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To Bayesian Optimisation and Beyond

Gaussian Processes as Decision Makers

Henry Moss

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Bayesian Search

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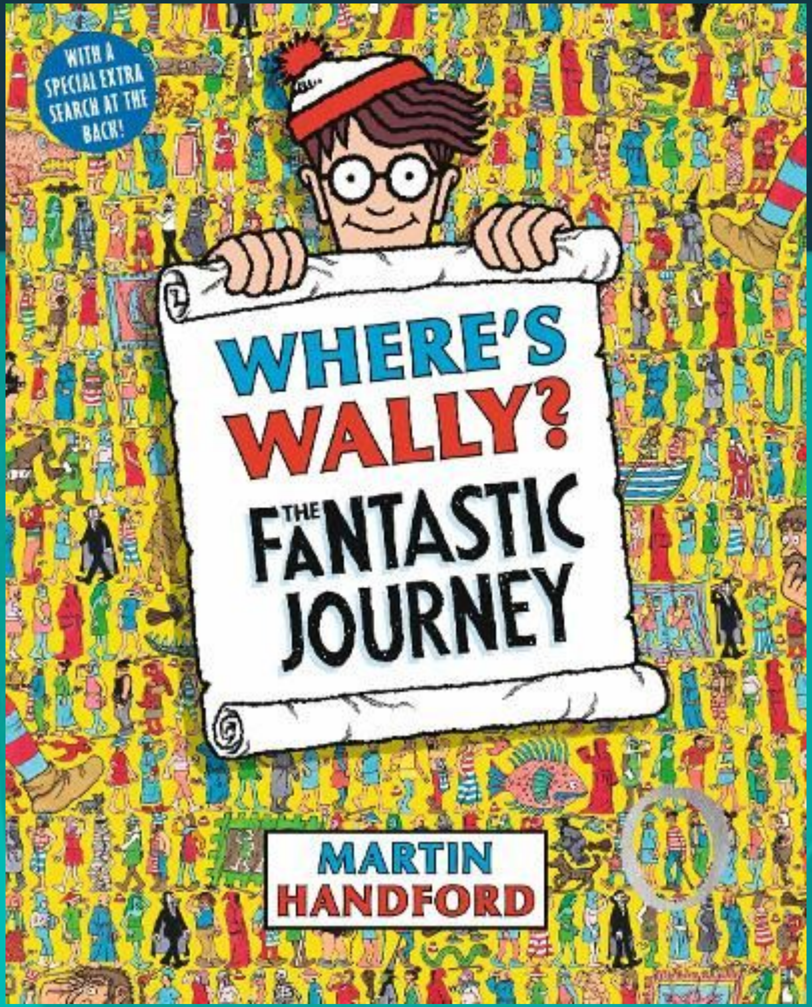
Bayesian Search



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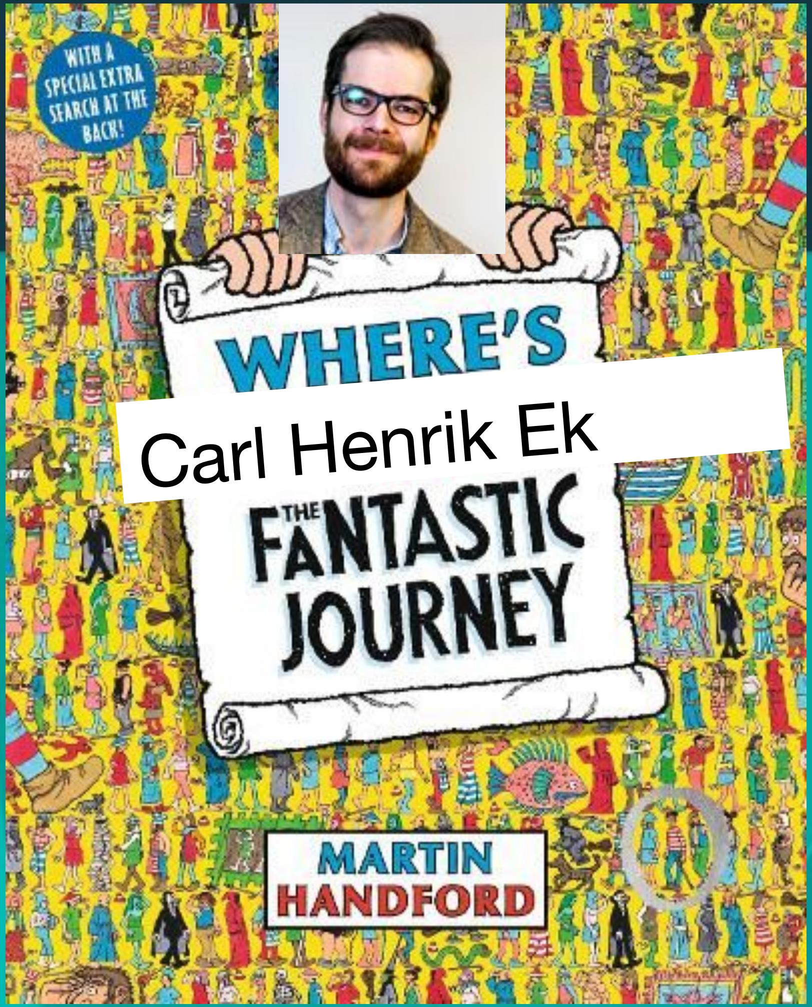
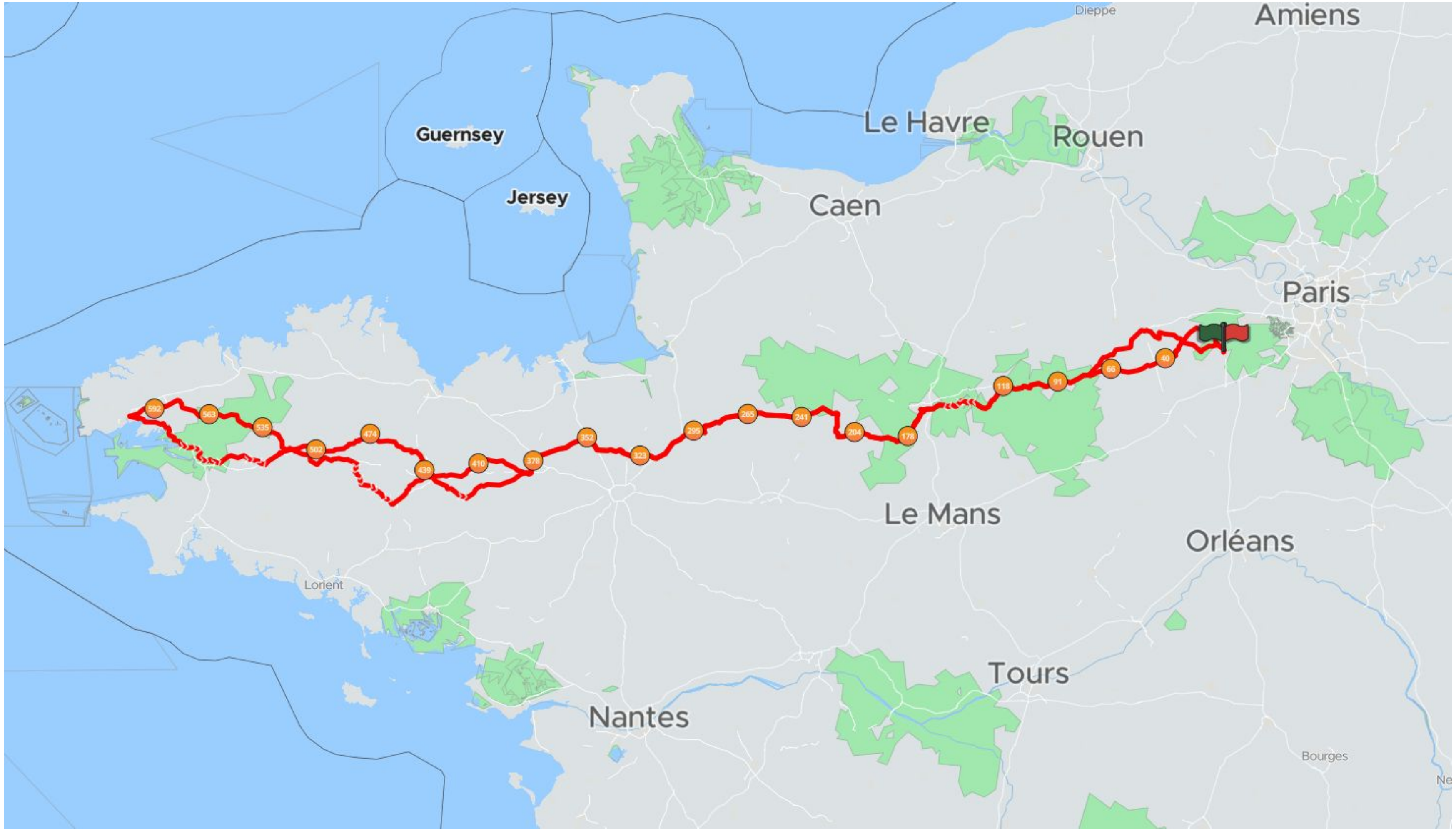
Bayesian Search



