rightarrow$ modified selection rule
  - h is now an estimated quantity $\rightarrow$ modified classification rules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Length (m)
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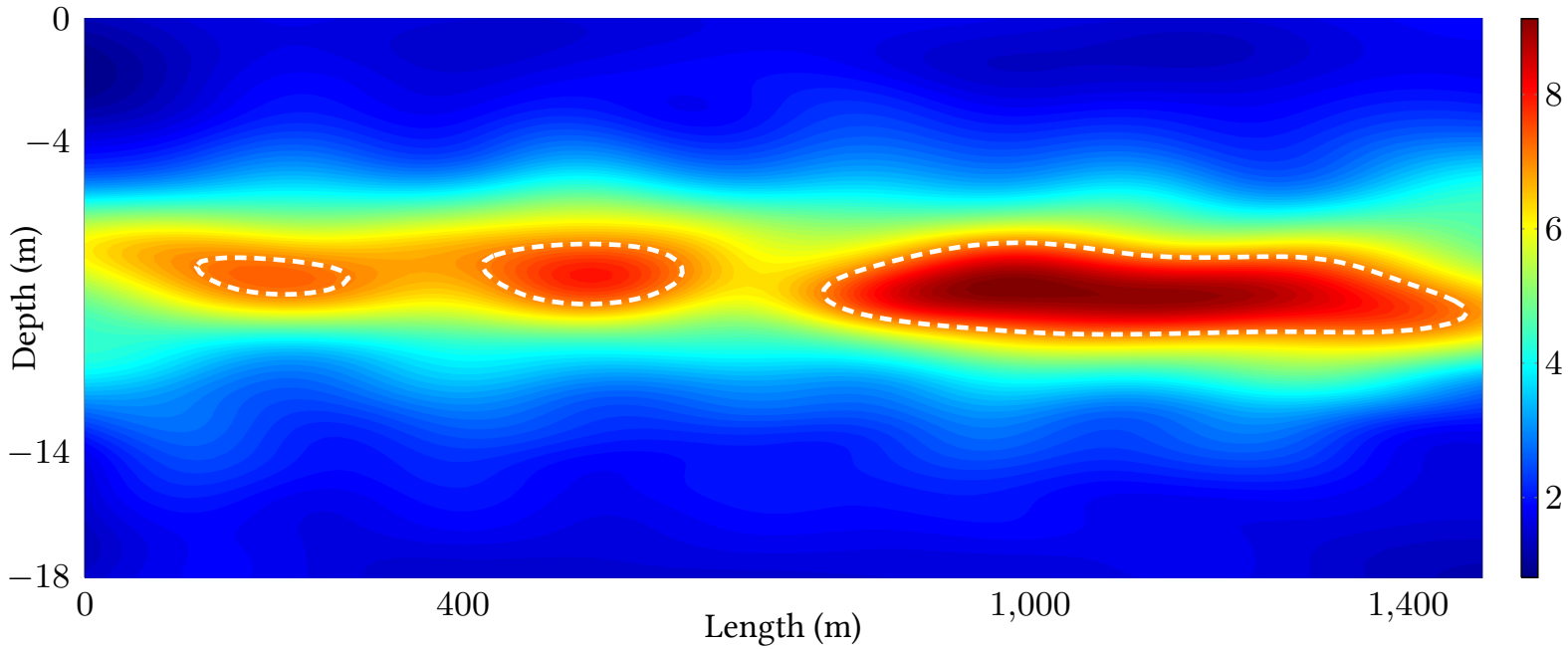
4
2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Length (m)
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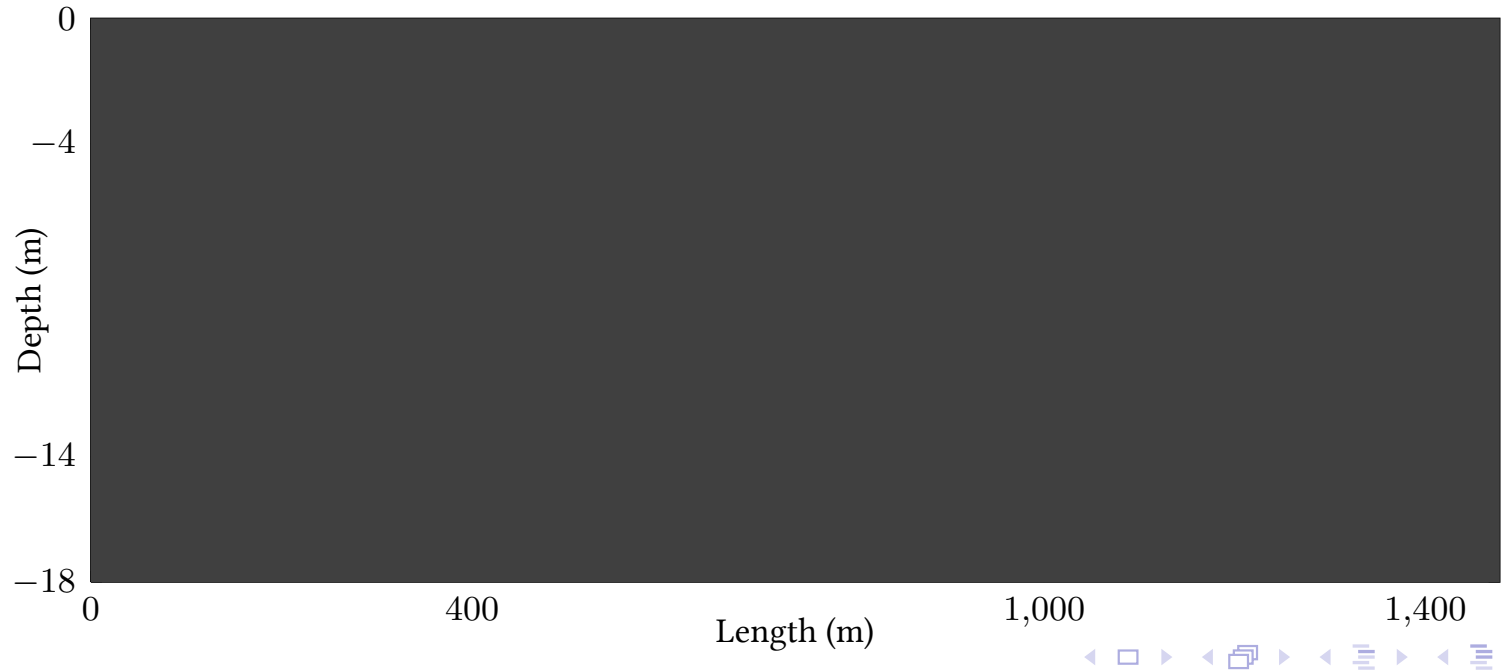
4
2

$t = 0$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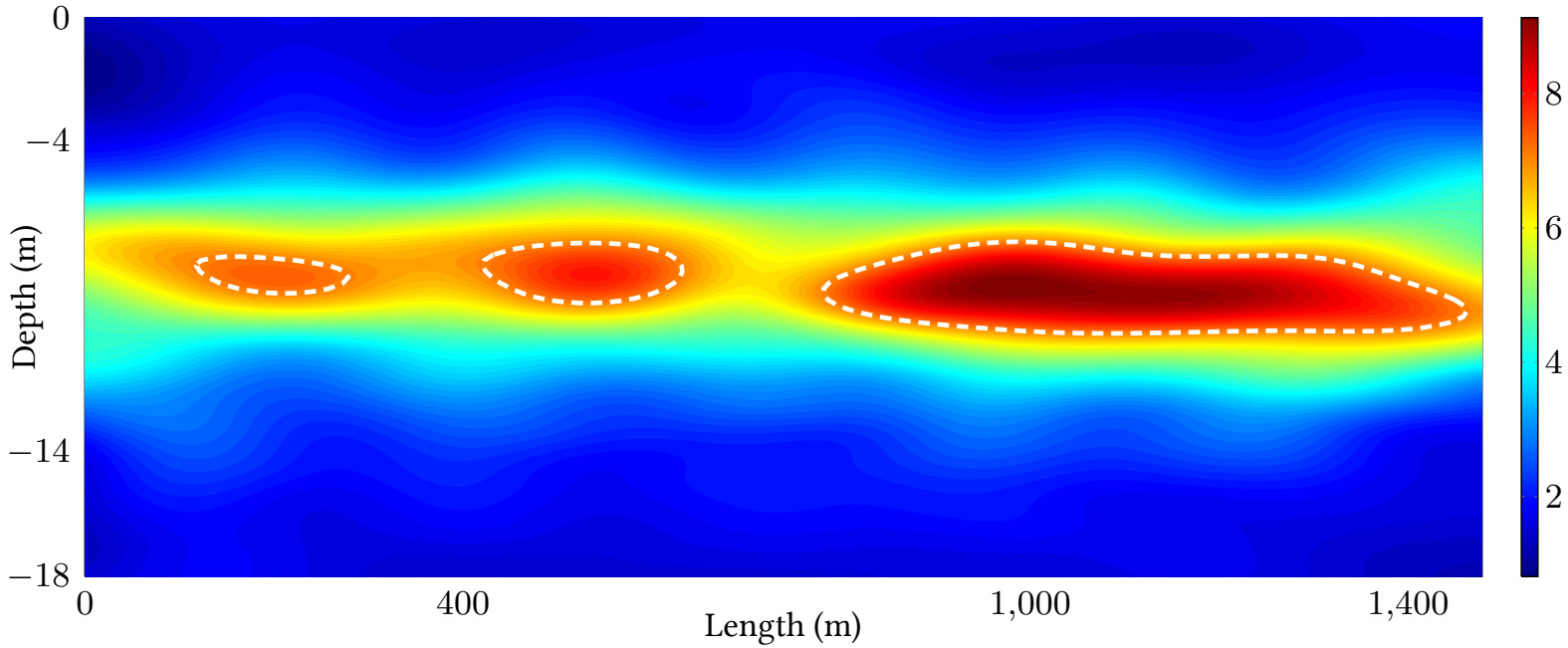
Length (m)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1,400
Length (m)
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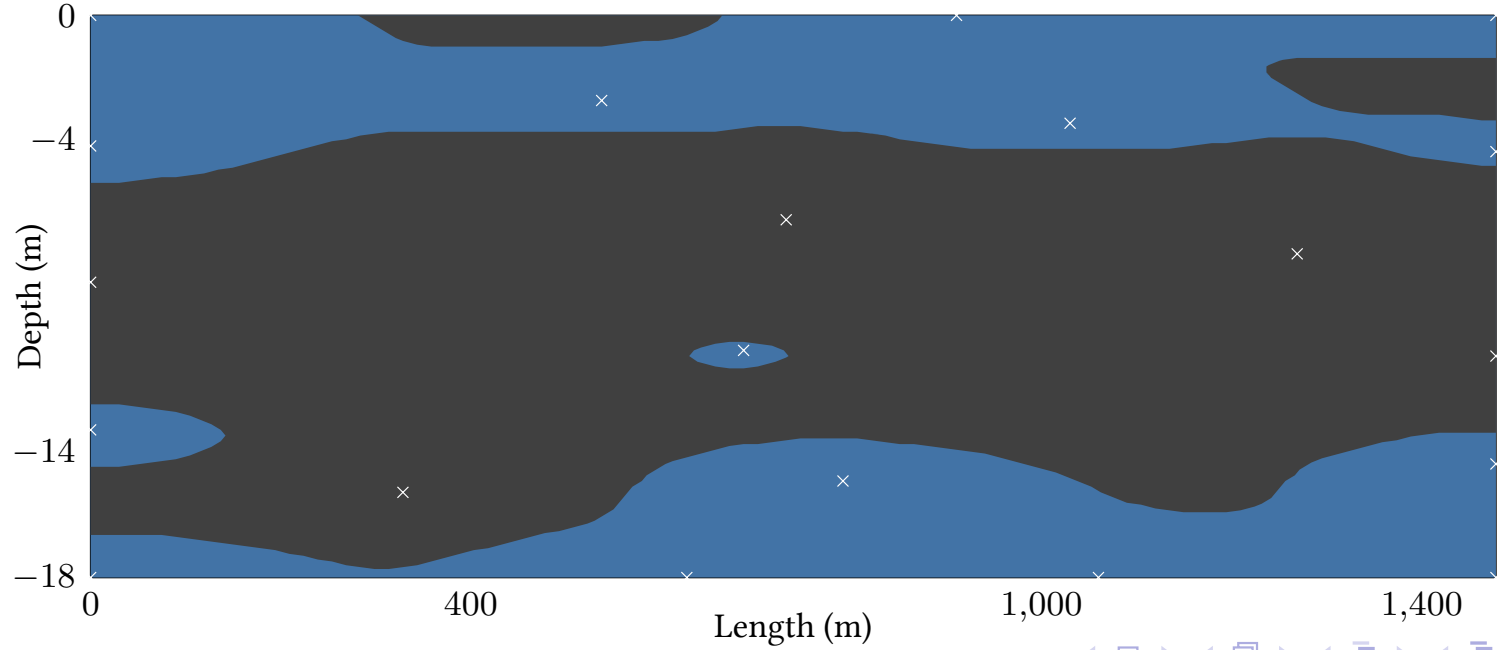
6
4
2

$t = 20$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−18
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0
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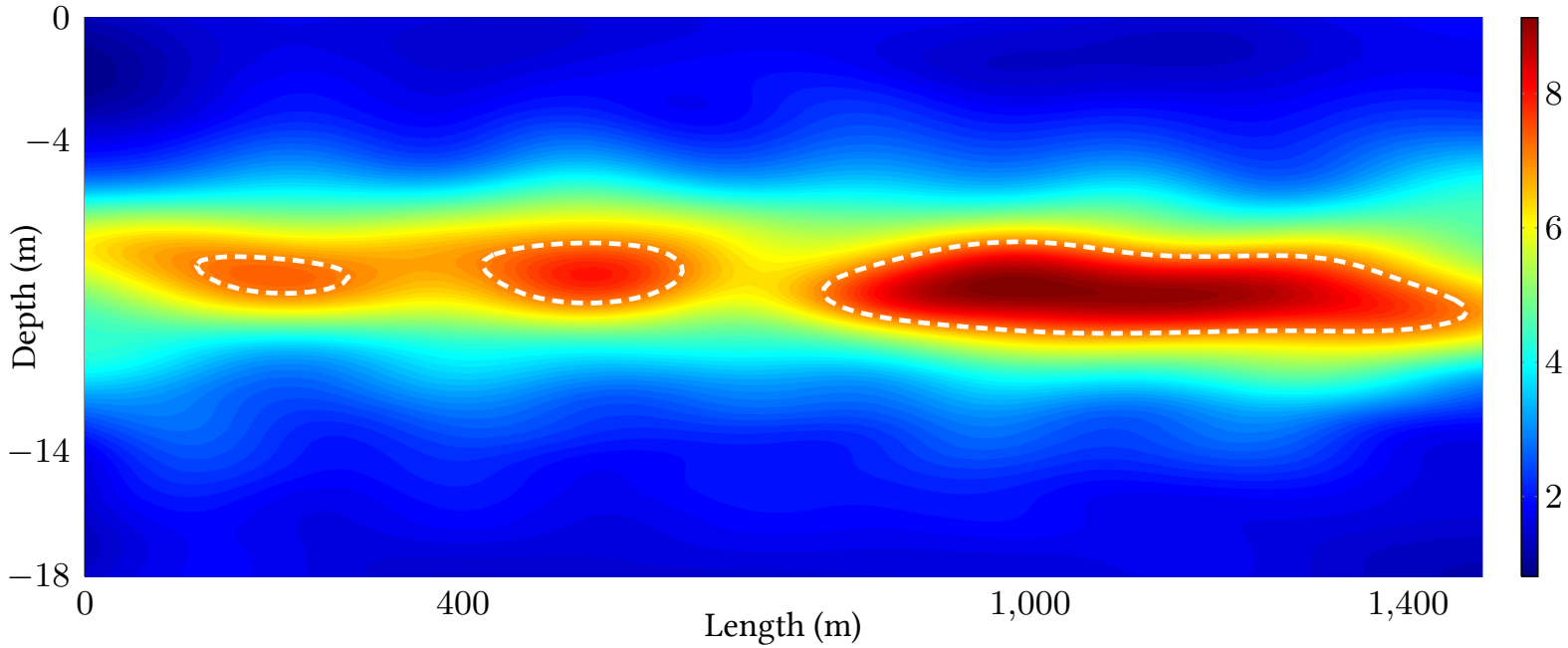
1,400
Length (m)


0
−4
−14
−18
Depth (m)
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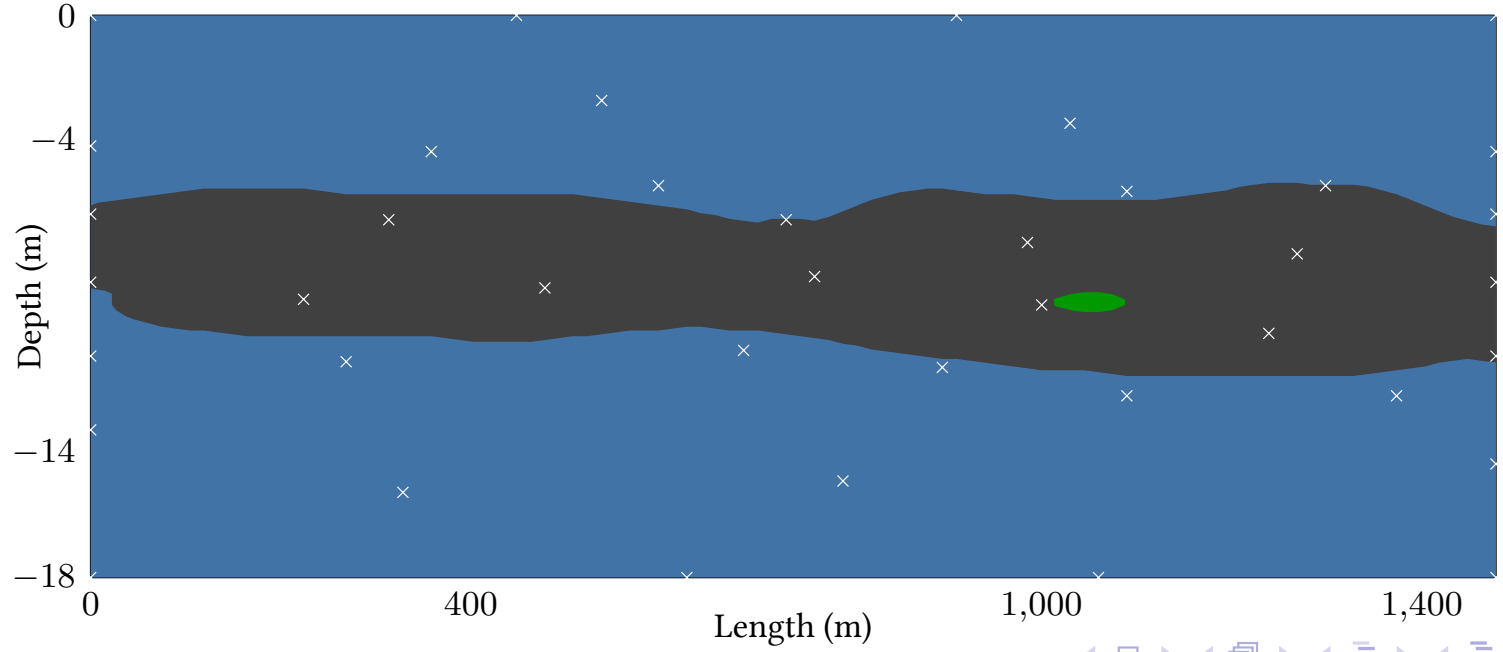
400
1,000
1,400
Length (m)
8
6
4
2

$t = 40$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Depth (m)
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1,000
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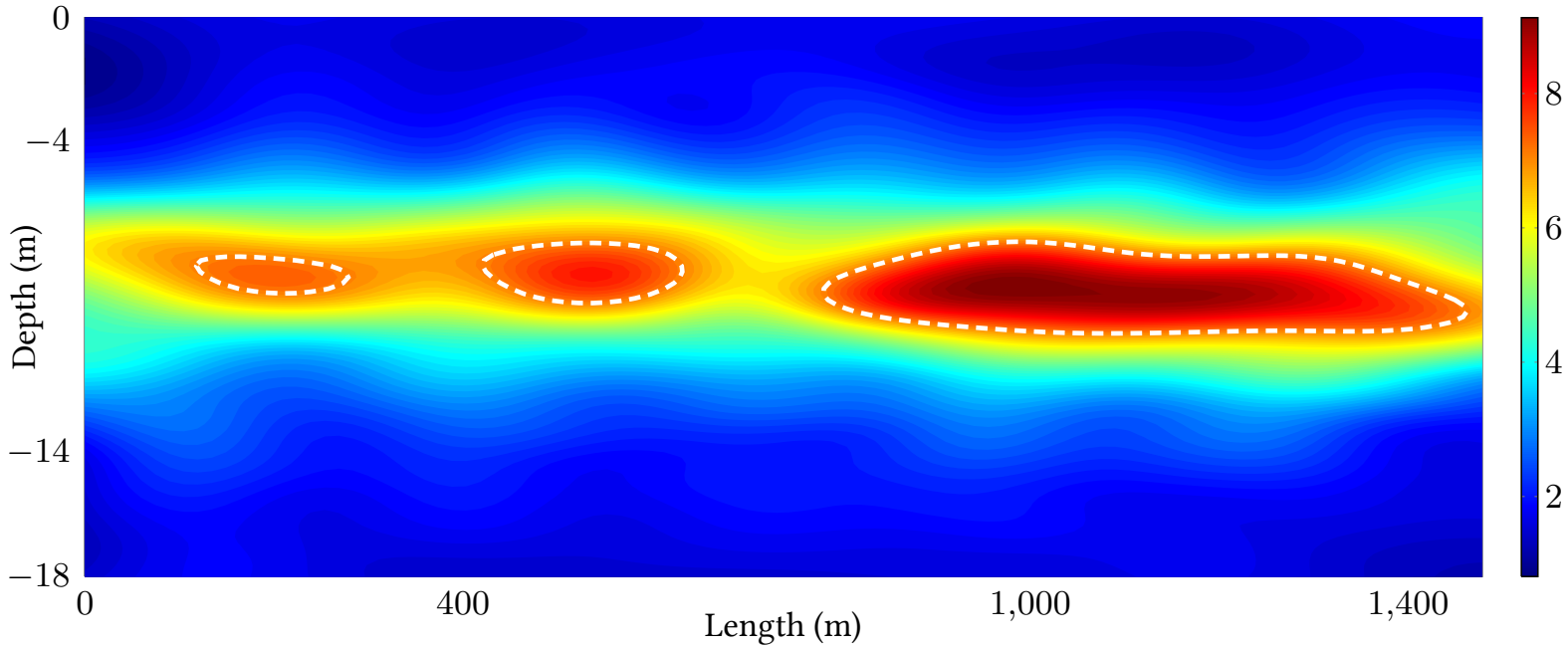
Length (m)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400
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1,400
Length (m)
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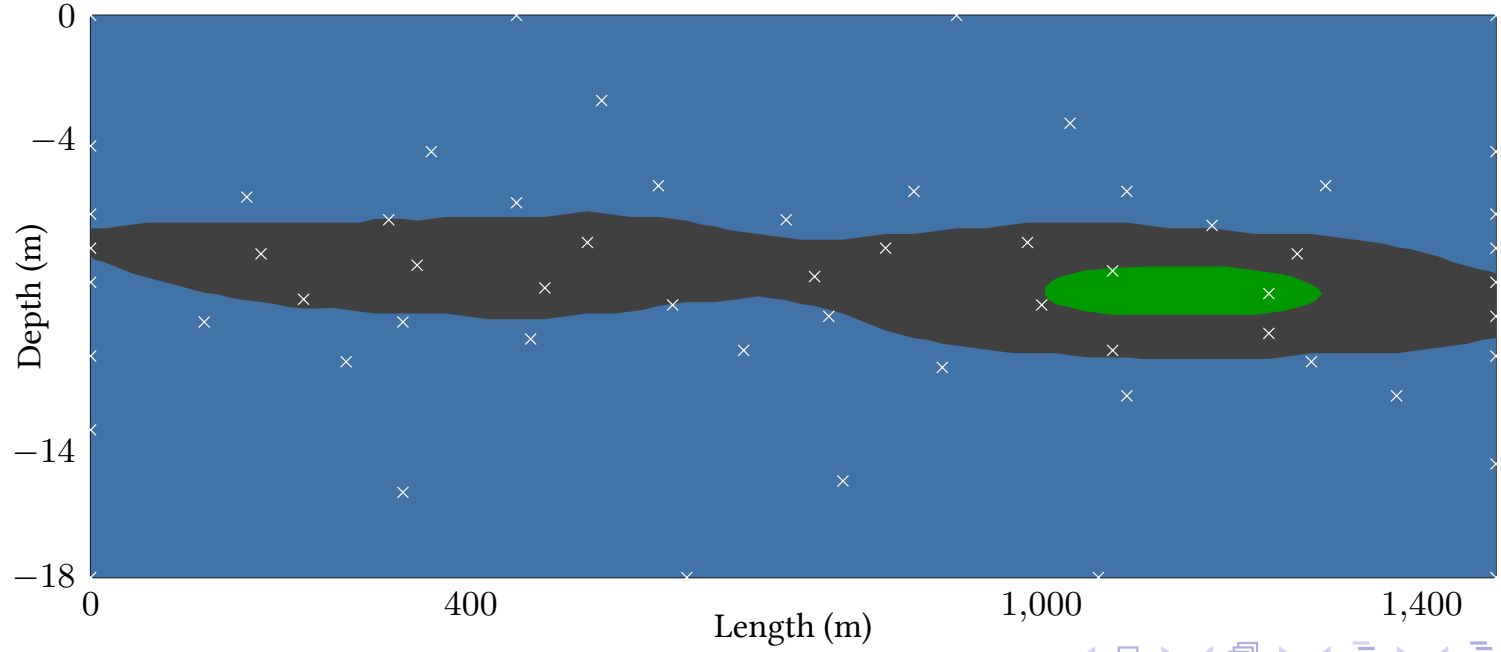
6
4
2

$t = 60$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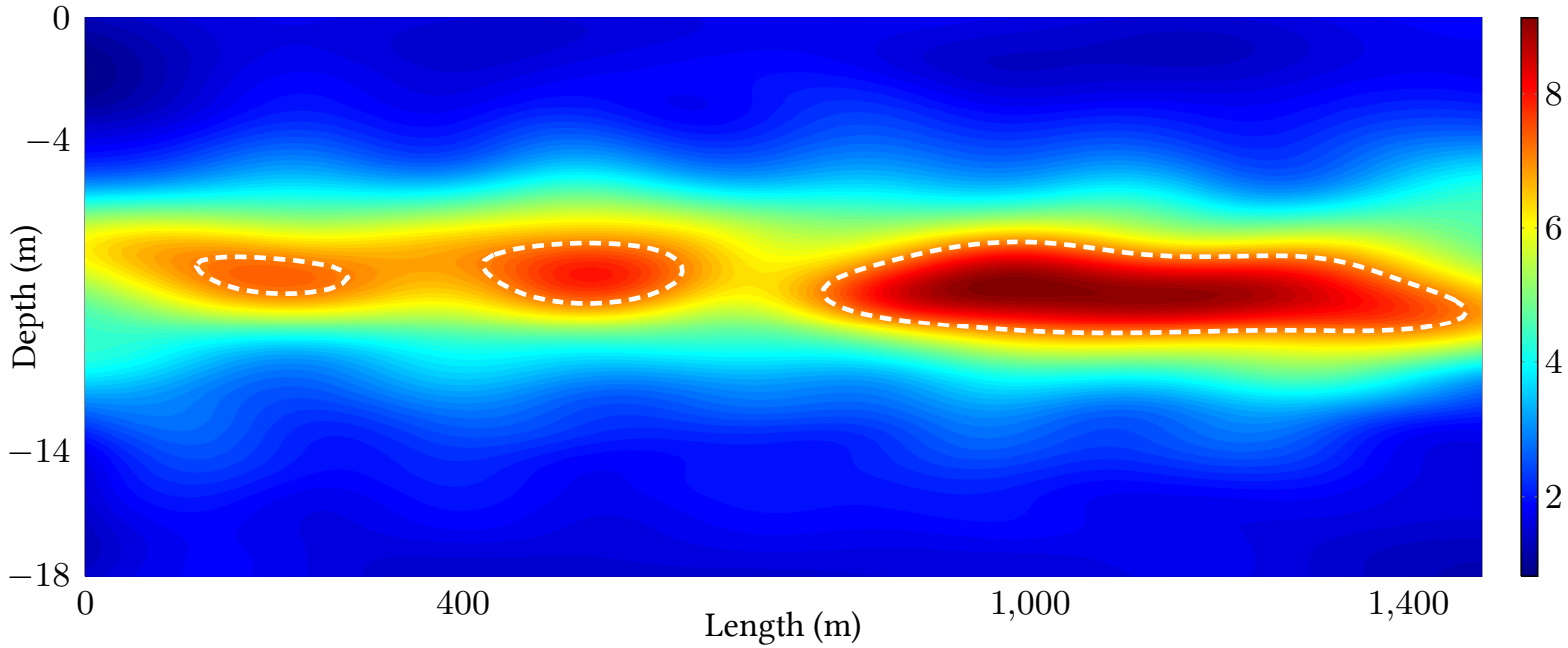
Length (m)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Length (m)
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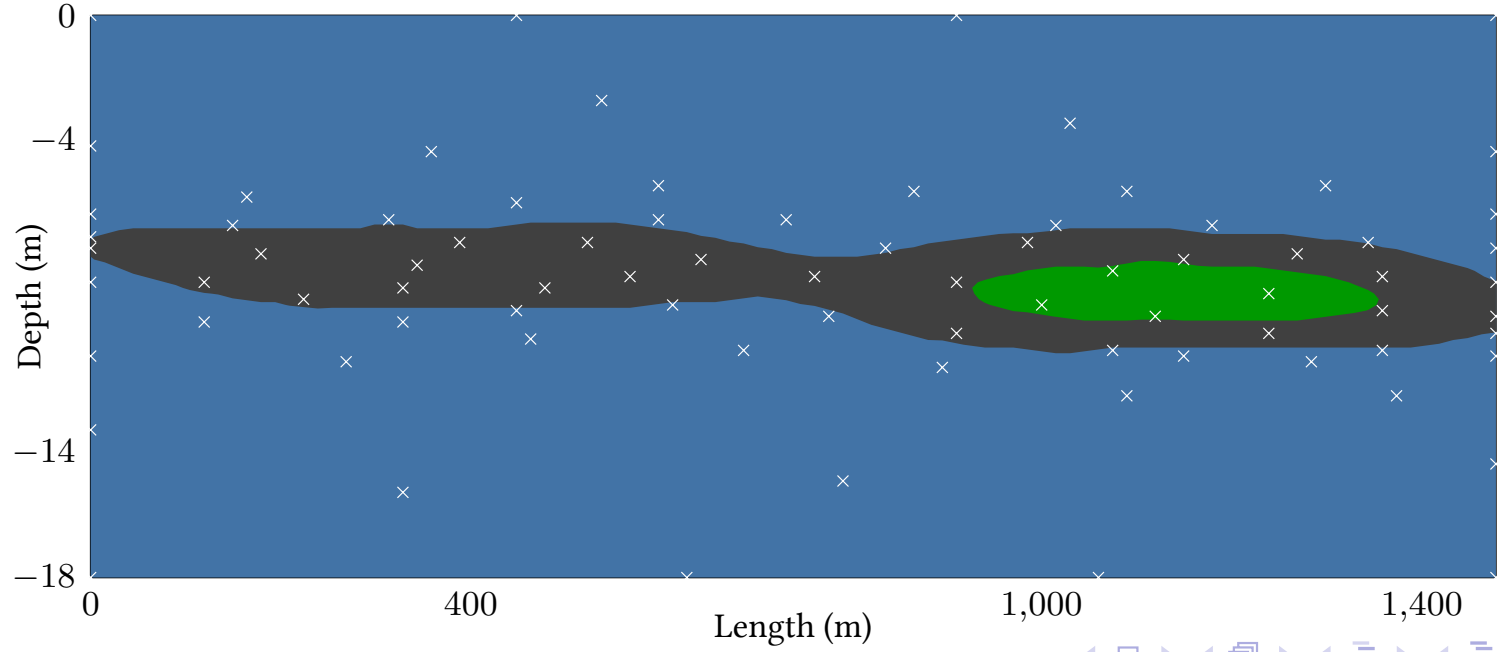
4
2

$t = 80$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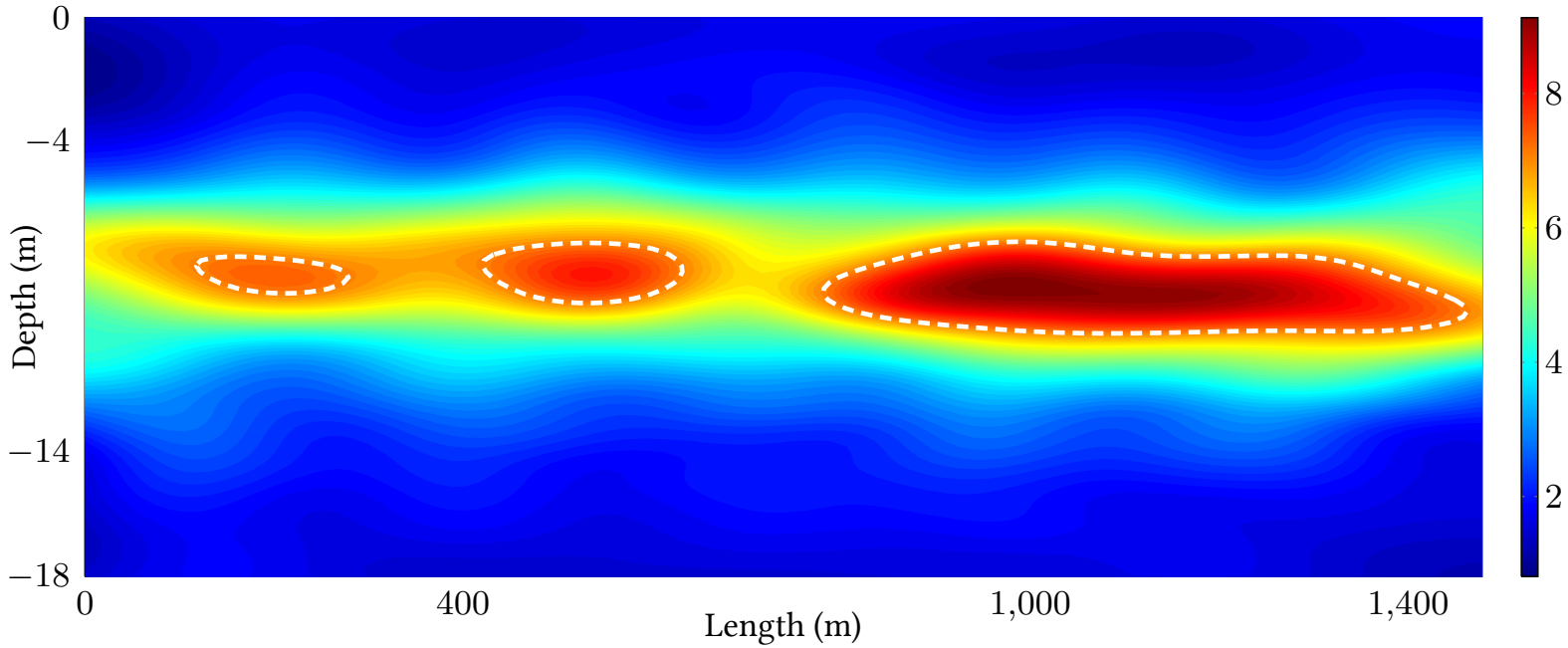
Length (m)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Depth (m)
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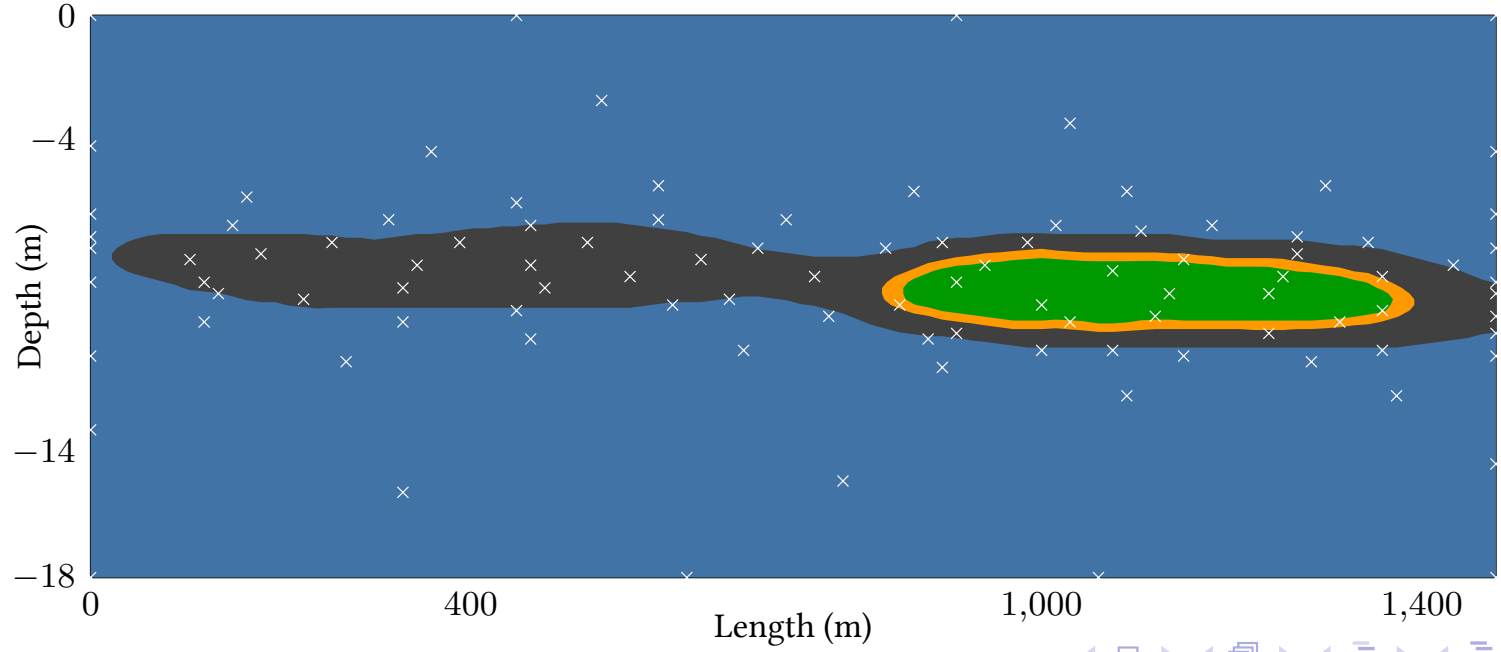
1,400
Length (m)
8
6
4
2