Where is Carl Henrik?



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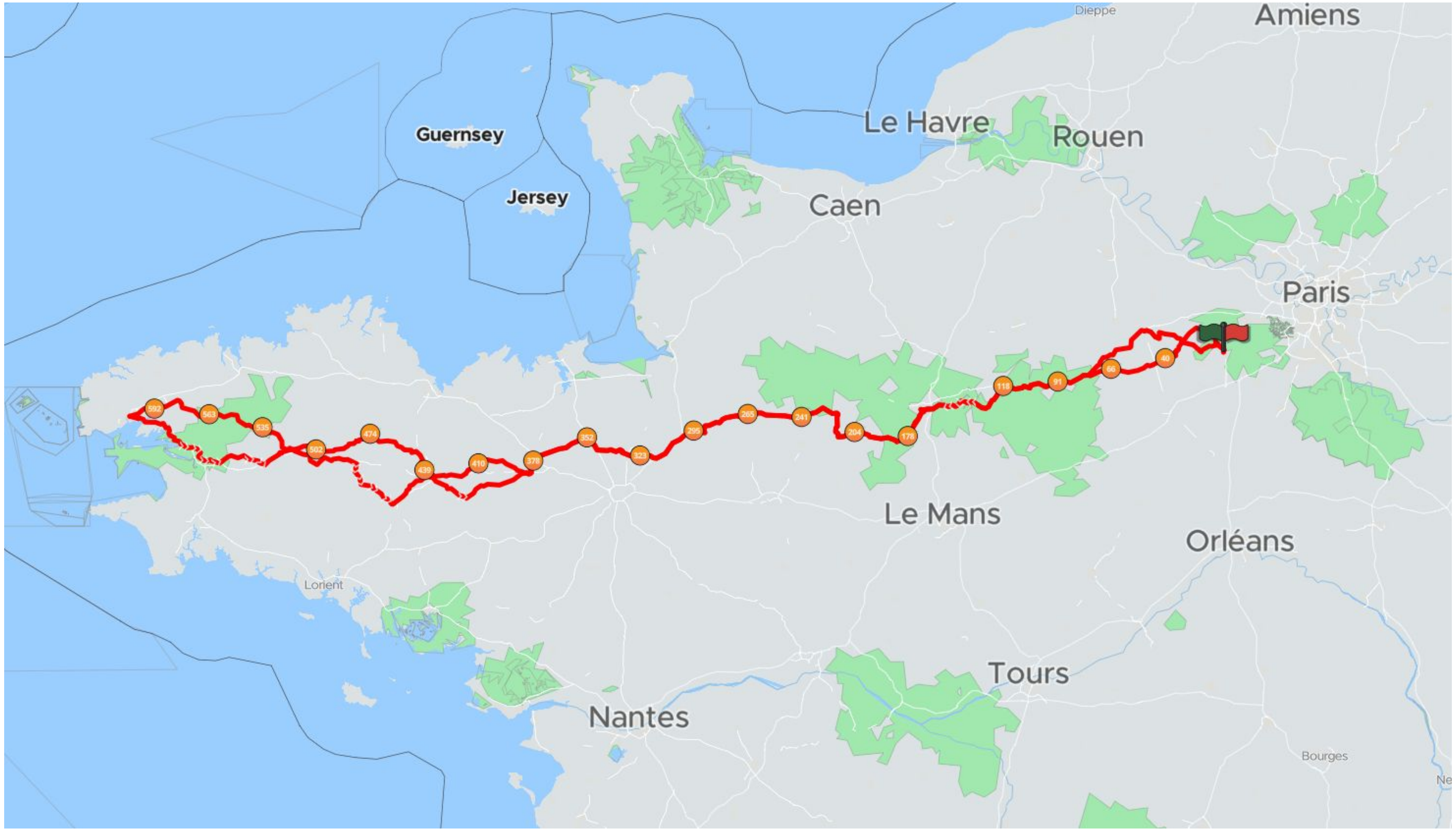
At 3:30 AM?