$t = 100$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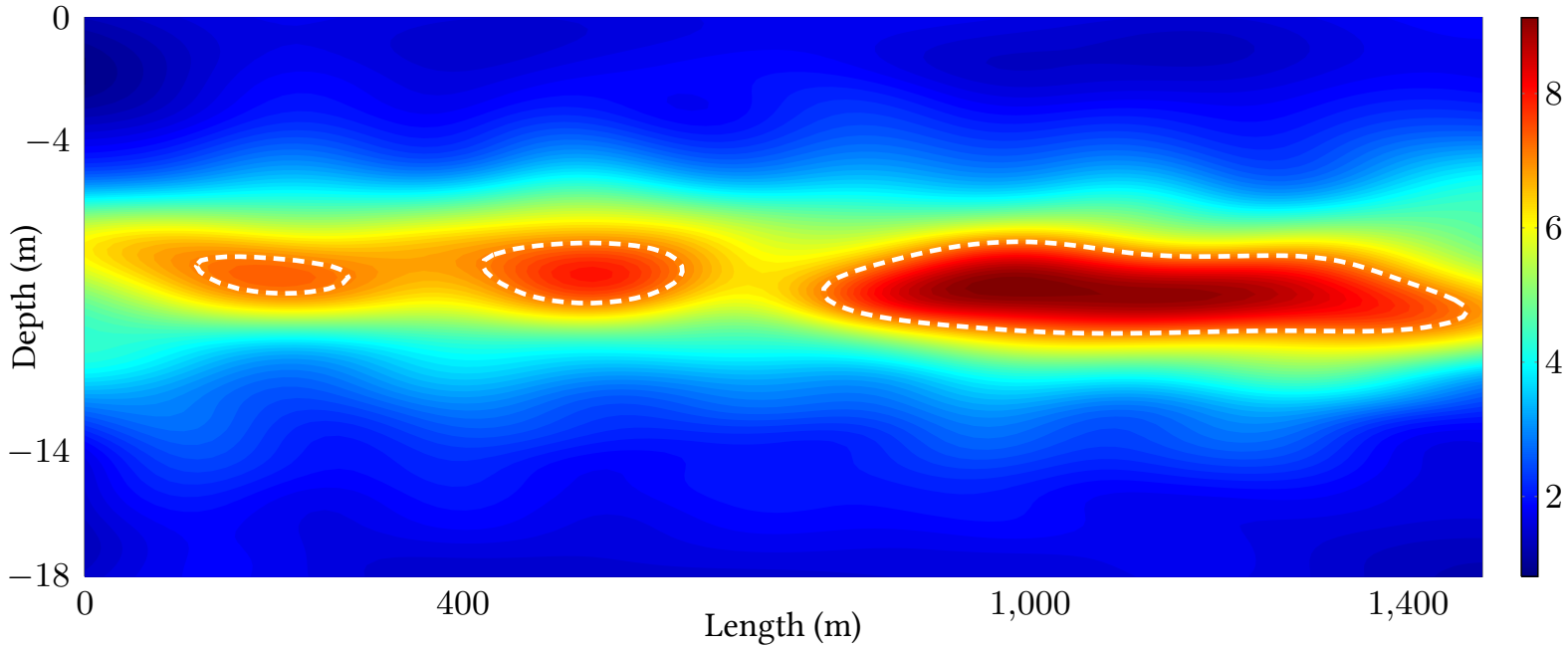
−14
−18
Depth (m)
0
400
1,000
1,400
Length (m)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Depth (m)
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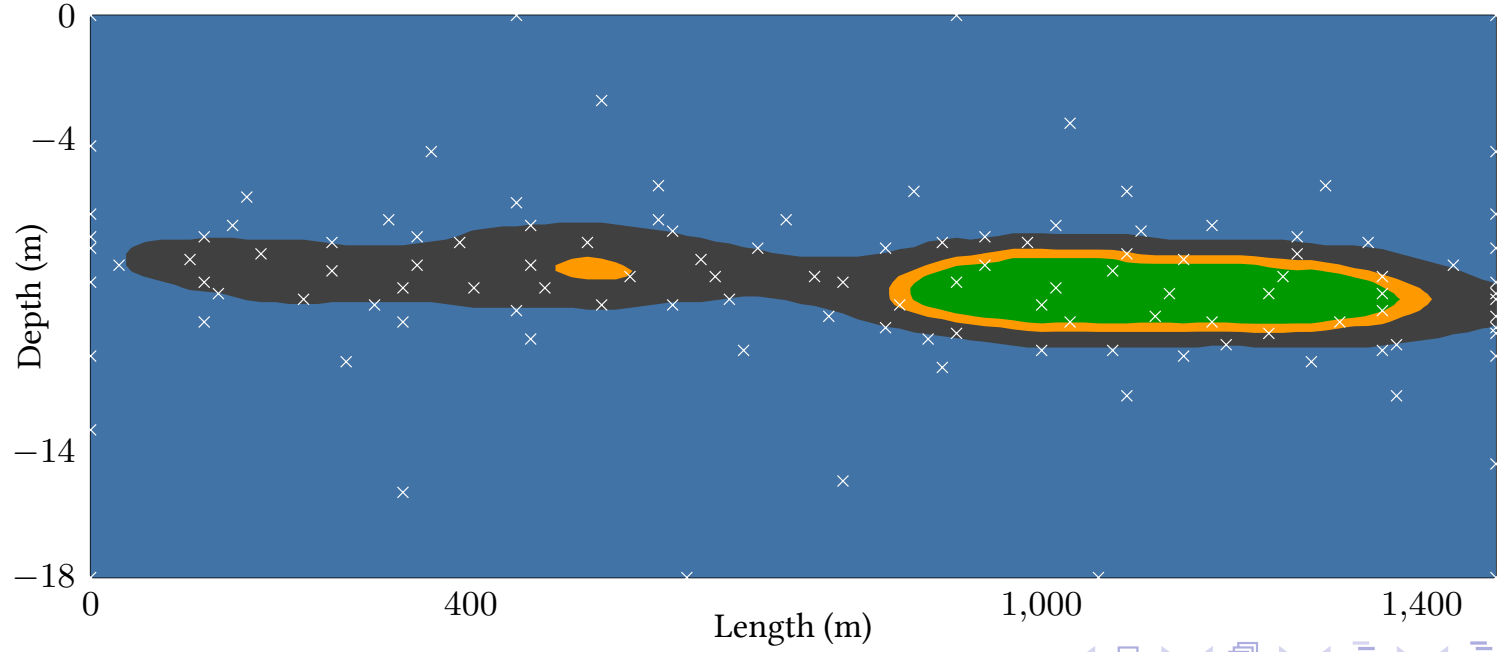
400
1,000
1,400
Length (m)
8
6
4
2

$t = 120$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Depth (m)
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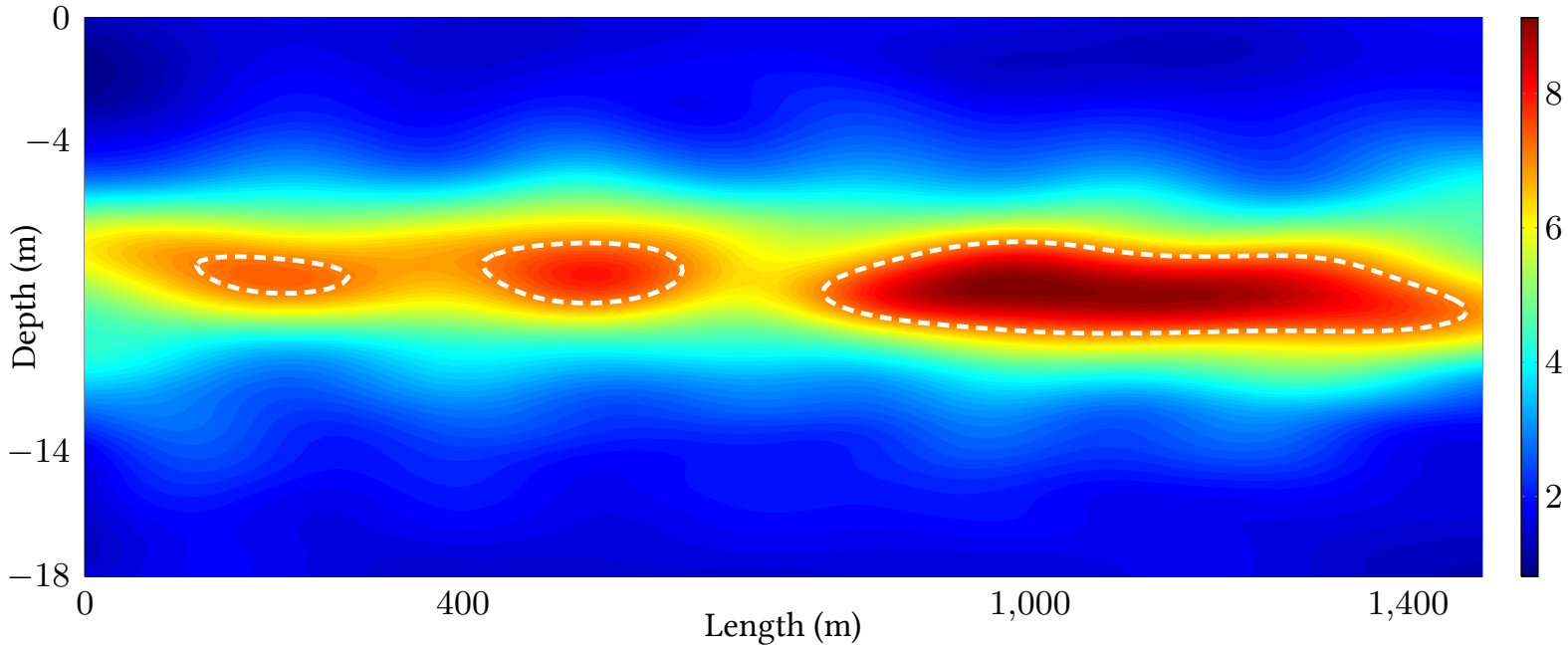
1,000
1,400
Length (m)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−18
Depth (m)
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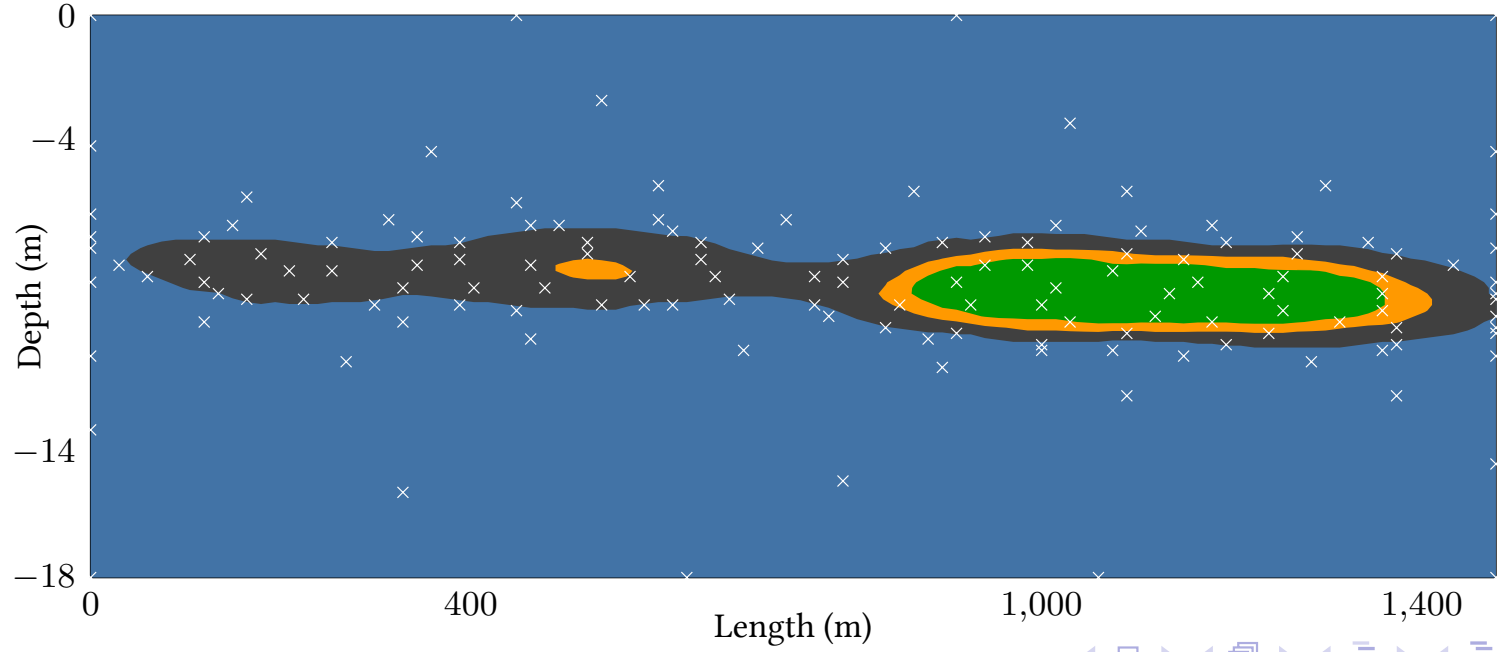
400
1,000
1,400
Length (m)
8
6
4
2

$t = 140$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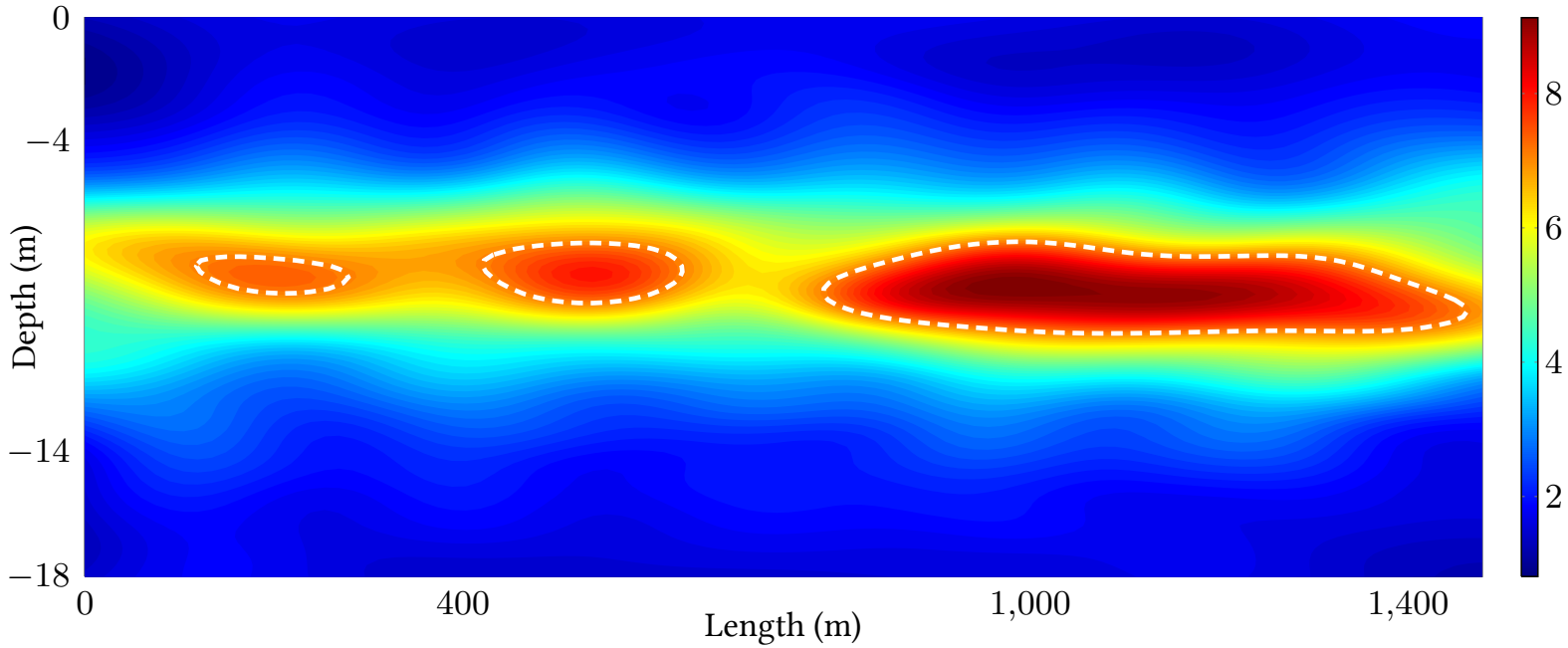
1,400
Length (m)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Depth (m)
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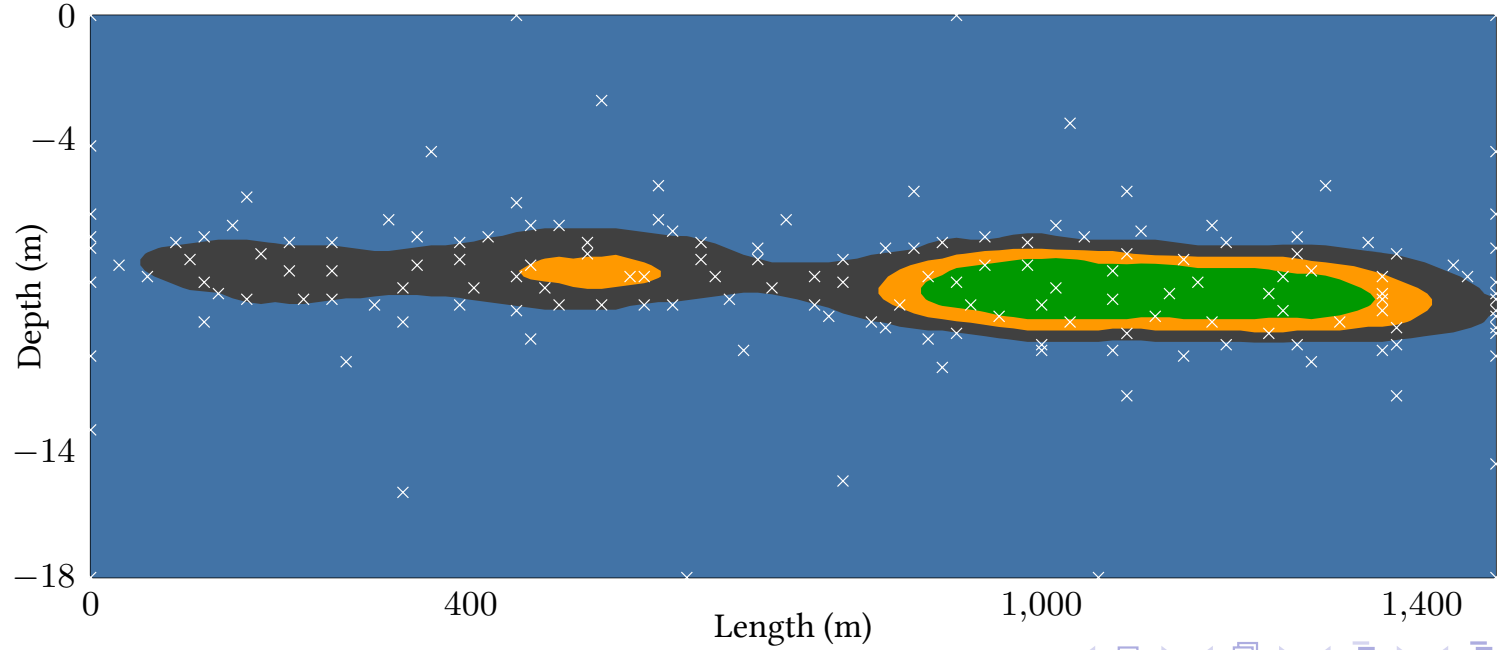
1,400
Length (m)
8
6
4
2

$t = 160$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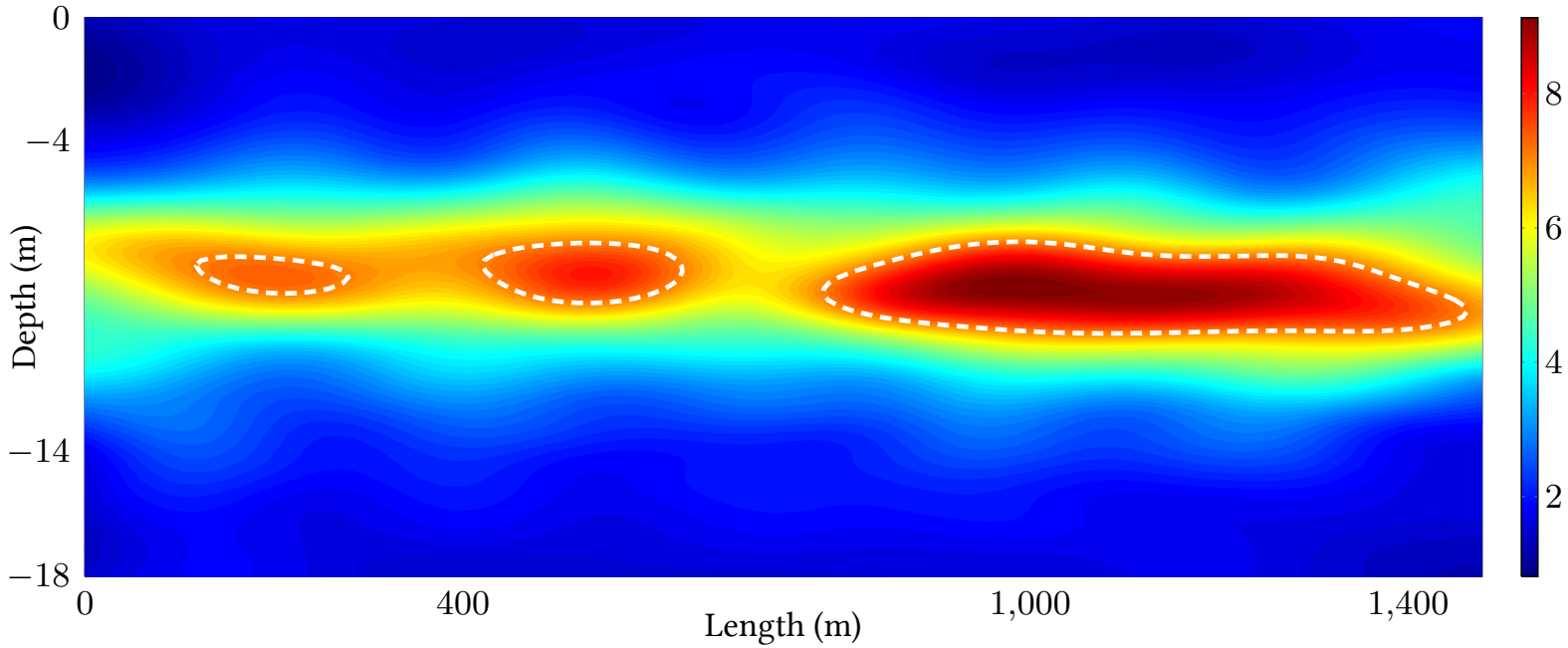
−18
Depth (m)
0
400
1,000
1,400
Length (m)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Depth (m)
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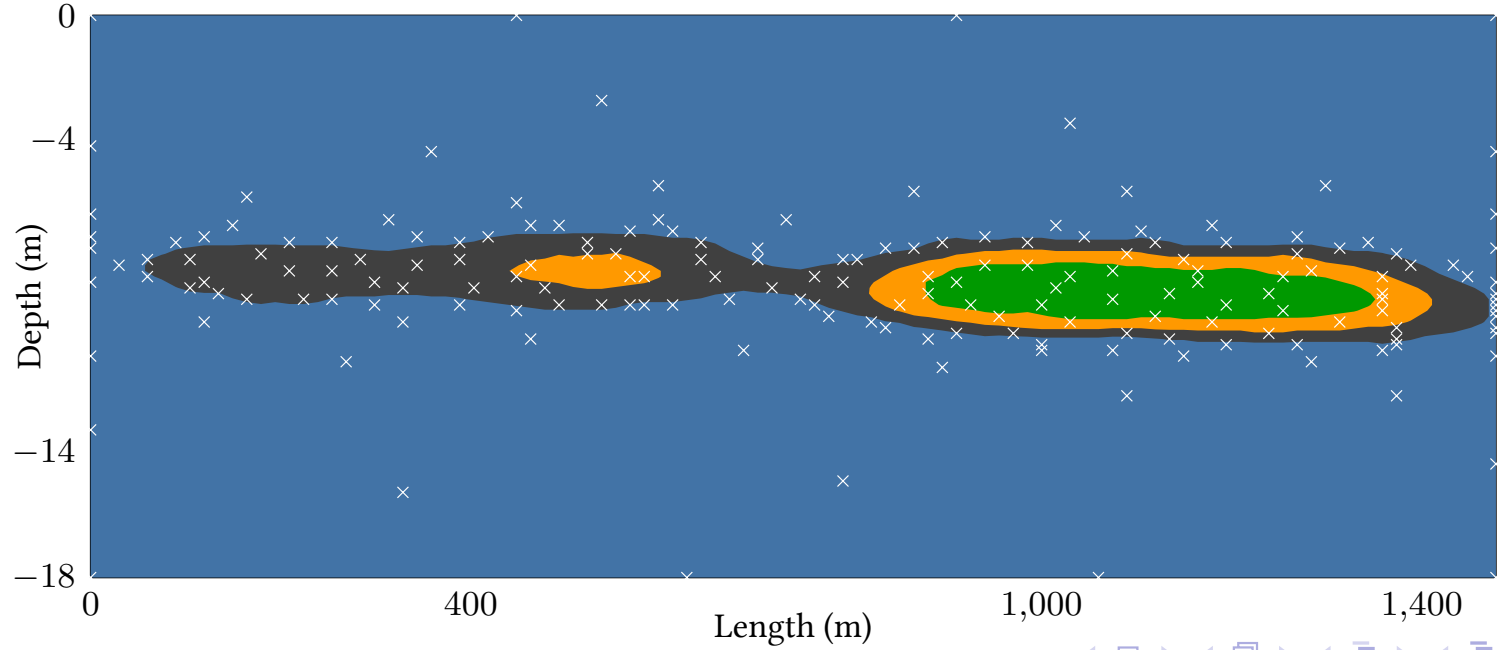
400
1,000
1,400
Length (m)
8
6
4
2

$t = 180$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Depth (m)
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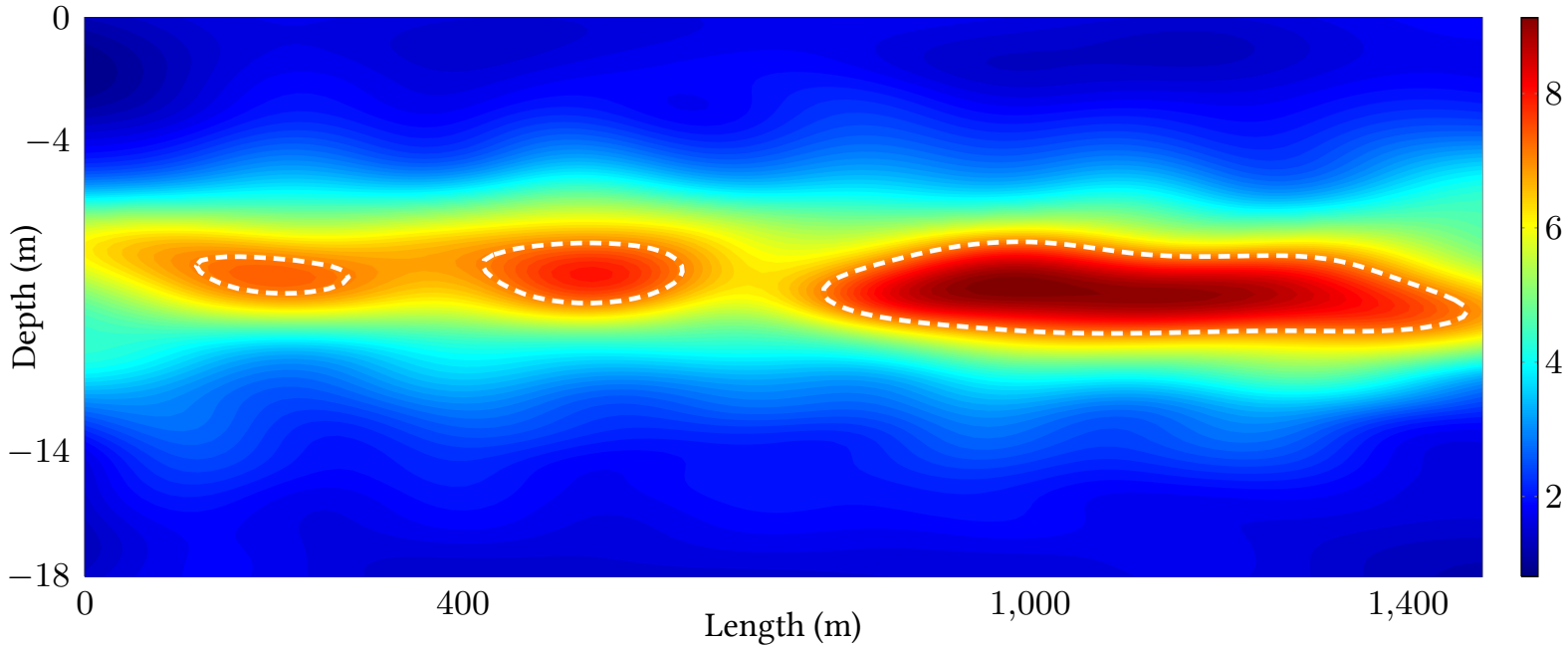
400
1,000
1,400
Length (m)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Depth (m)
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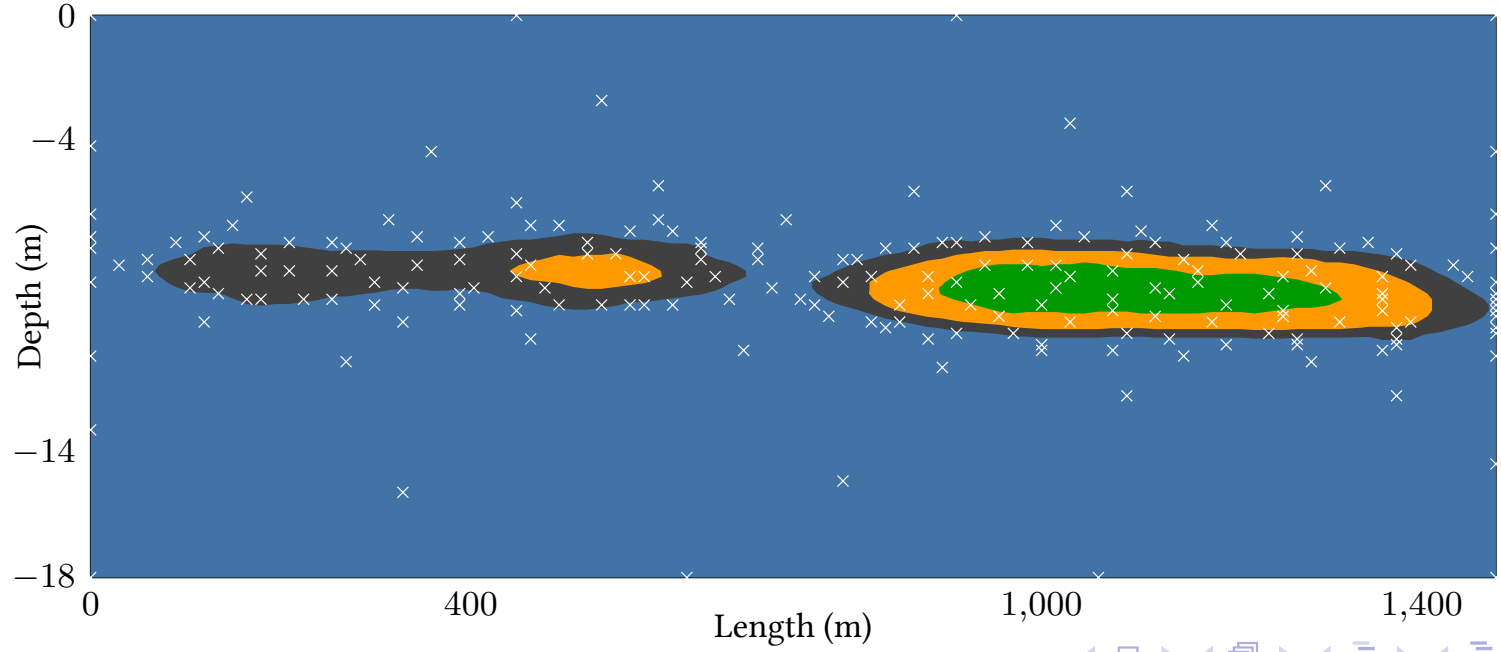
1,400
Length (m)
8
6
4
2

$t = 200$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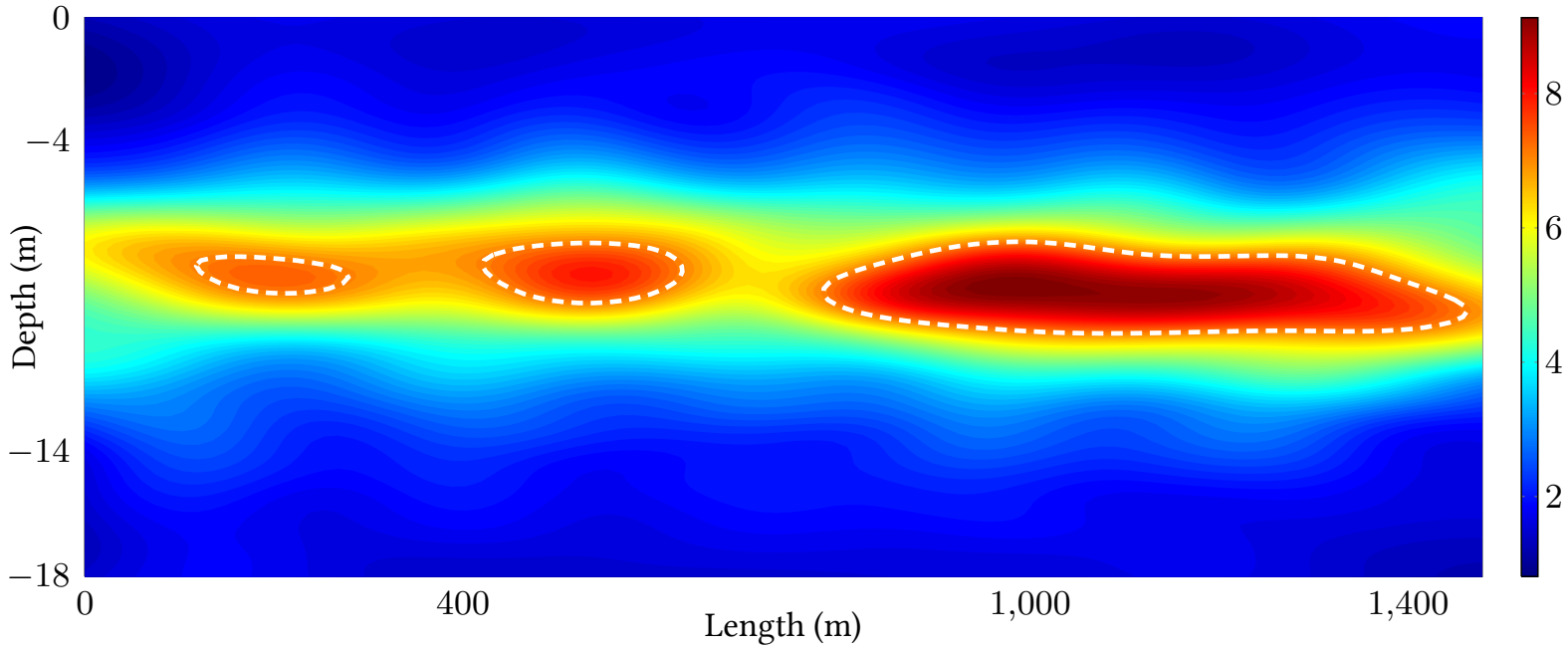
−18
Depth (m)
0
400
1,000
1,400
Length (m)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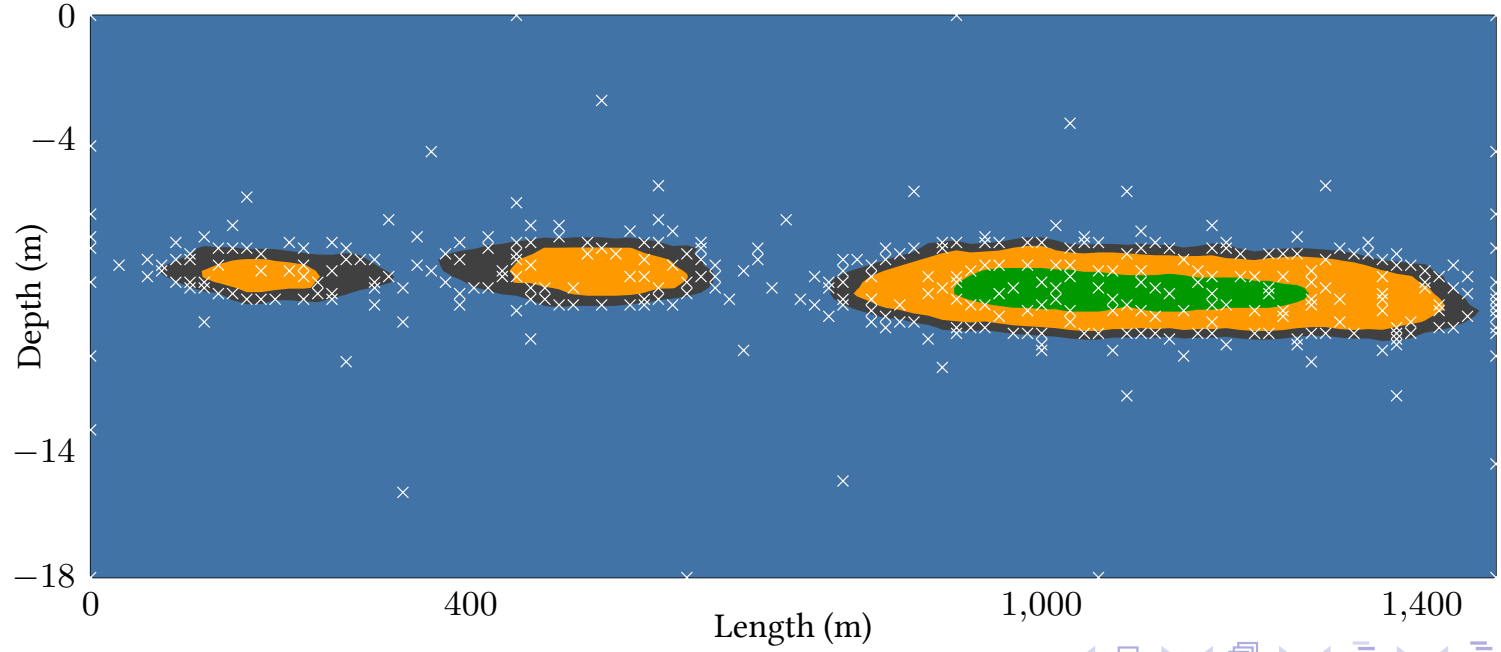
−4
−14
−18
Depth (m)
0
400
1,000
1,400
Length (m)
8
6
4
2