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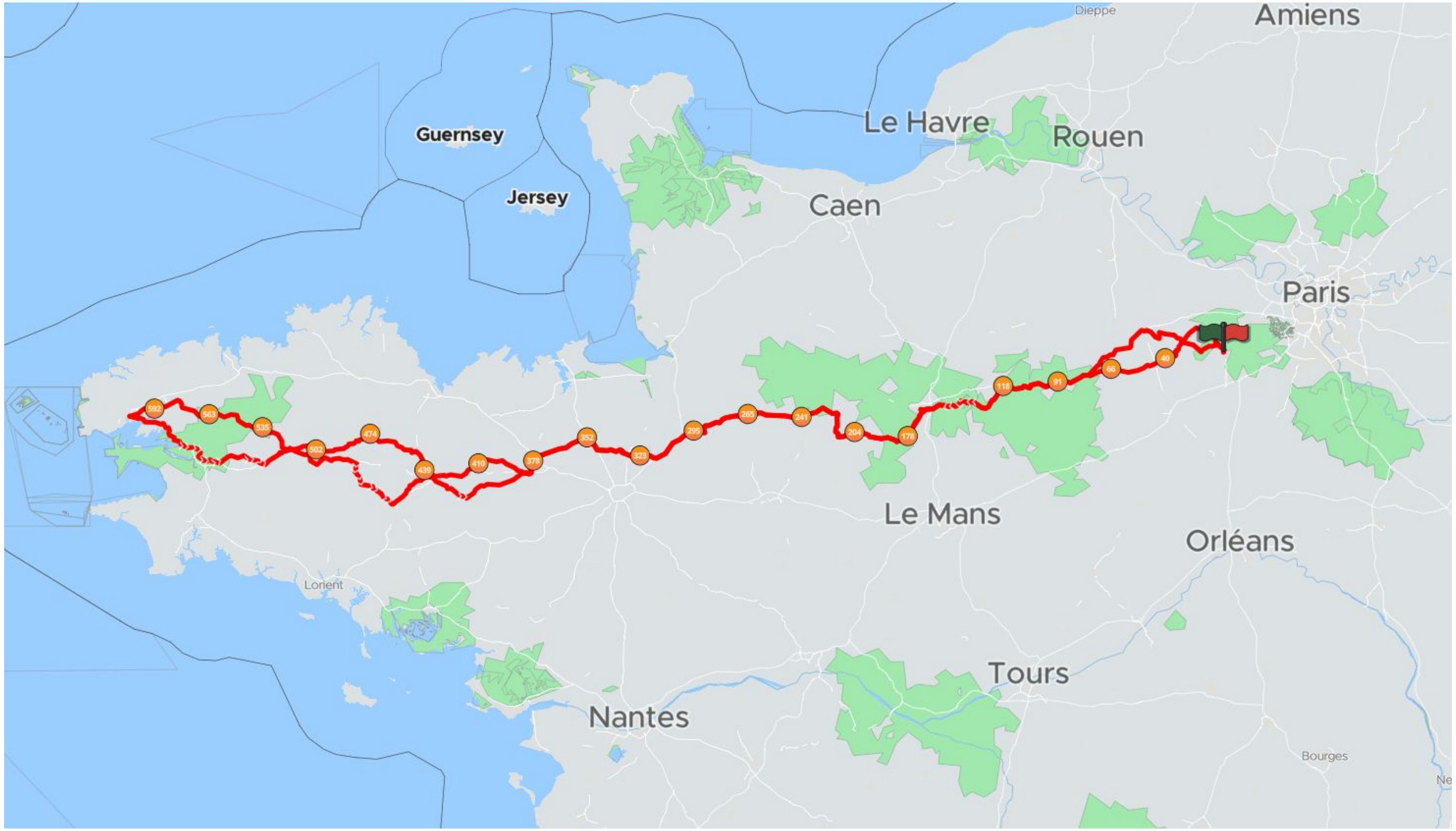

$$d = v \times t$$

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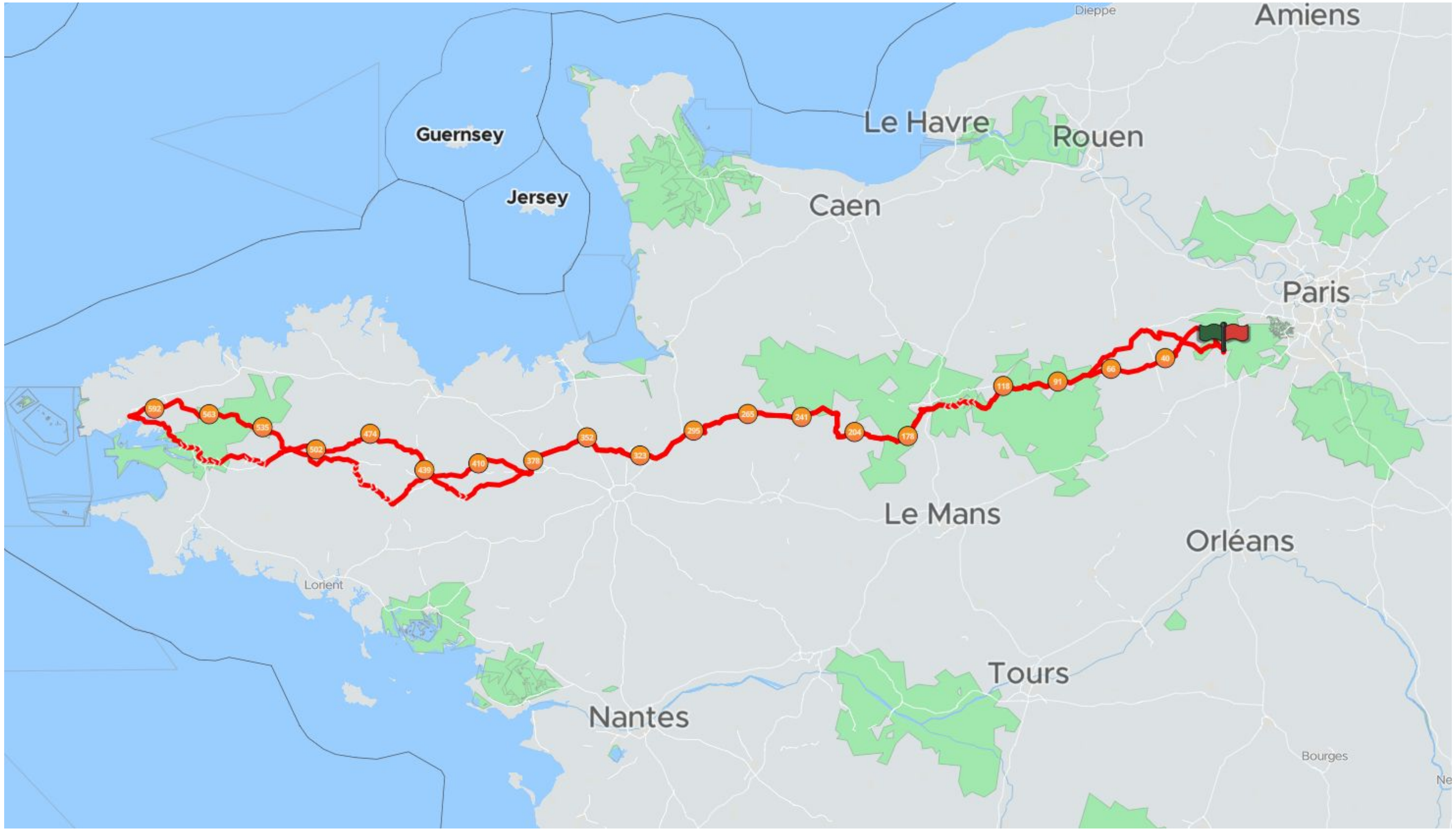

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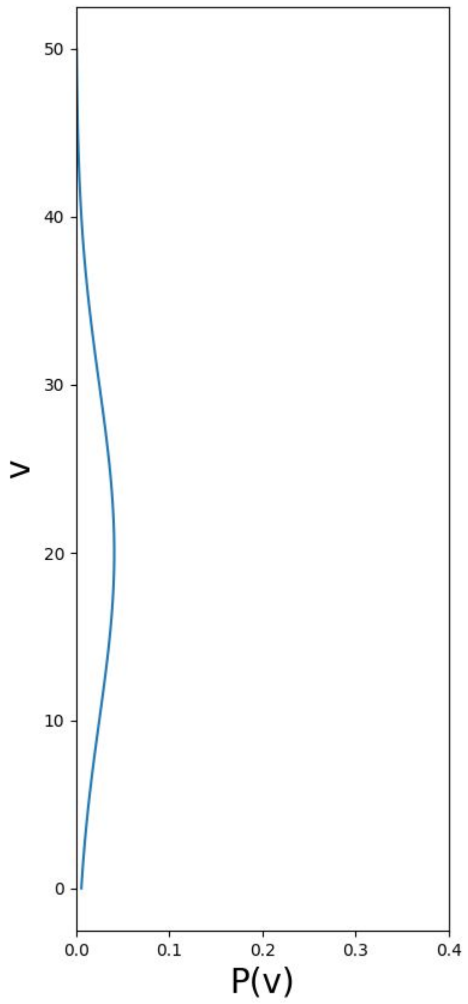