$t = 340$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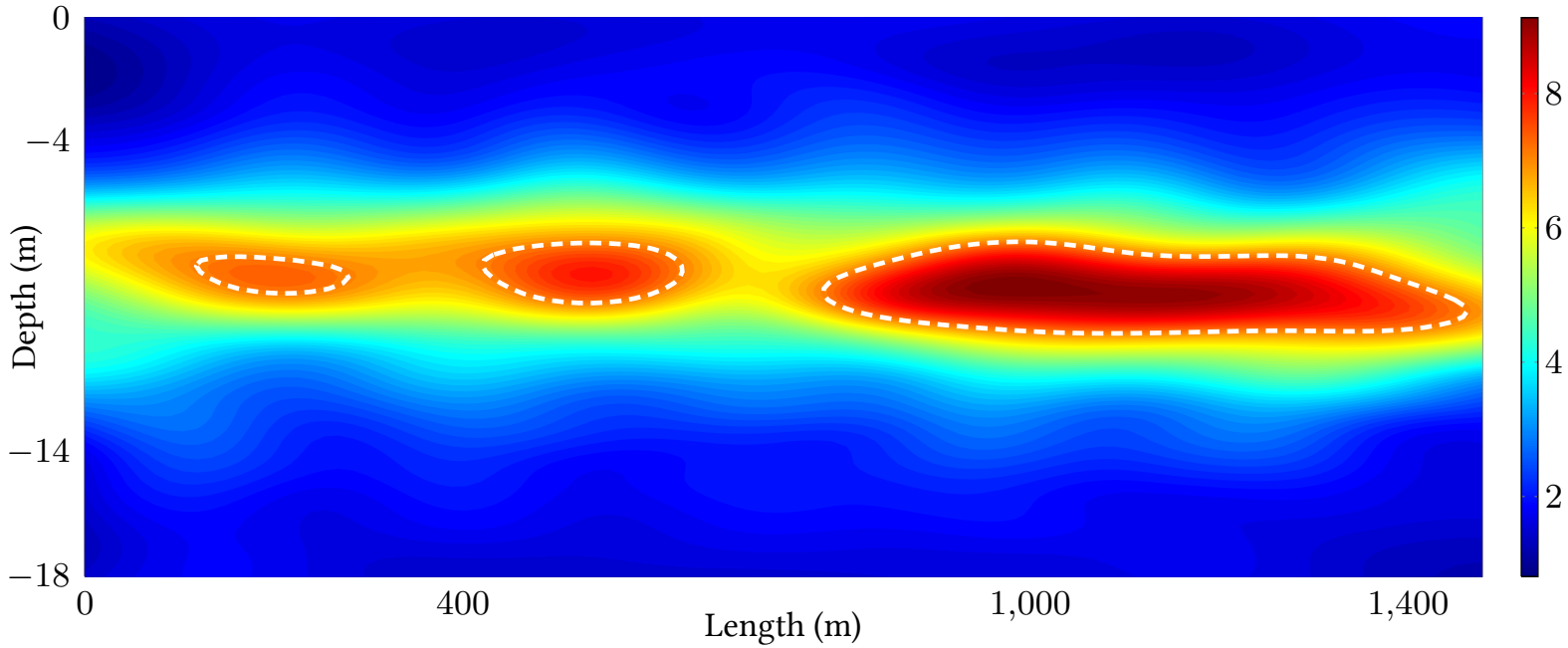
−14
−18
Depth (m)
0
400
1,000
1,400
Length (m)


0
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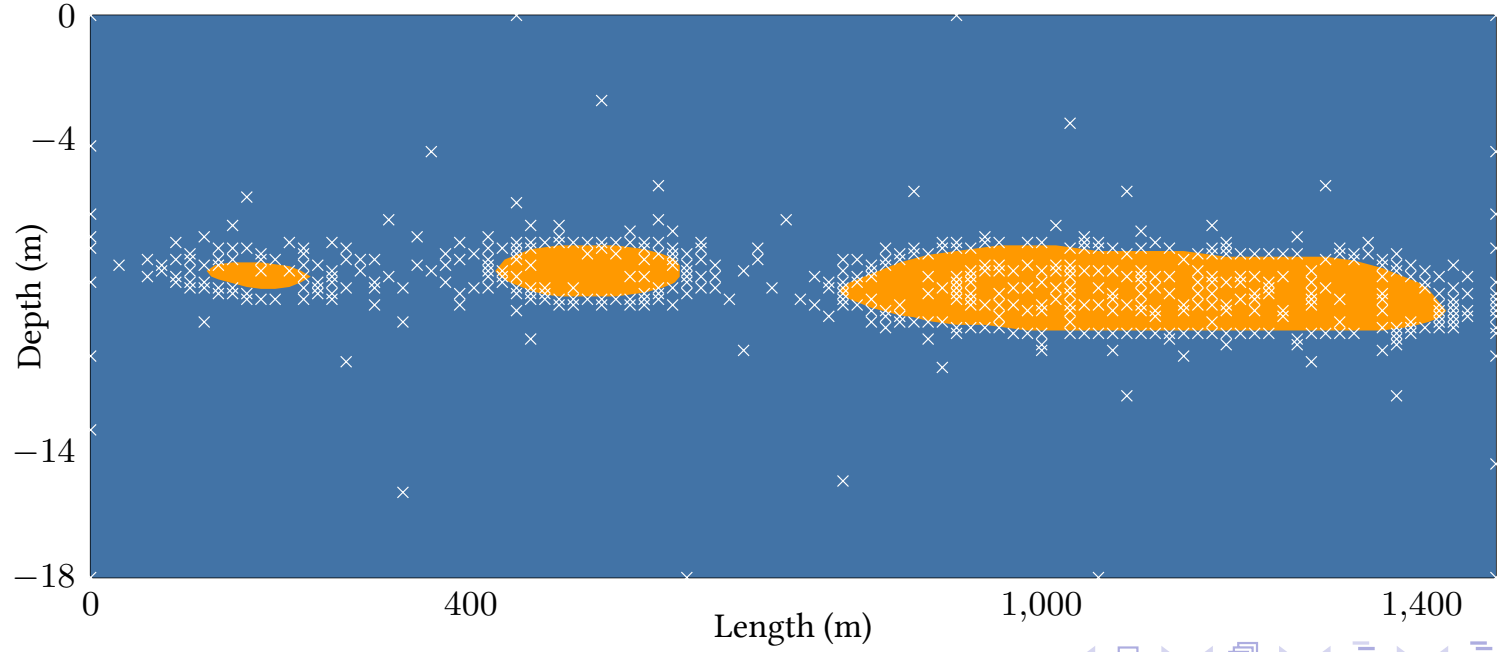
−14
−18
Depth (m)
0
400
1,000
1,400
Length (m)
8
6
4
2

$t = 486$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−18
Depth (m)
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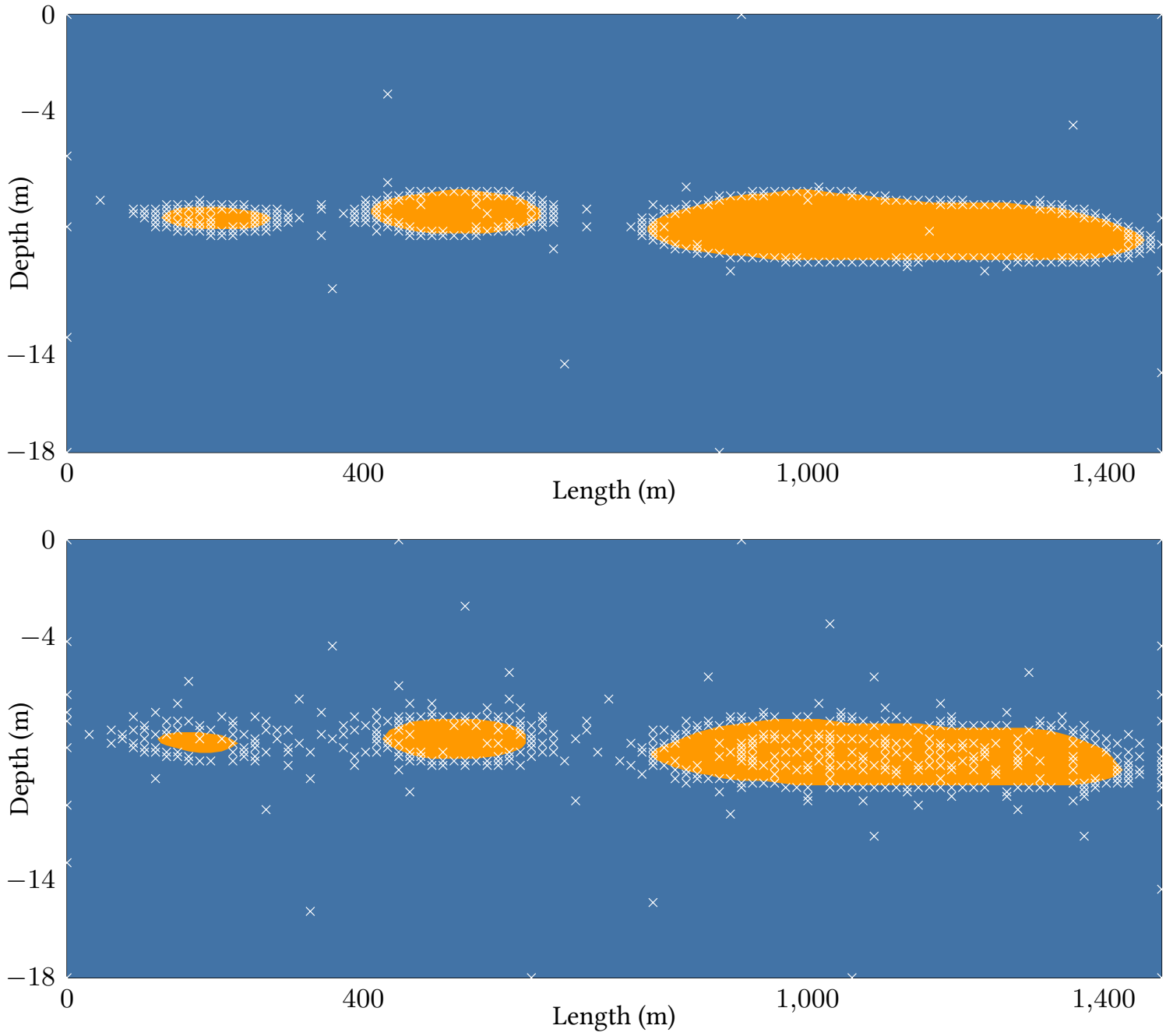
400
1,000
1,400
Length (m)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−4
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Depth (m)
0
400
1,000
1,400
Length (m)
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−4
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−18
Depth (m)
0
400
1,000
1,400
Length (m)

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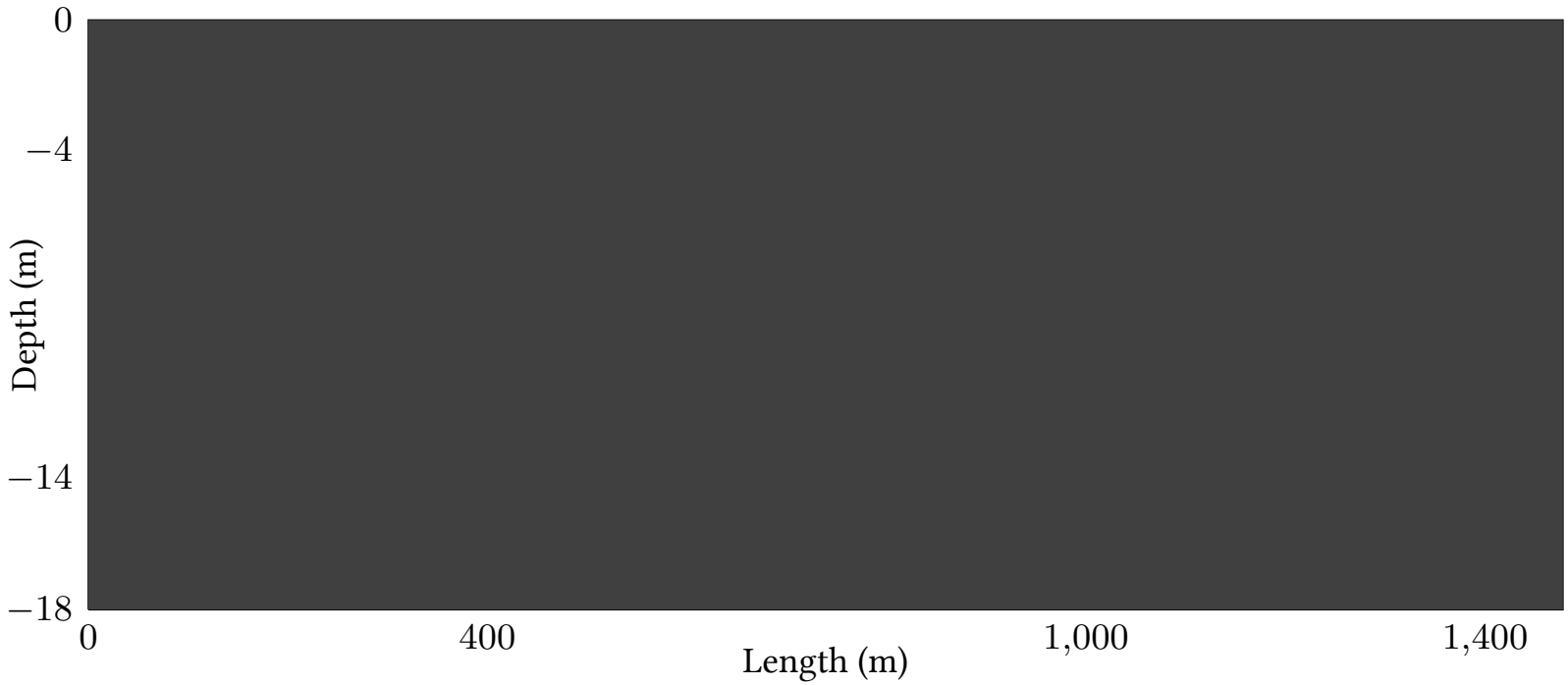

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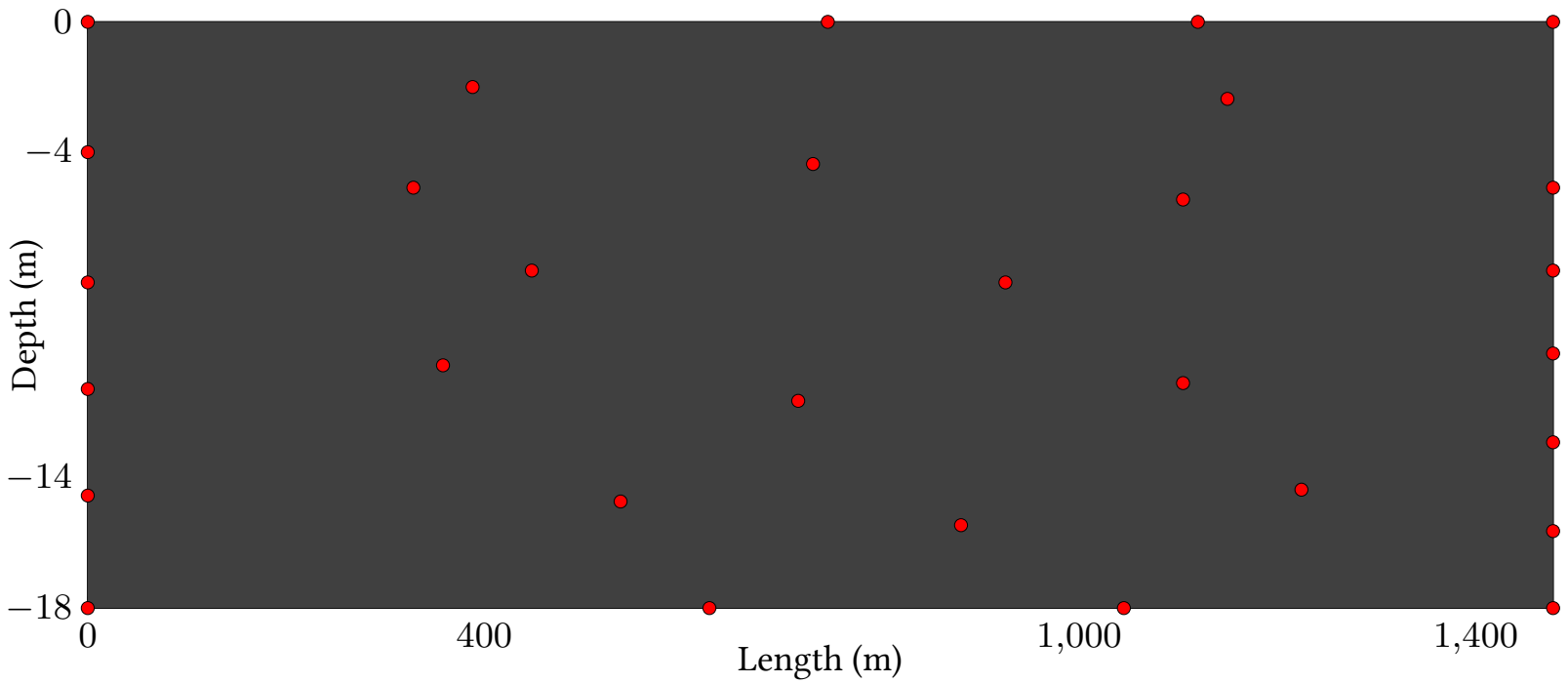

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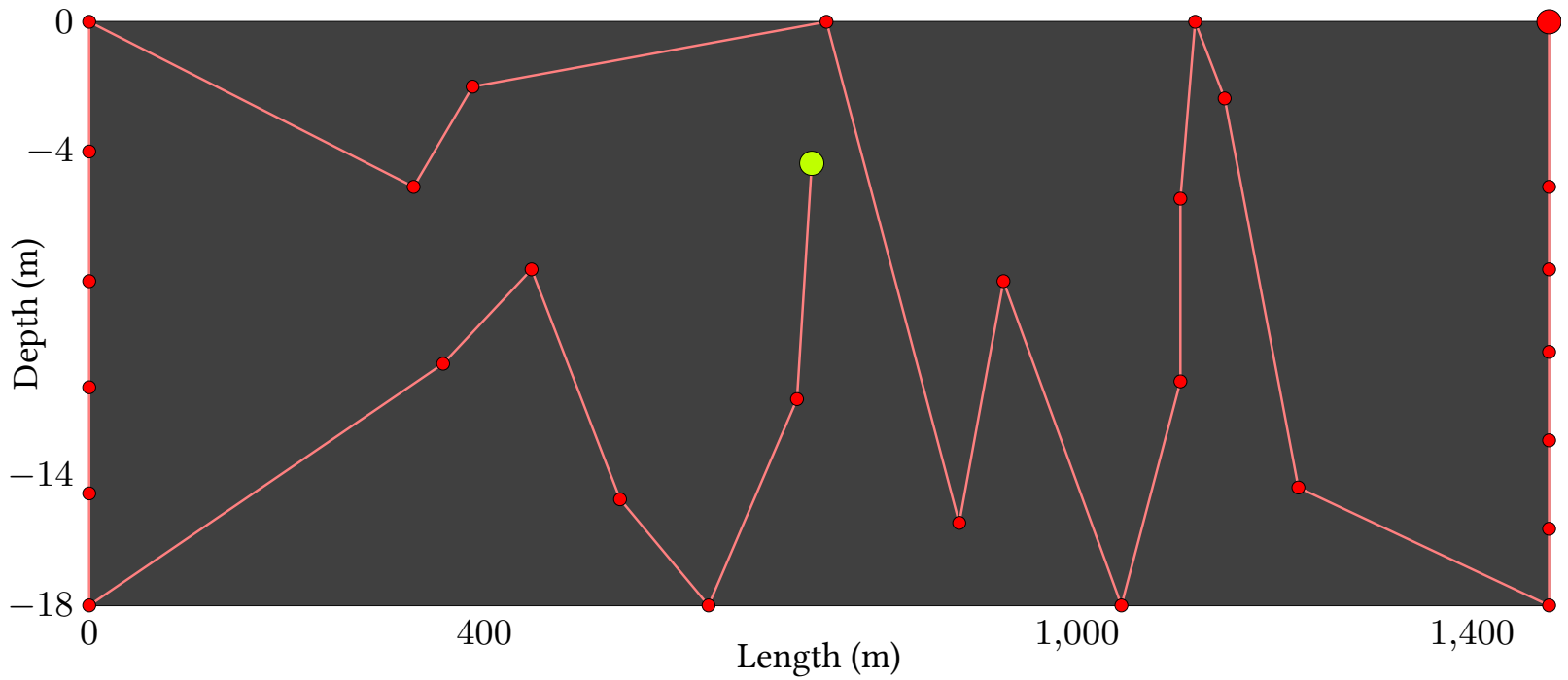

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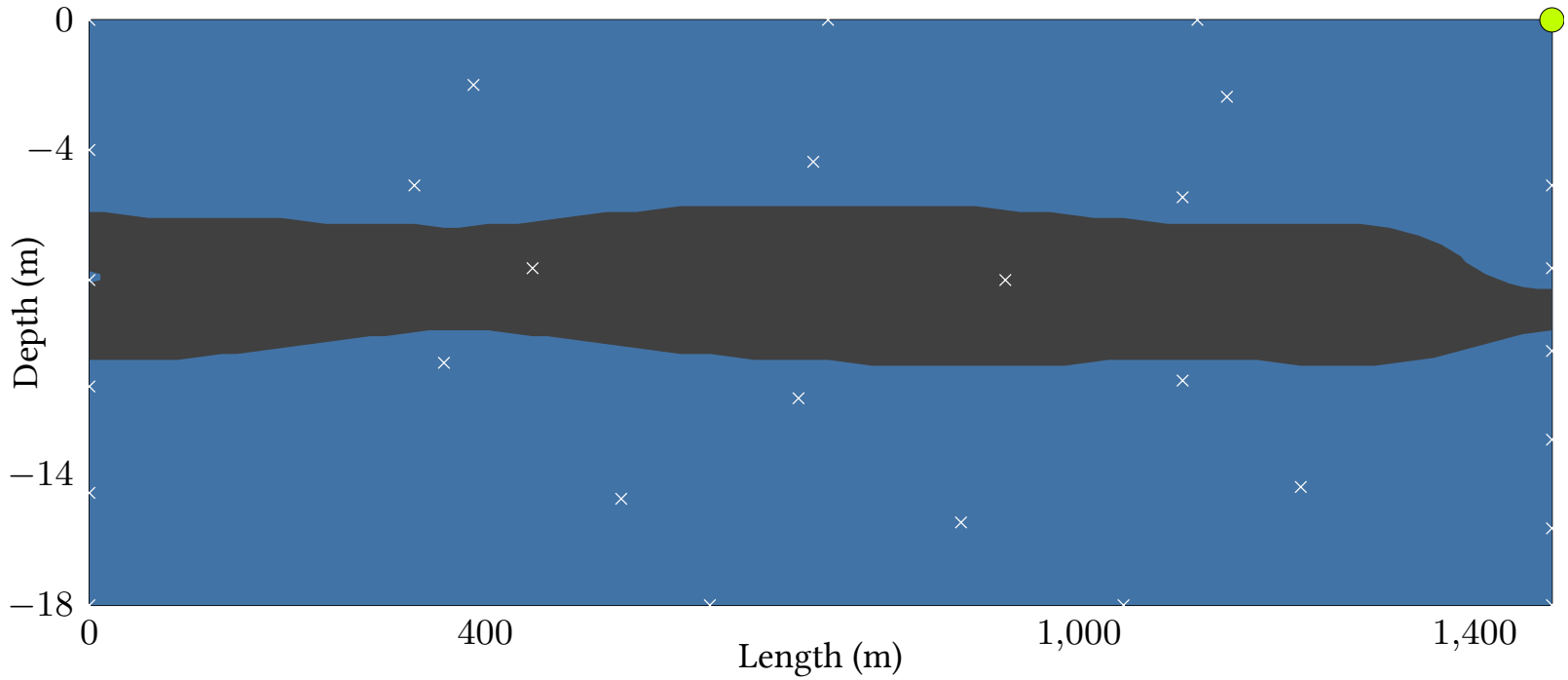

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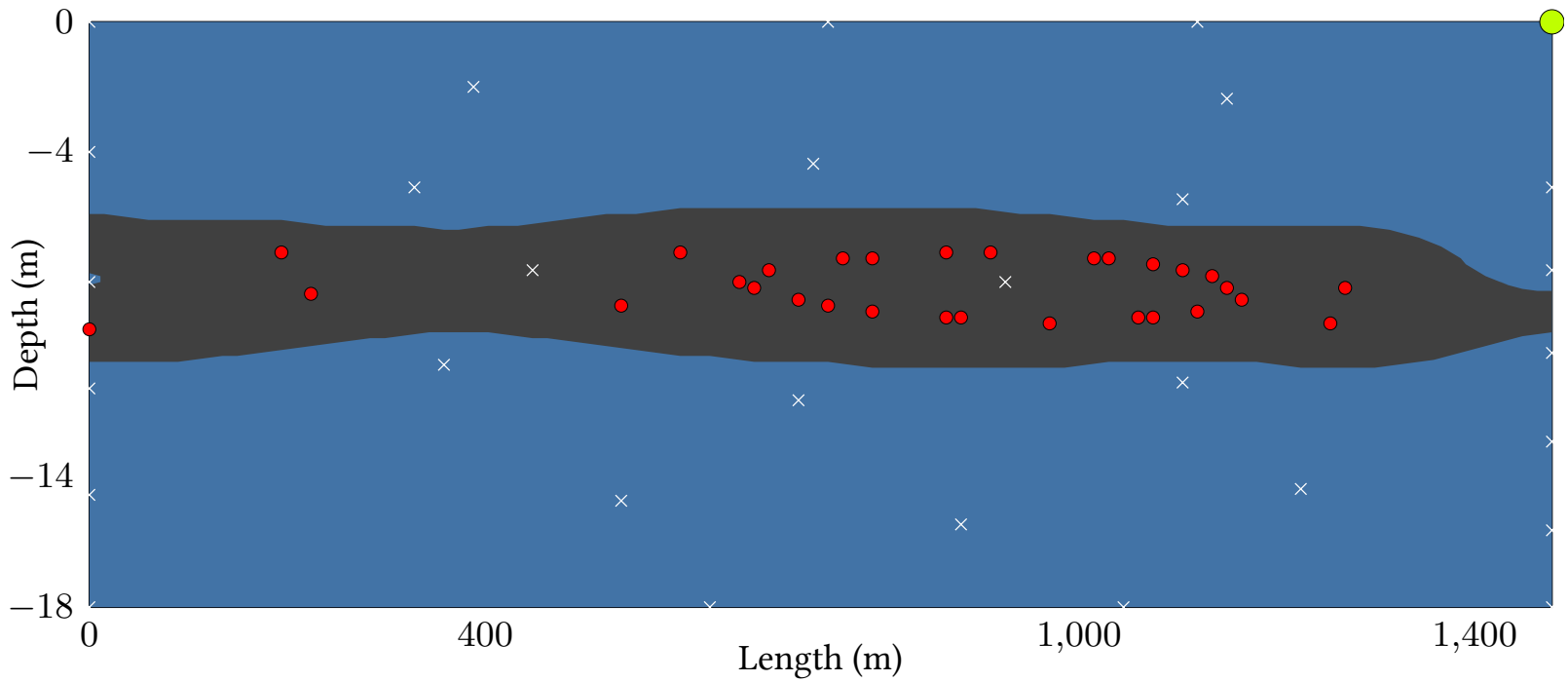

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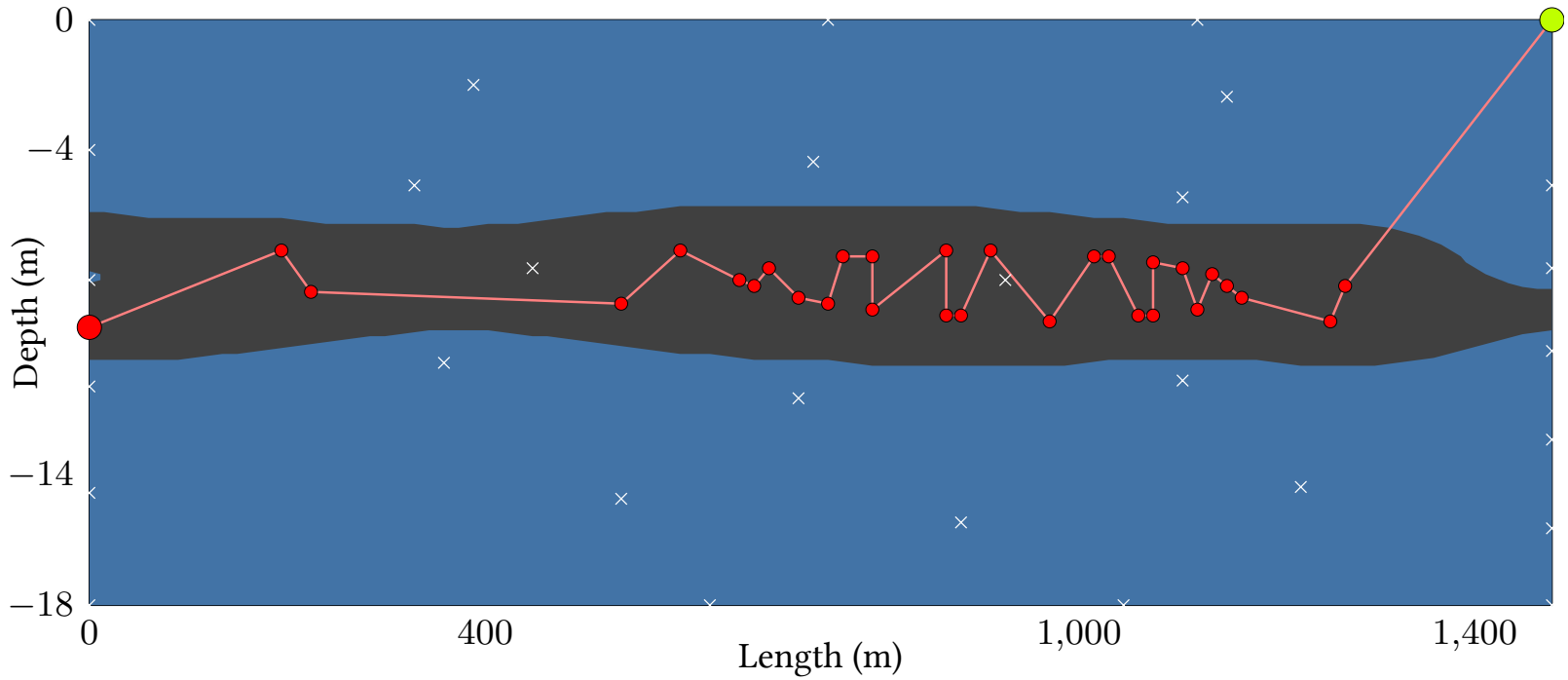

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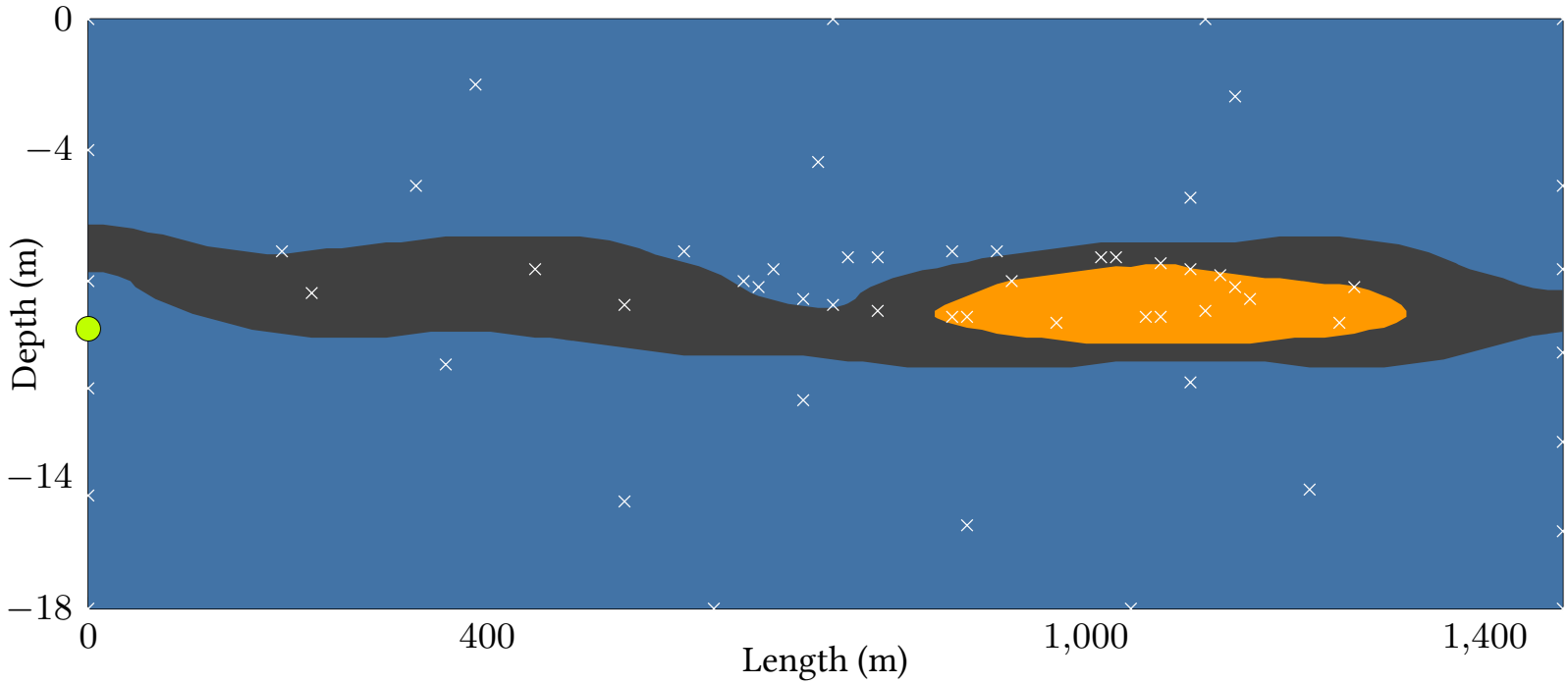

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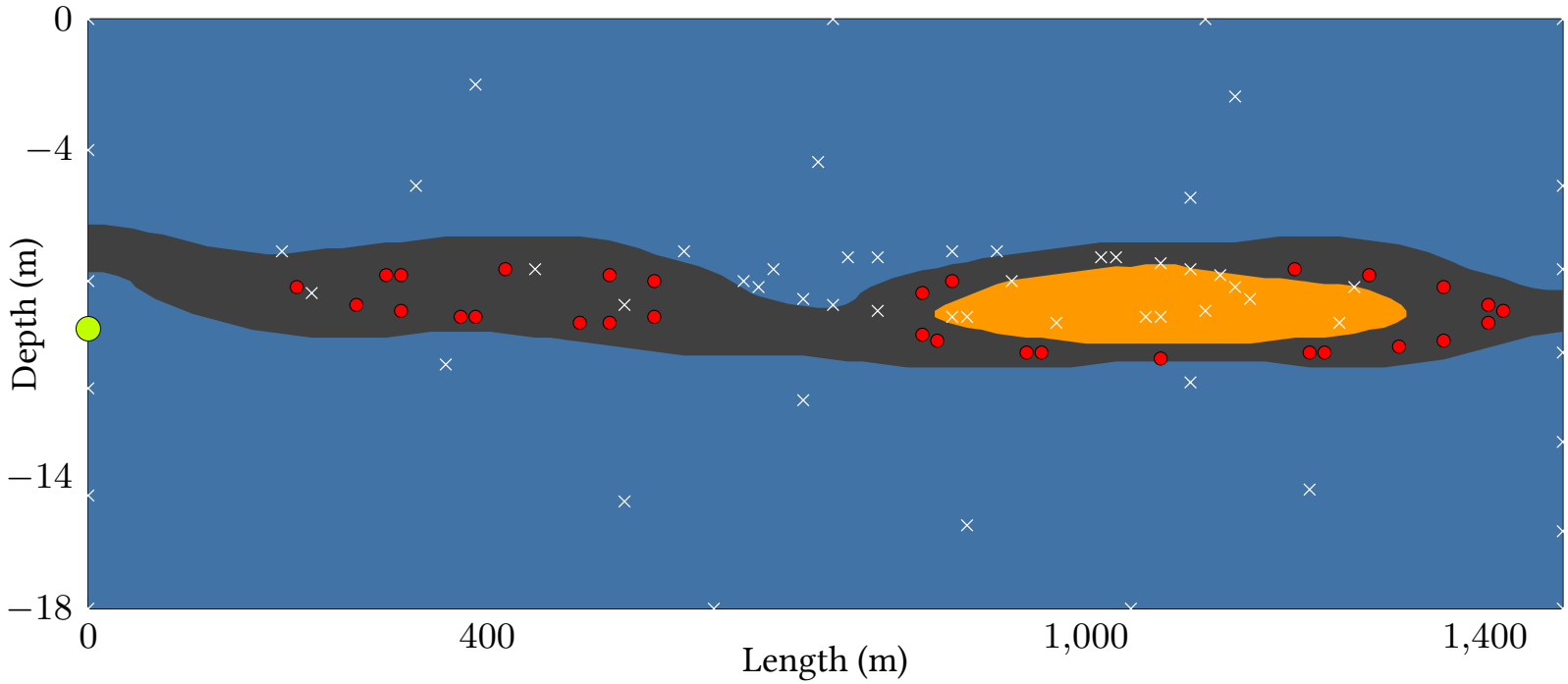