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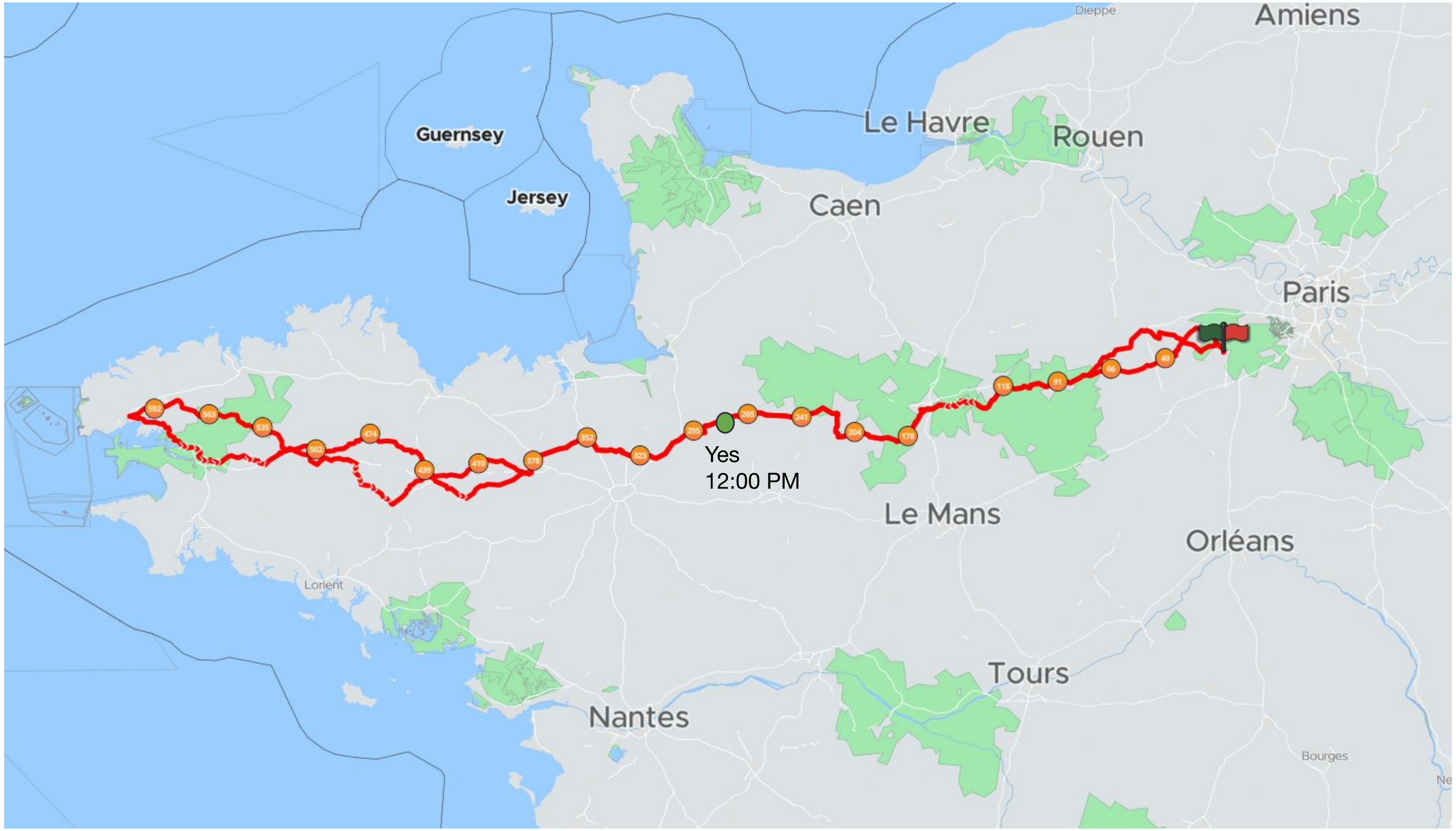

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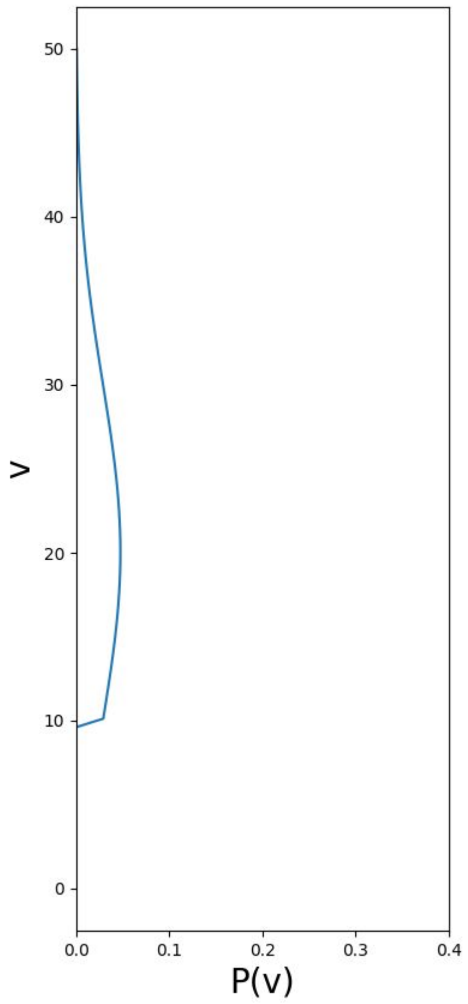