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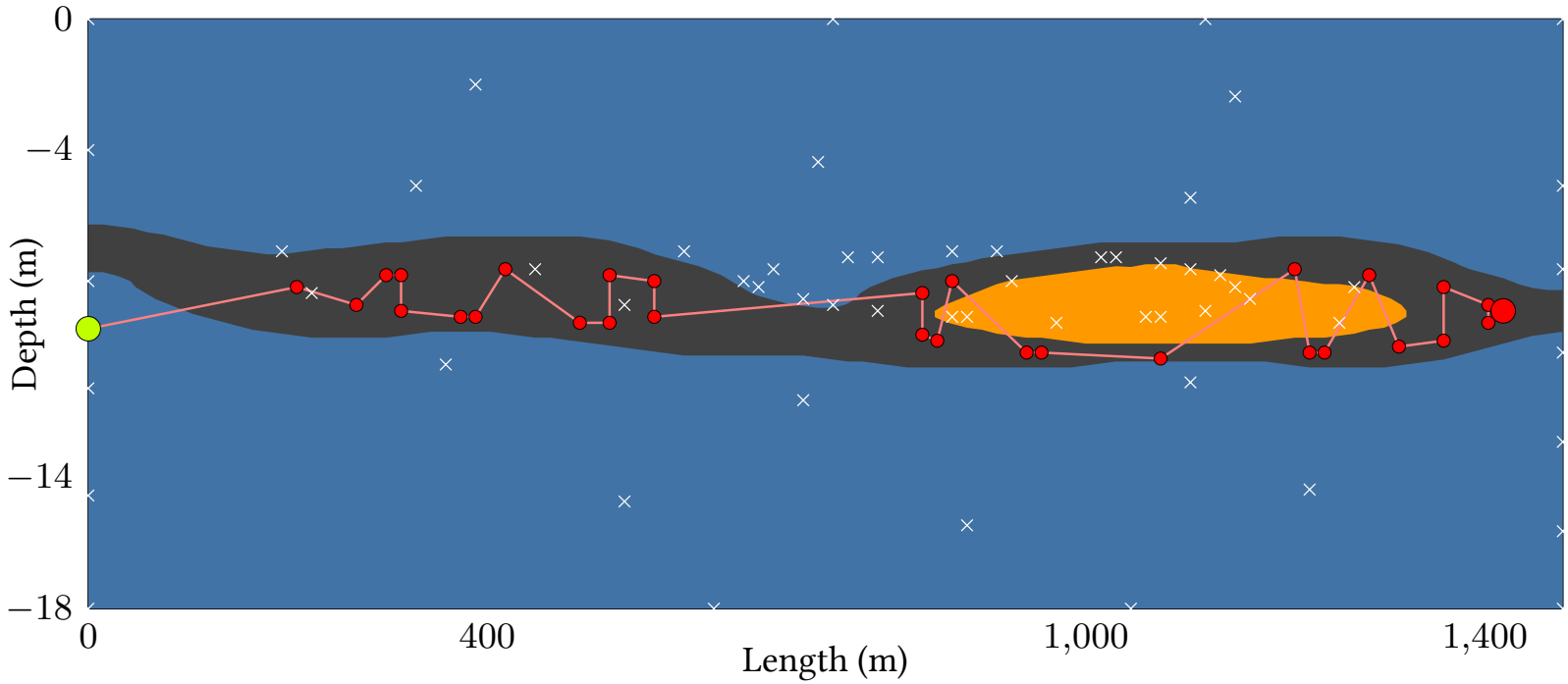

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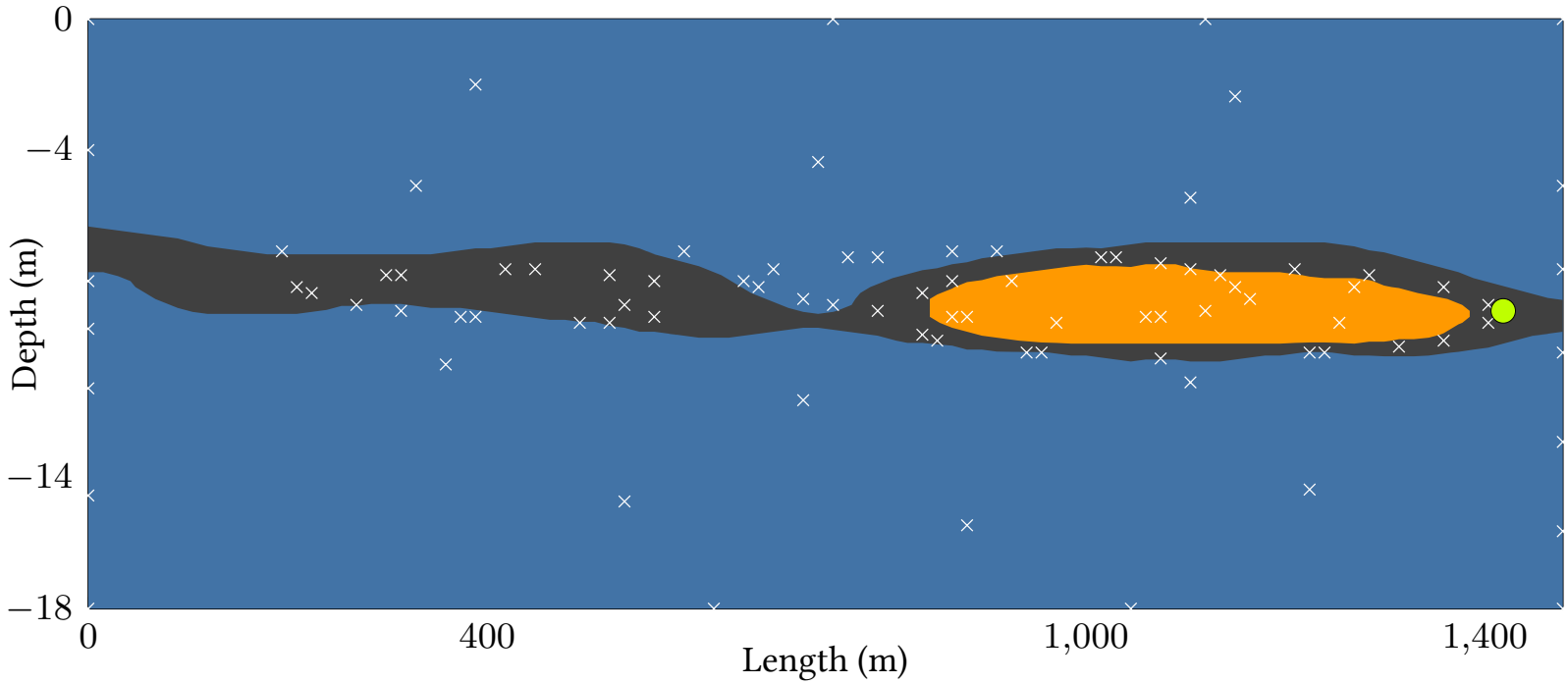

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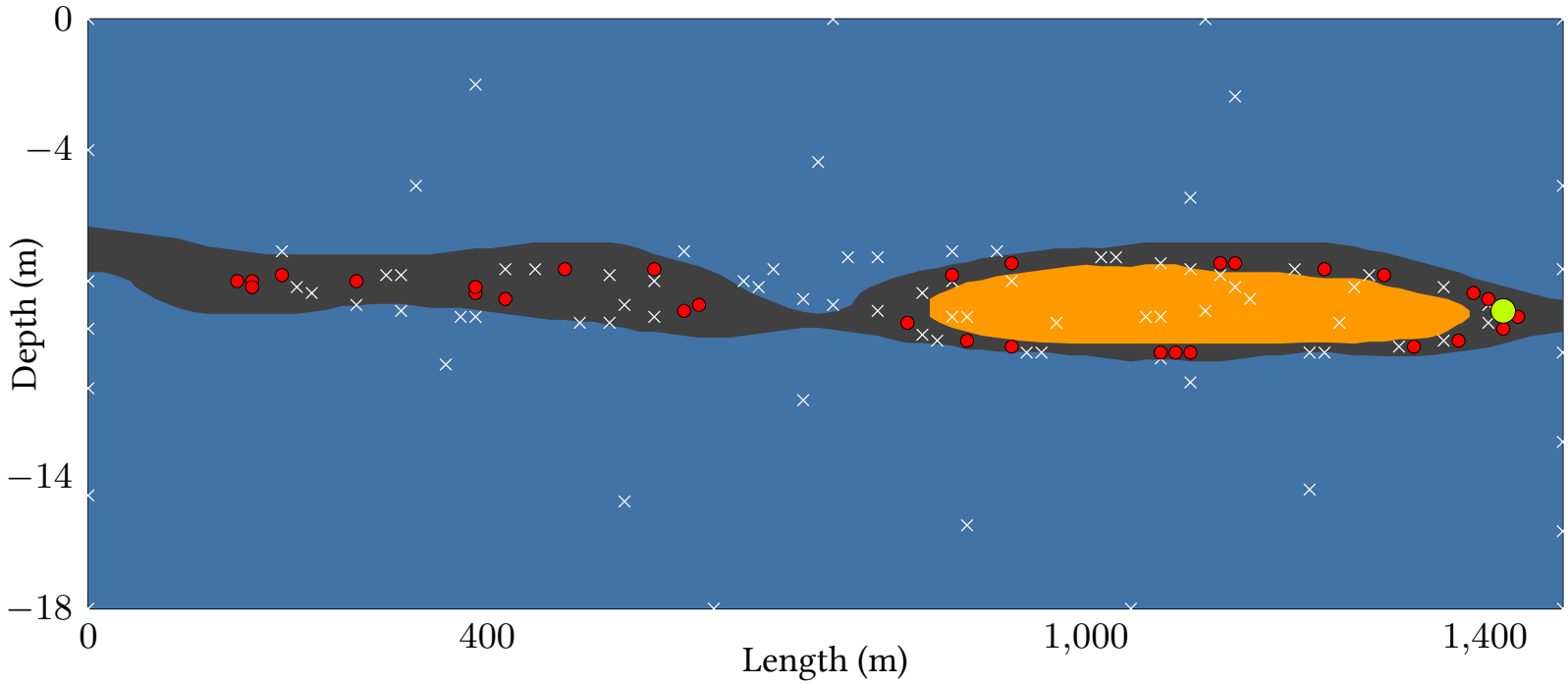

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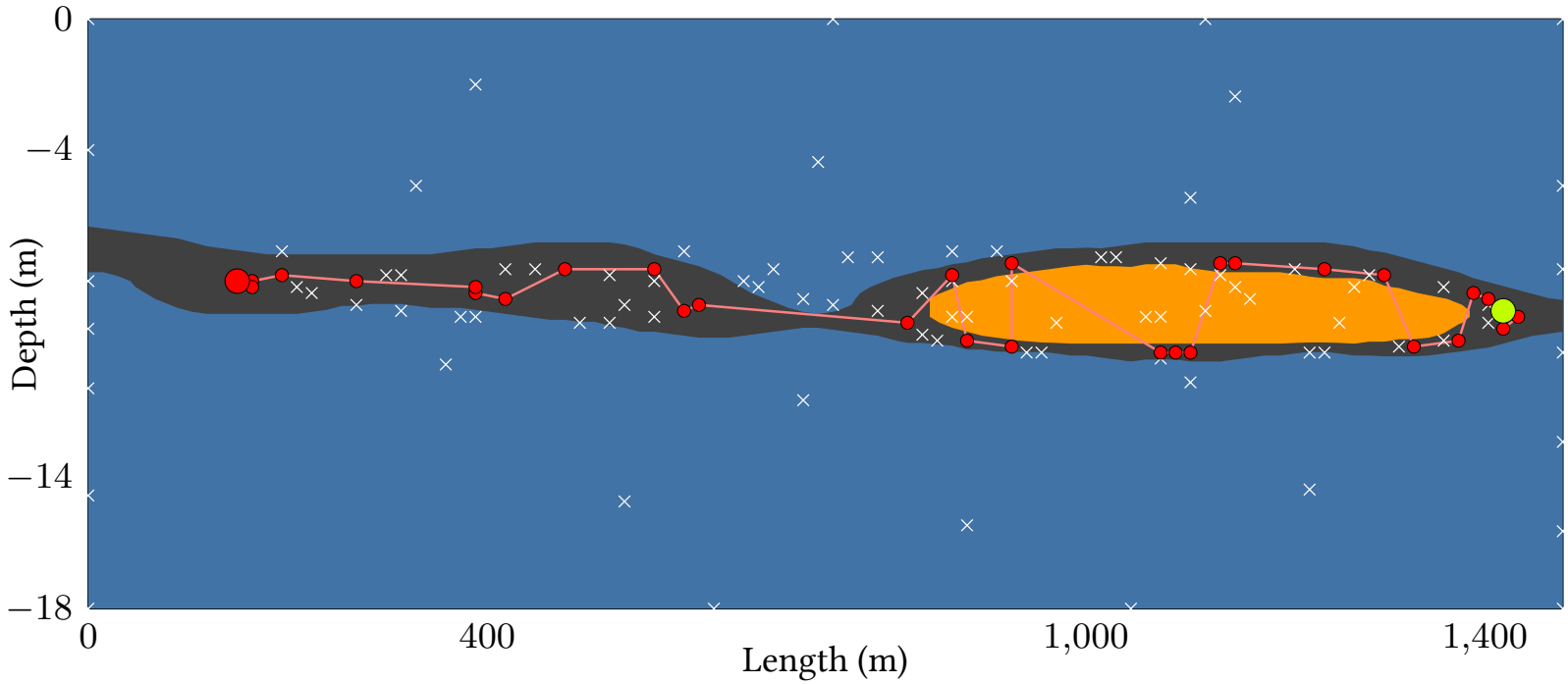

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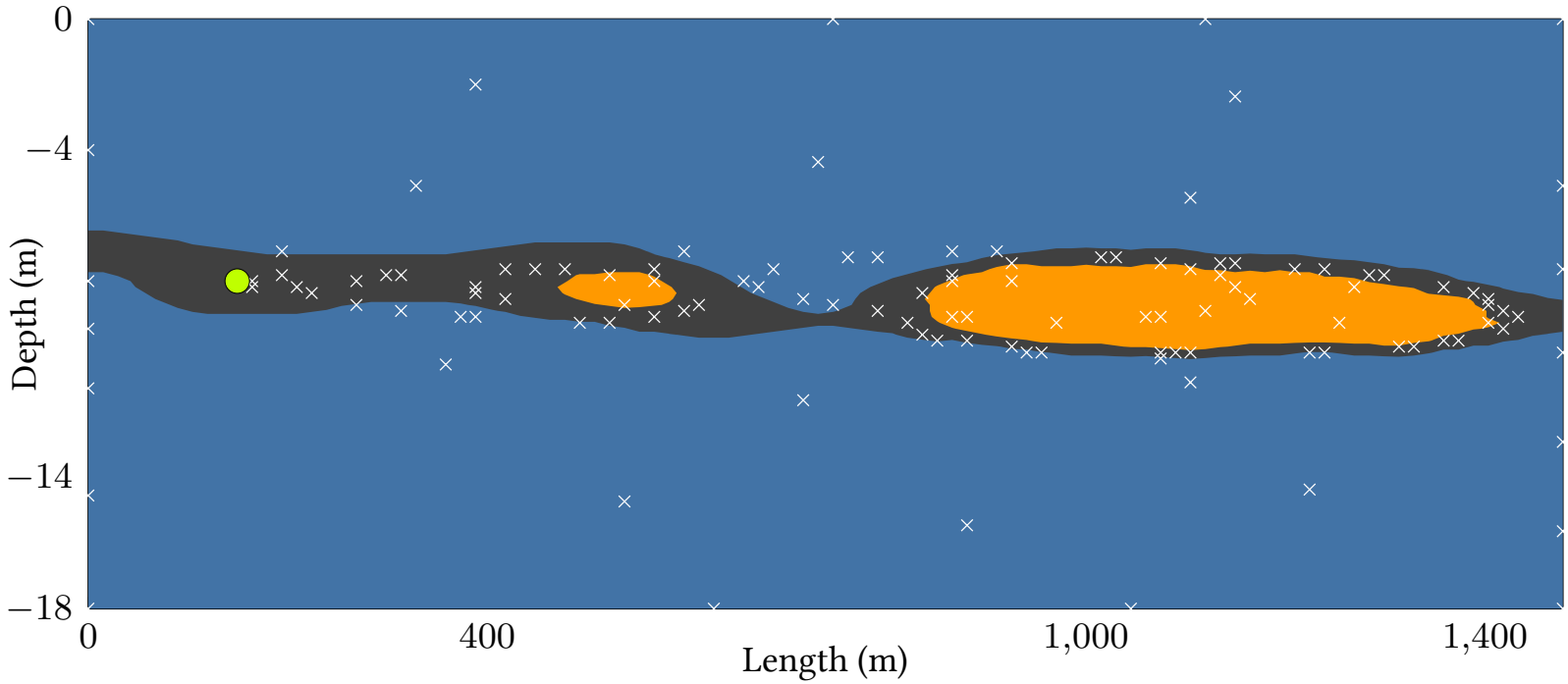

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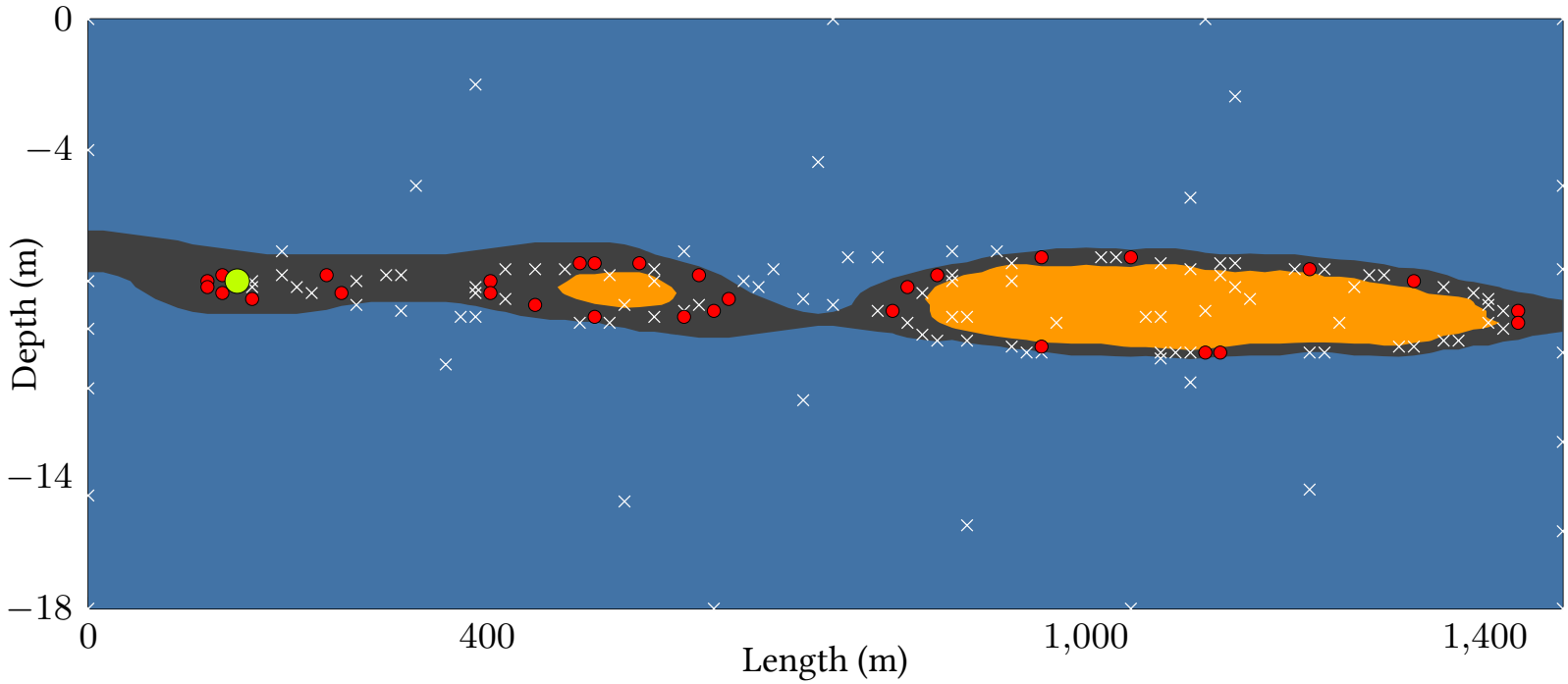