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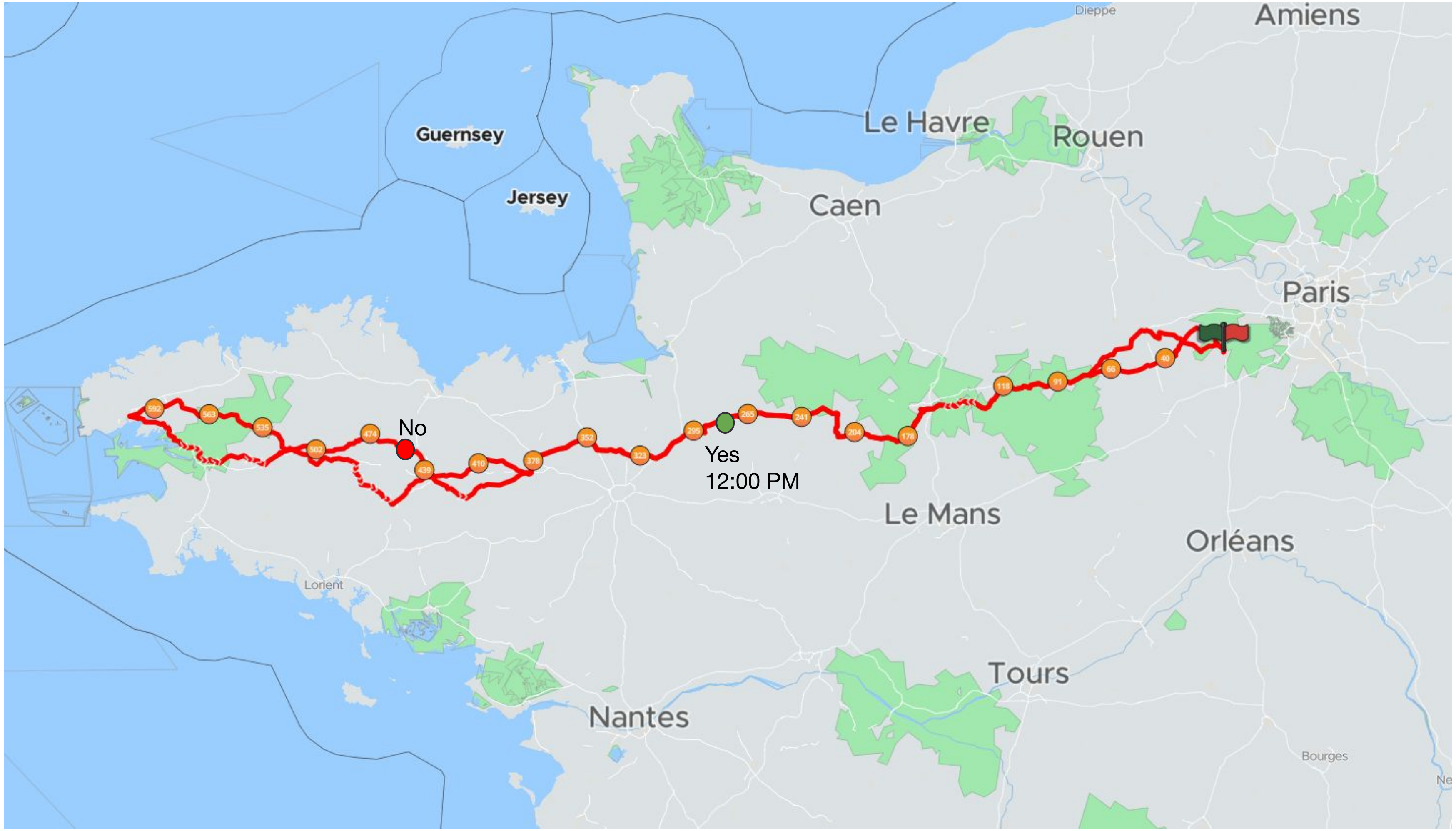

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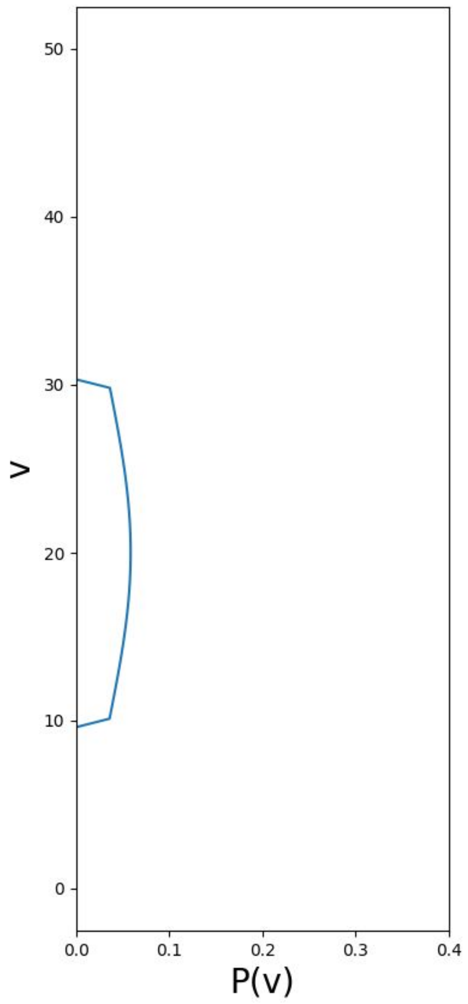

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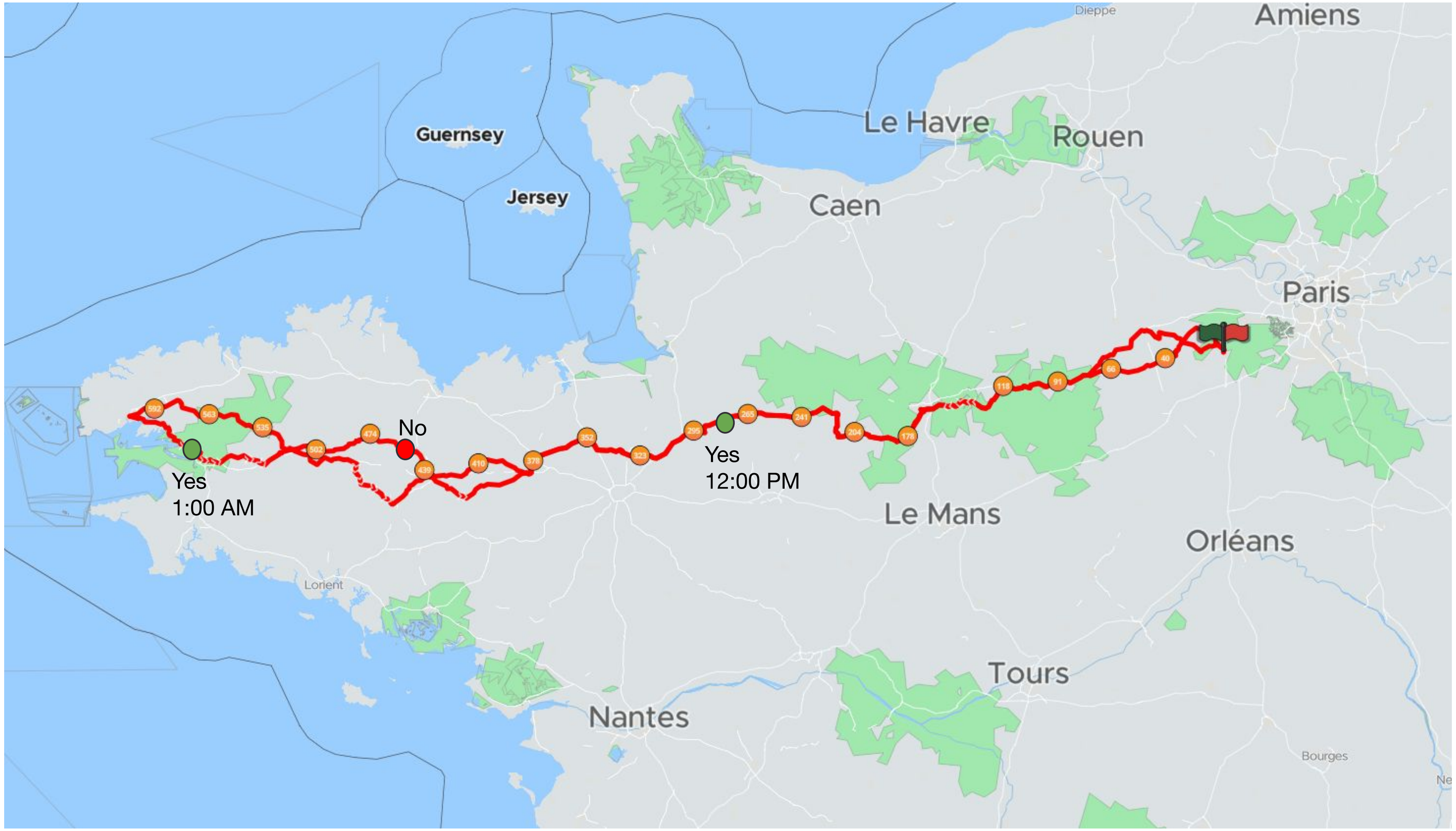