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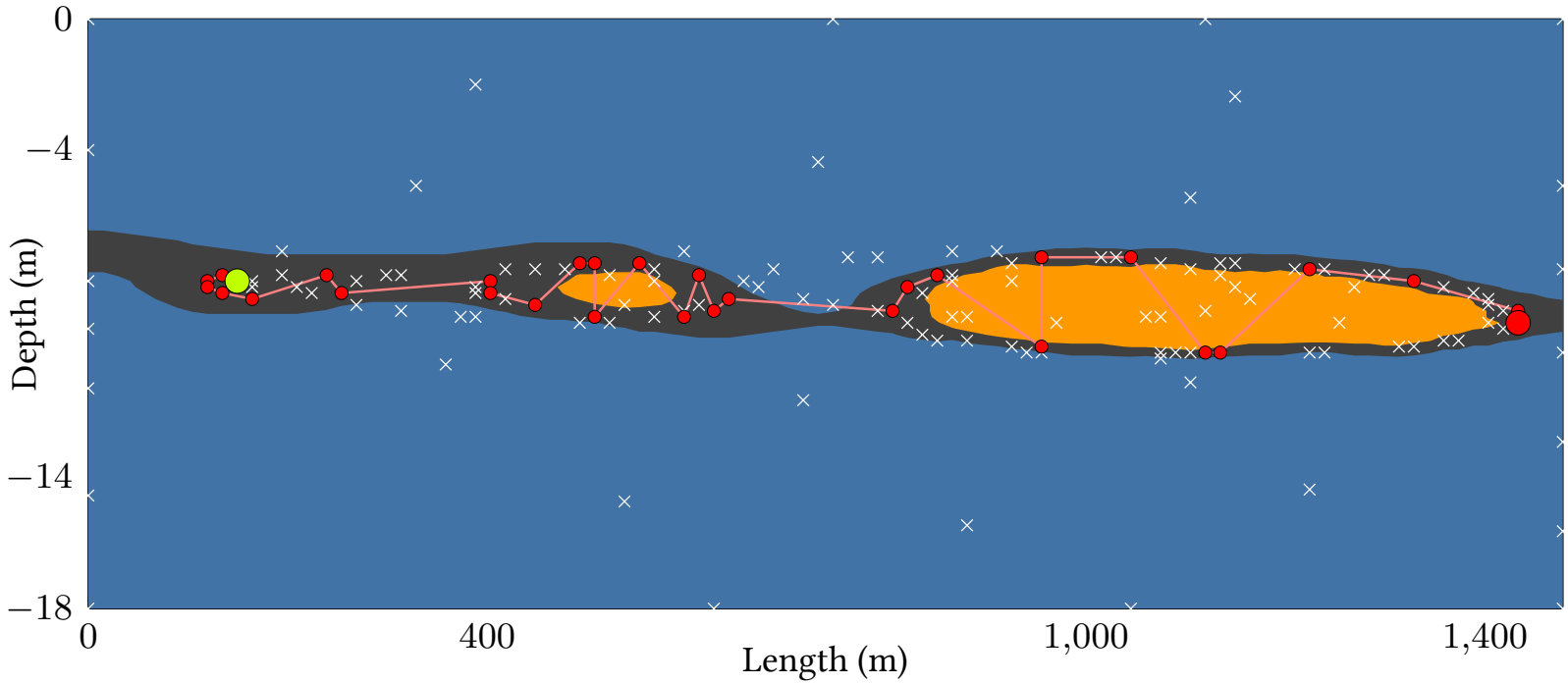

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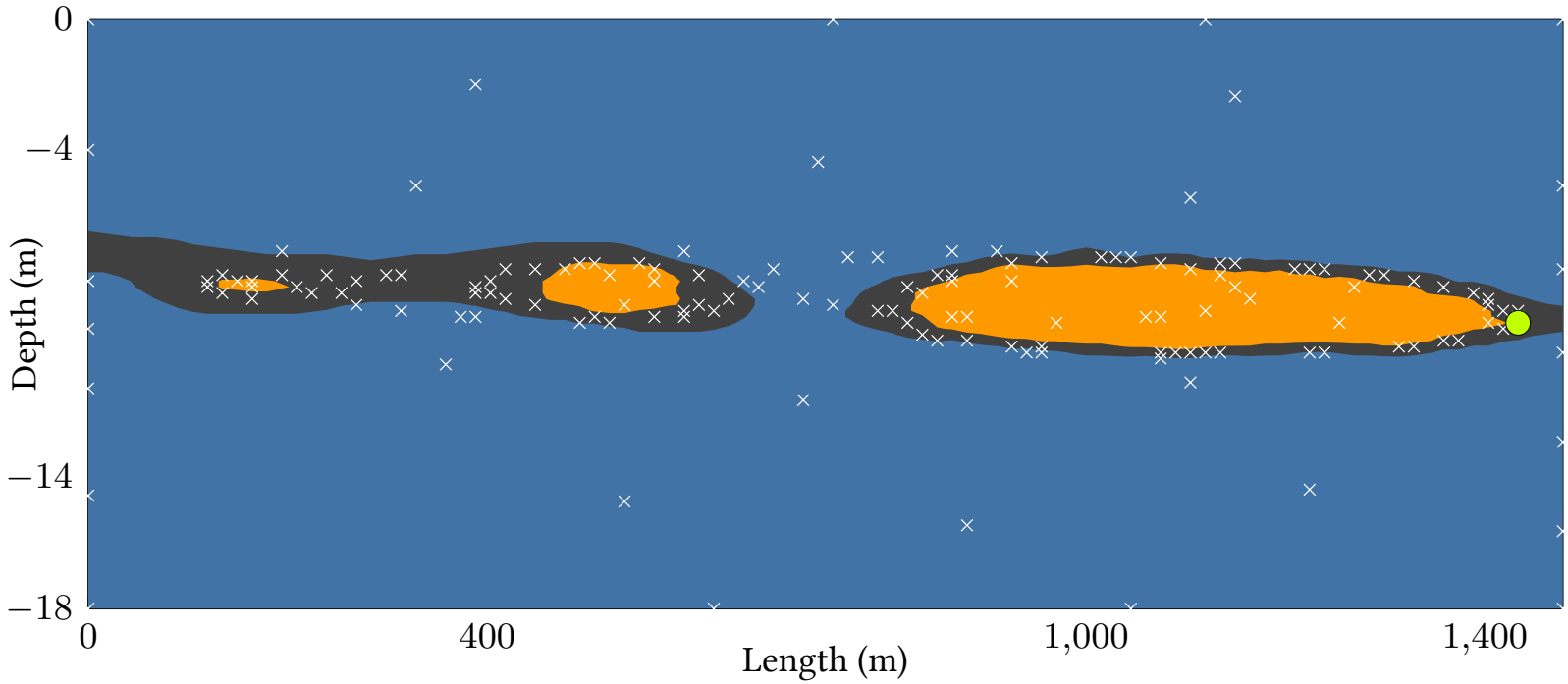

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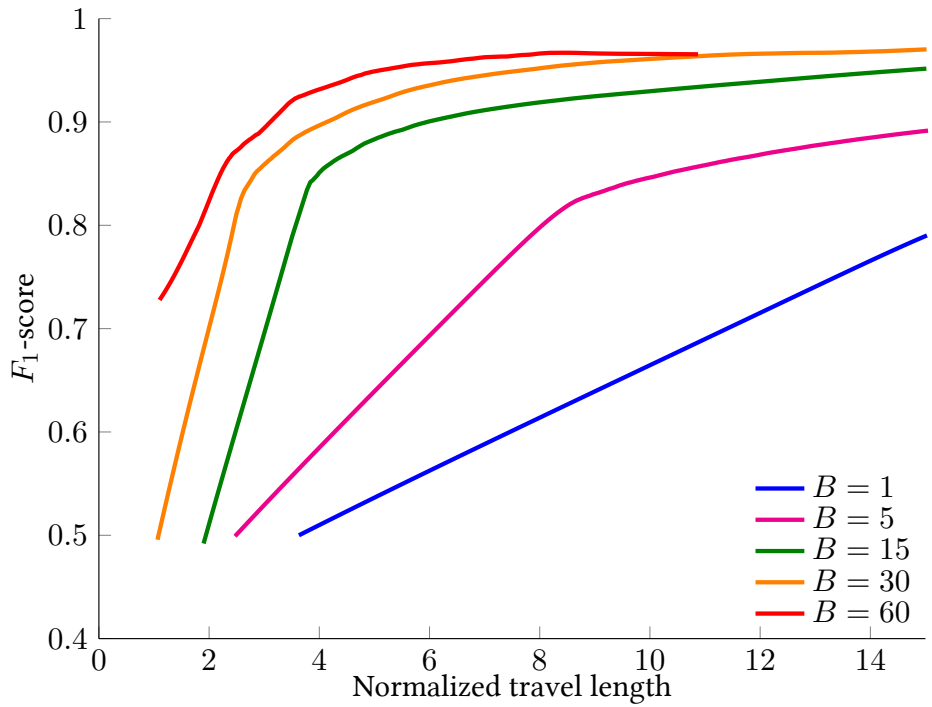

Come to the poster session for more...

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

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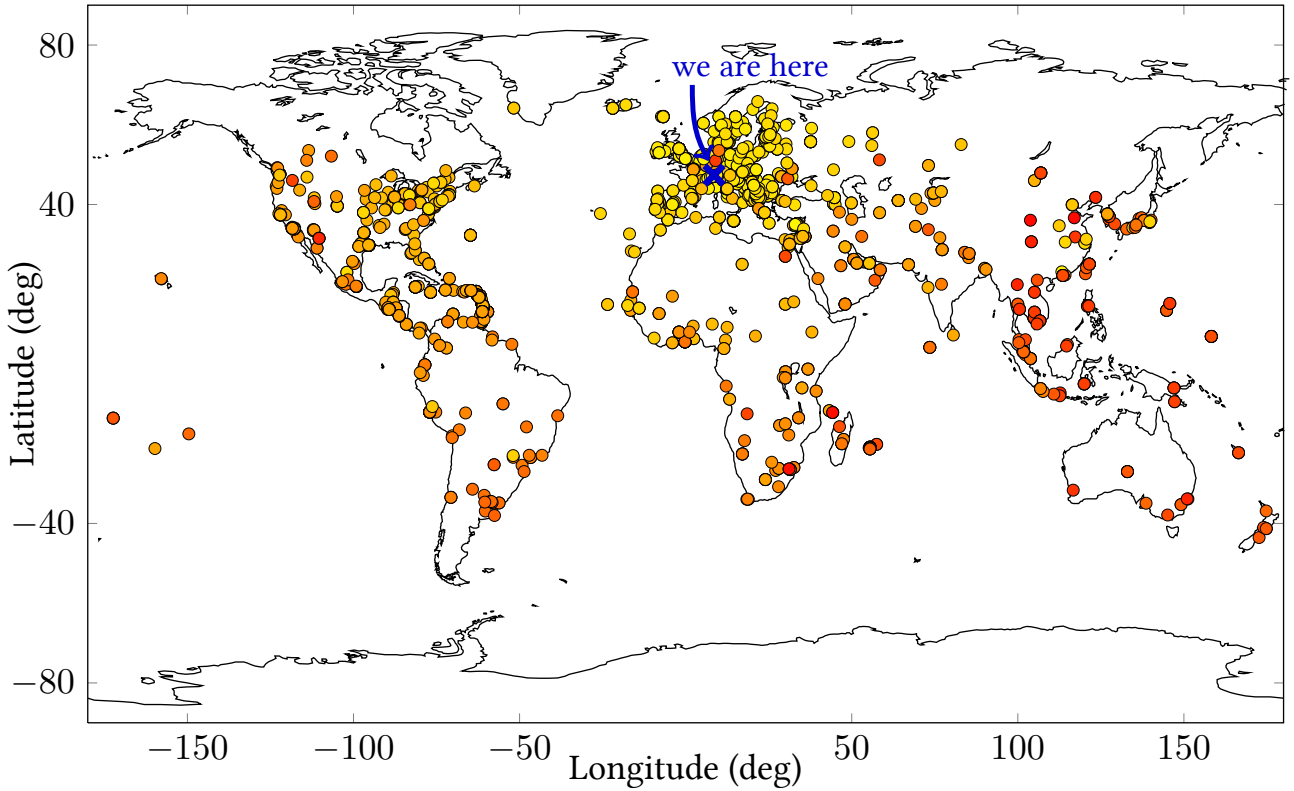
- ...applications: estimate world regions of low internet latency



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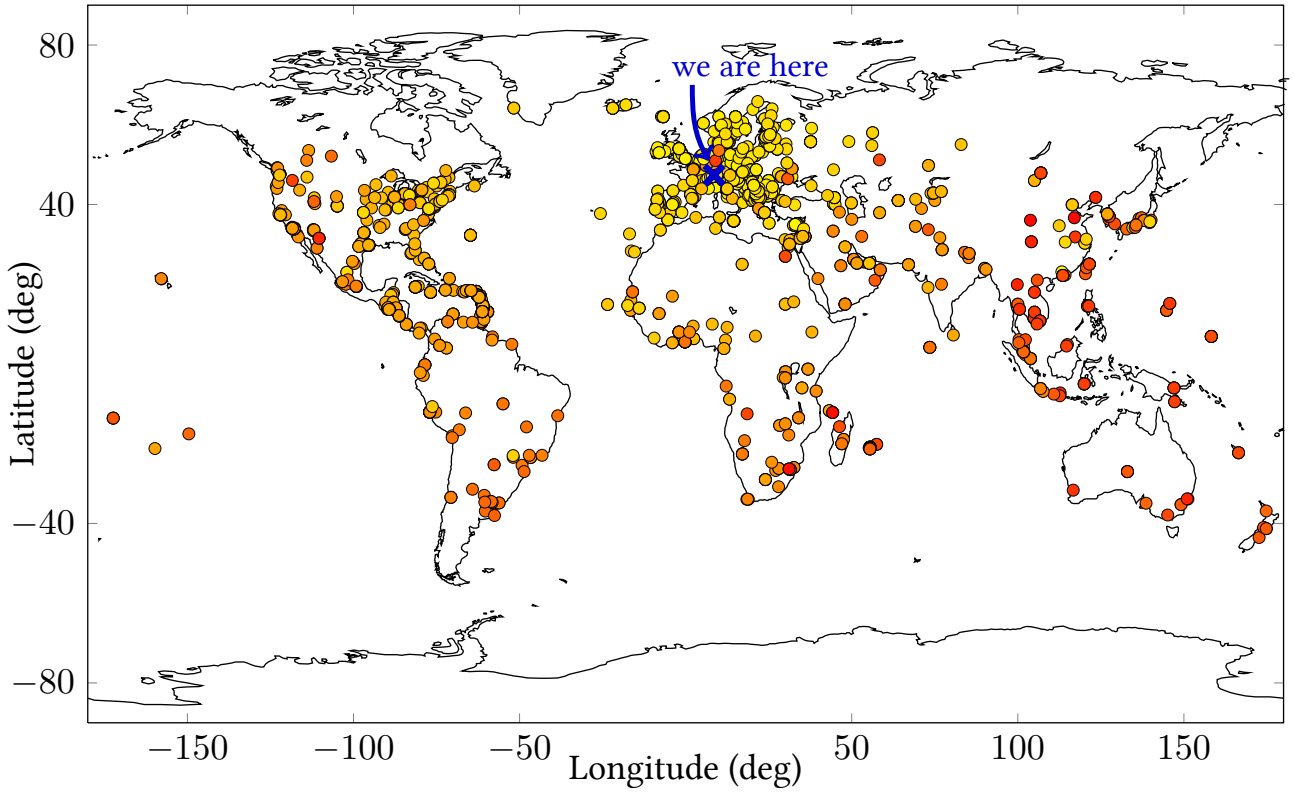

- ...results: why does LSE greatly outperform "straddle" in some cases?

Summary

- LSE algorithm:

Summary

- LSE algorithm:
  - Theoretical guarantees

Theorem (Convergence of LSE)

For any $h \in \mathbb{R}$, $\delta \in (0,1)$, 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

$$\frac{T}{\beta_T \hat{\gamma}_T} \geq \frac{C_1}{4\epsilon^2},$$

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- LSE algorithm:
  - Theoretical guarantees
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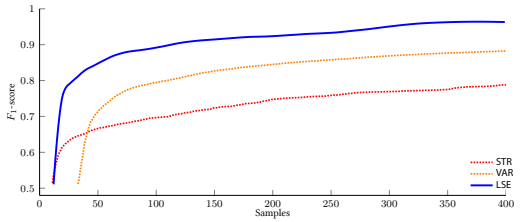

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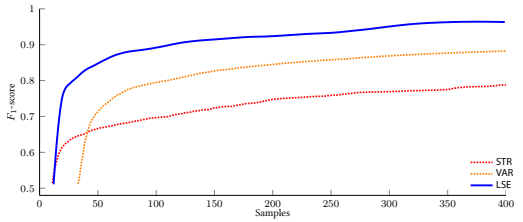

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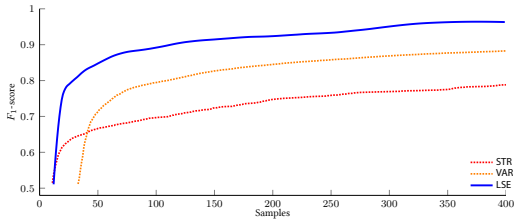

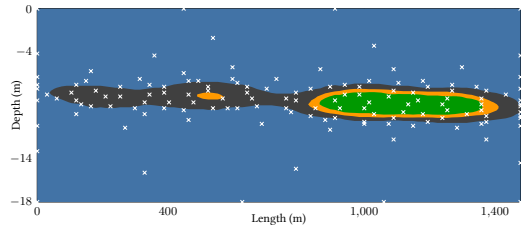

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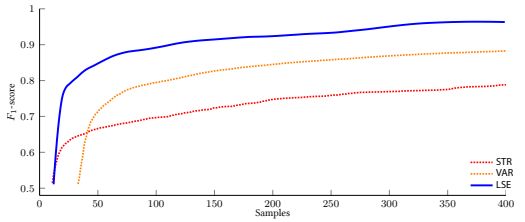

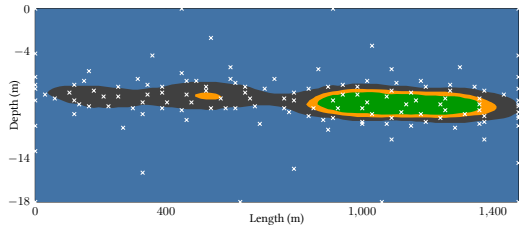

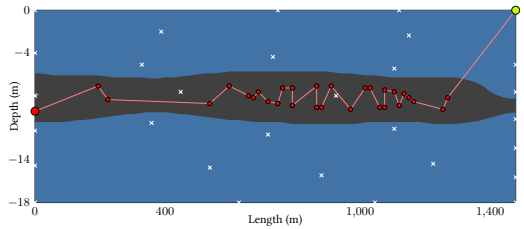

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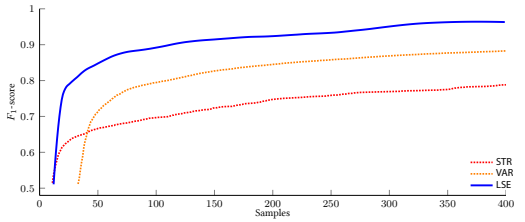

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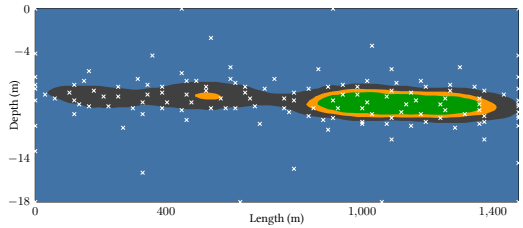

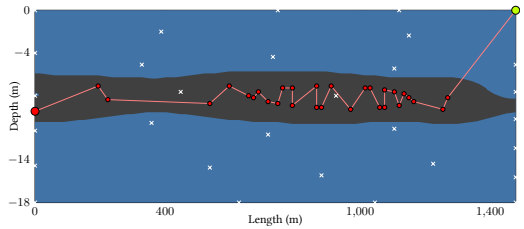

- Look out for algae when swimming in Lake Zurich! ☺