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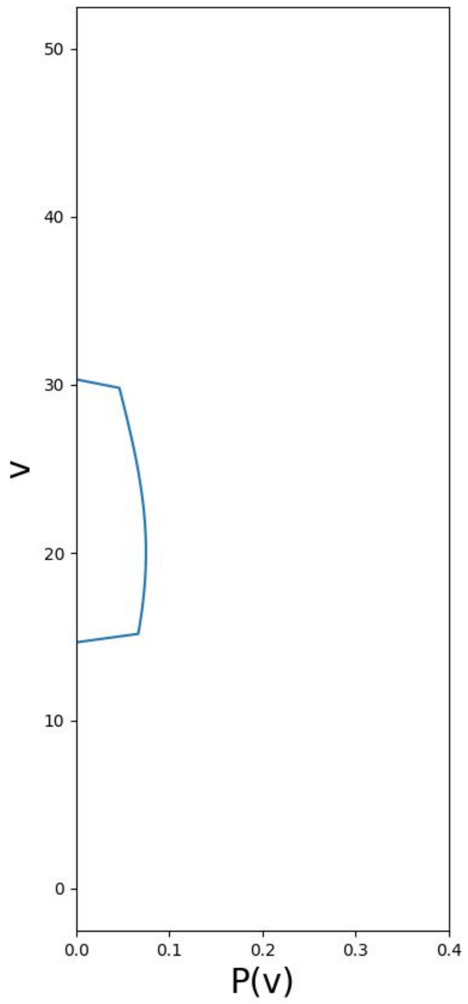

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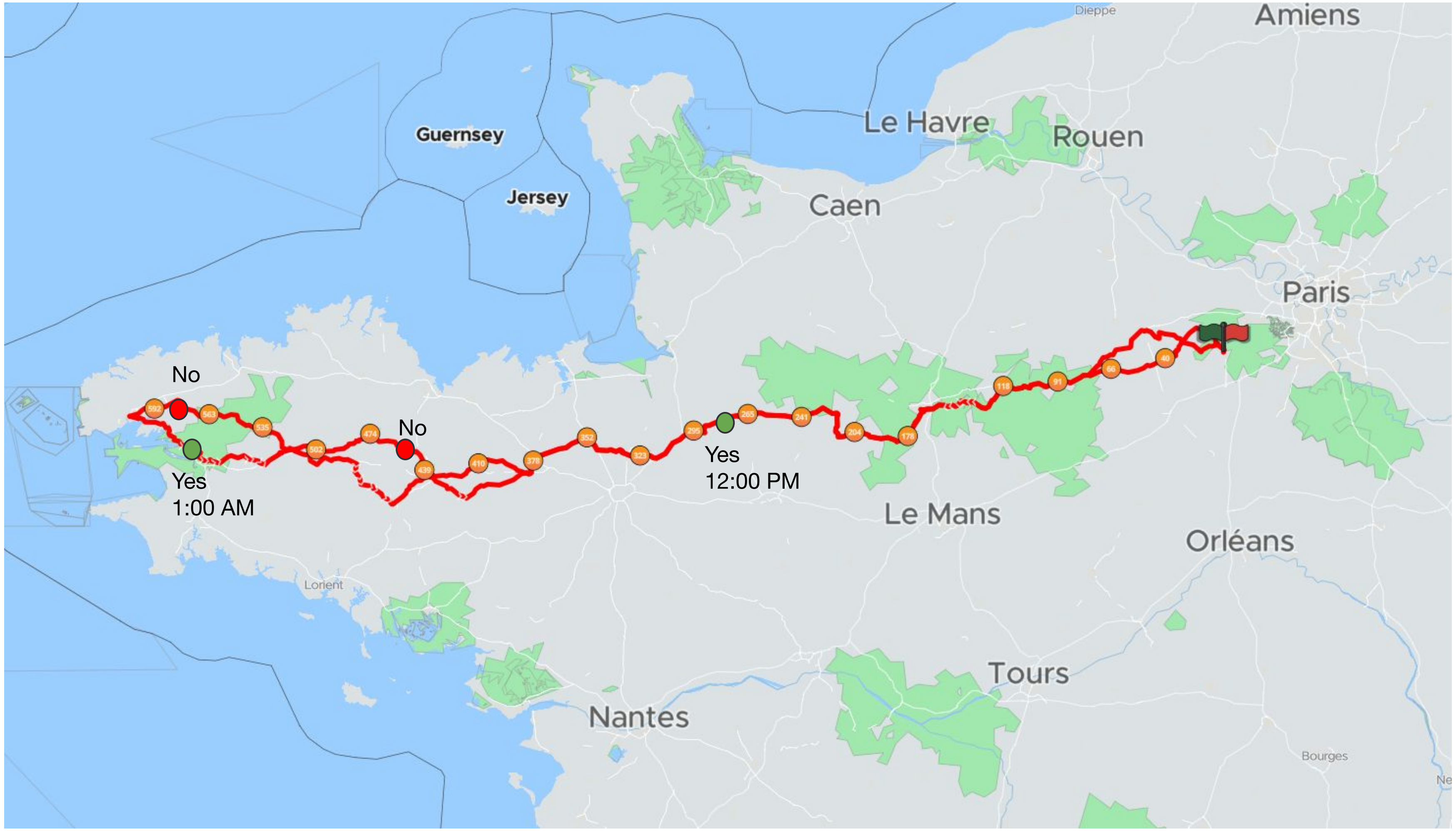

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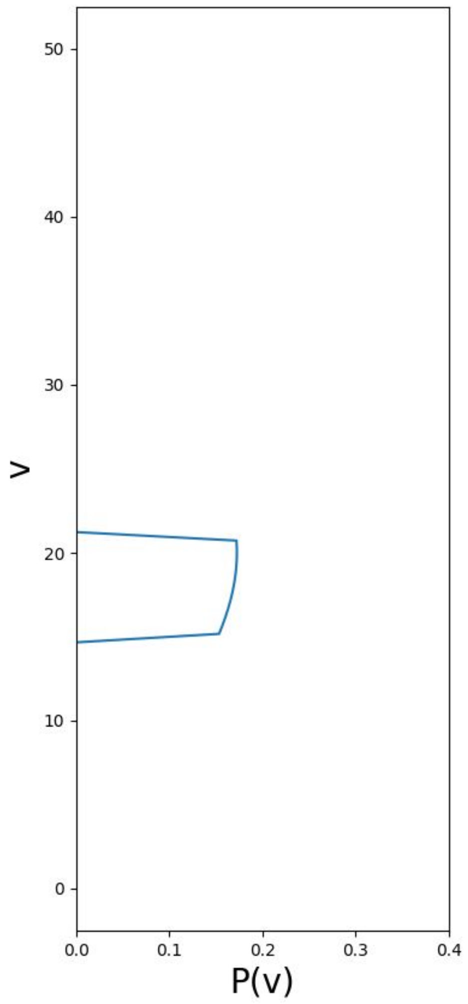

Where is Carl Henrik?

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But can we do better than **random**???

What is Active Learning?

Bayesian search for learning functions

Sequential data collection

Let's make use of uncertainty estimates to make better models

Sequential data collection

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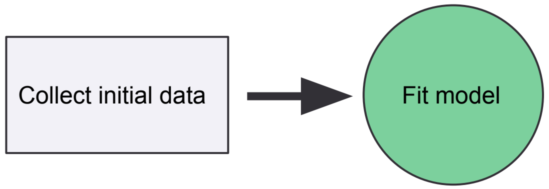
Collect initial data

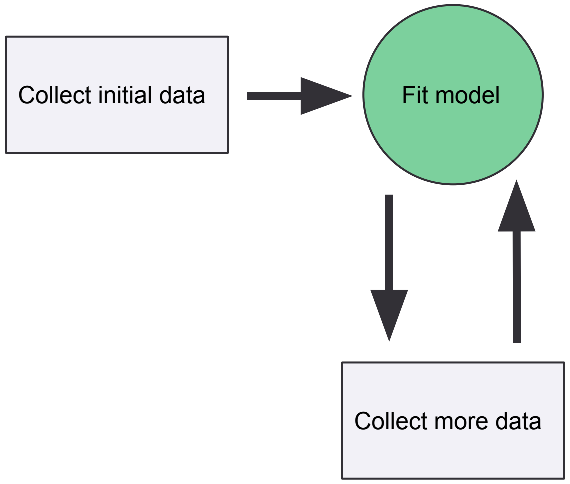
Sequential data collection

Let's make use of uncertainty estimates to make better models



Sequential data collection

Let's make use of uncertainty estimates to make better models



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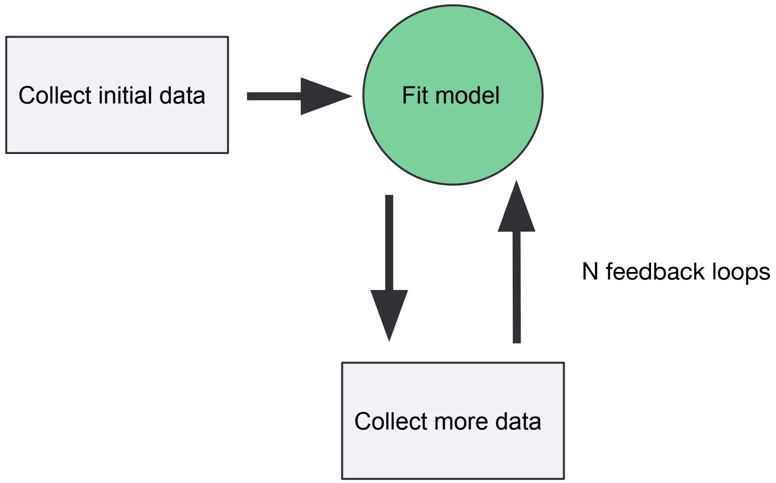

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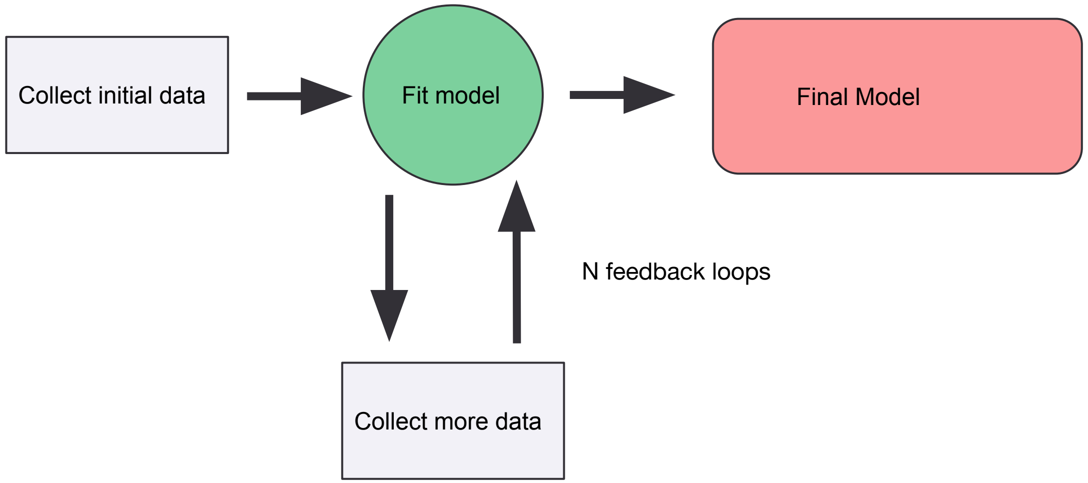

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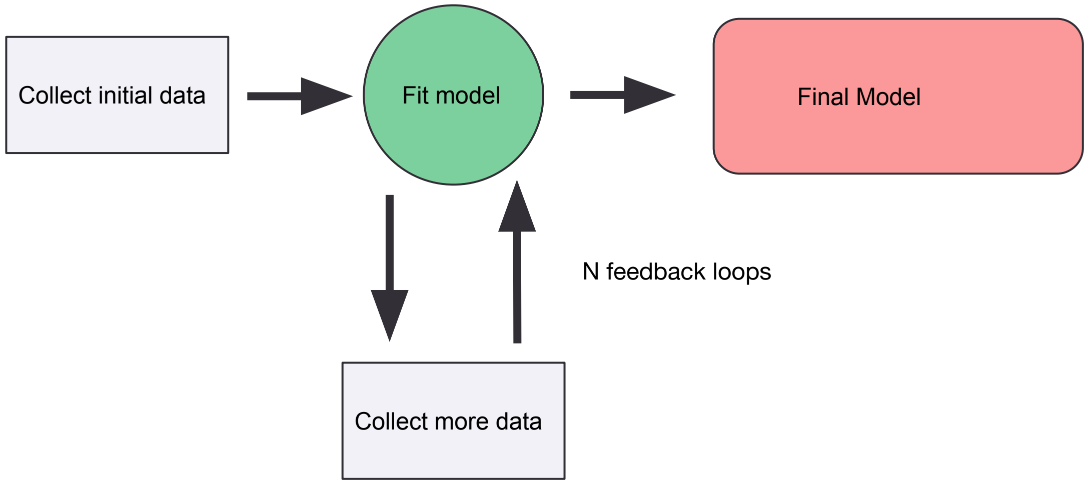

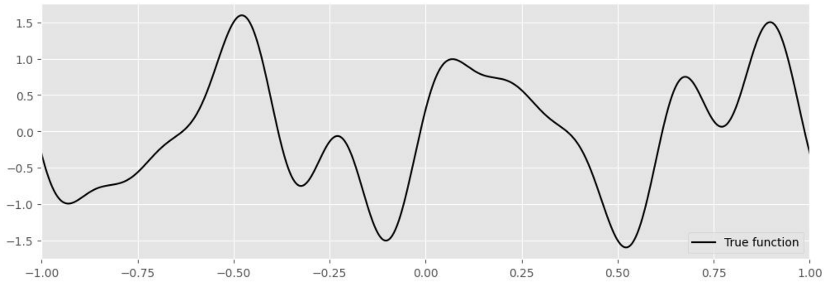

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Sequential data collection

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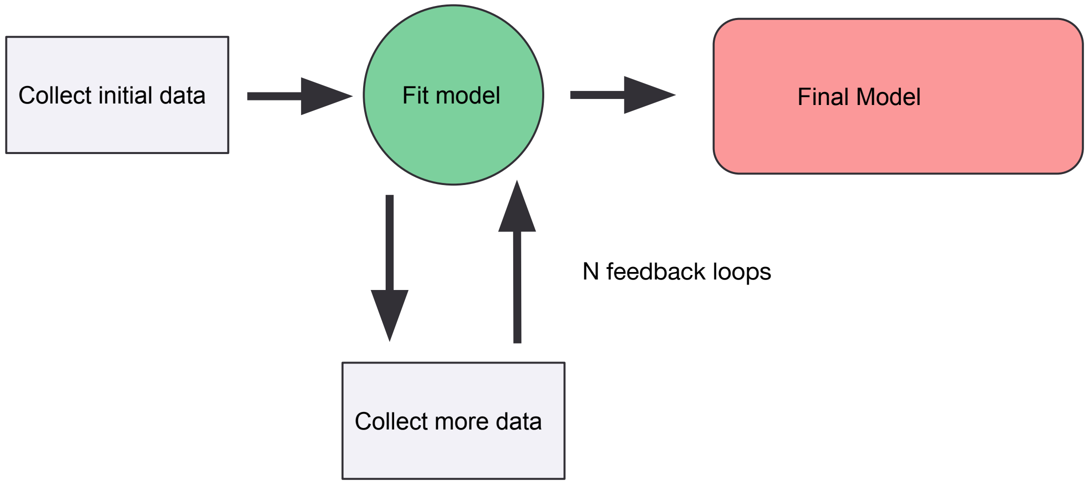

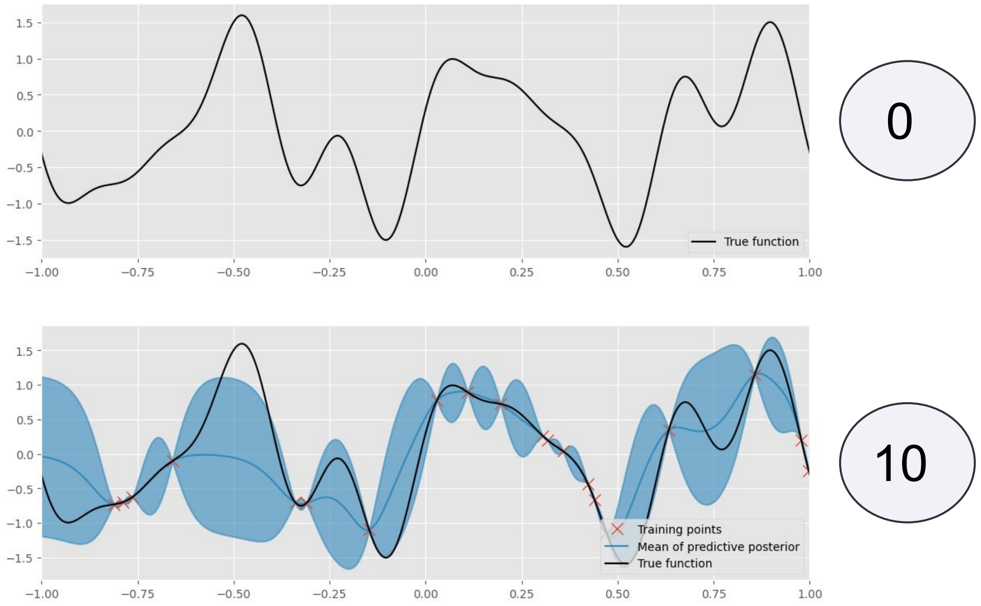

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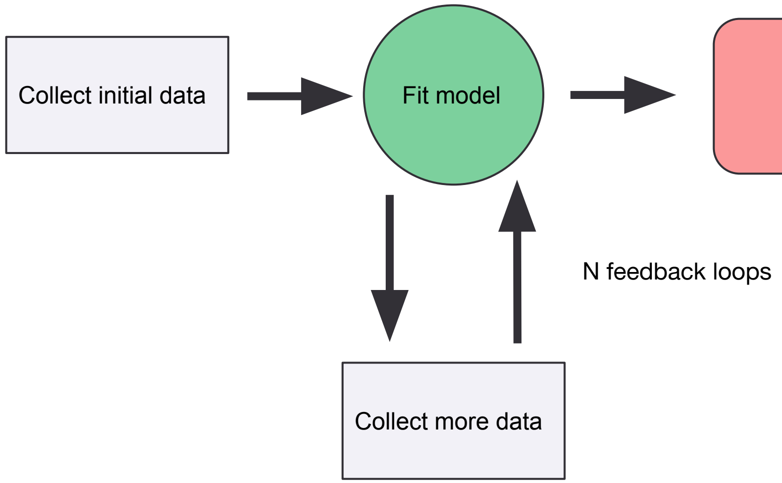

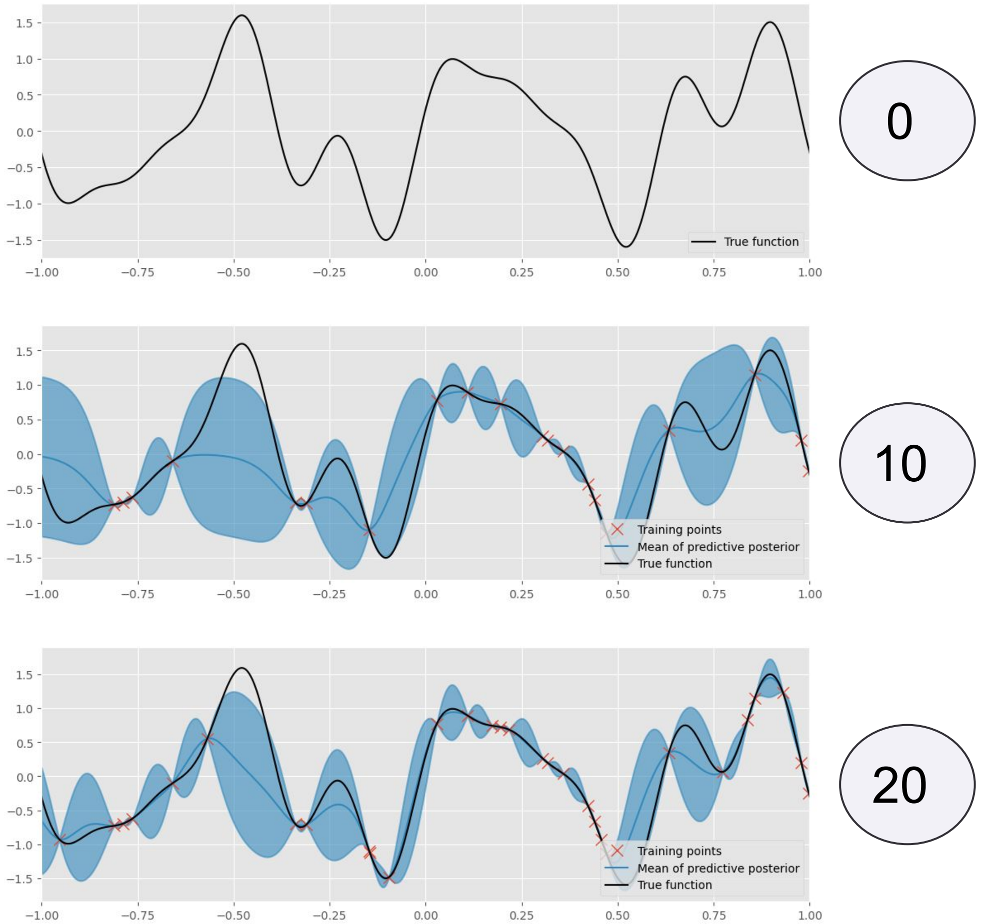

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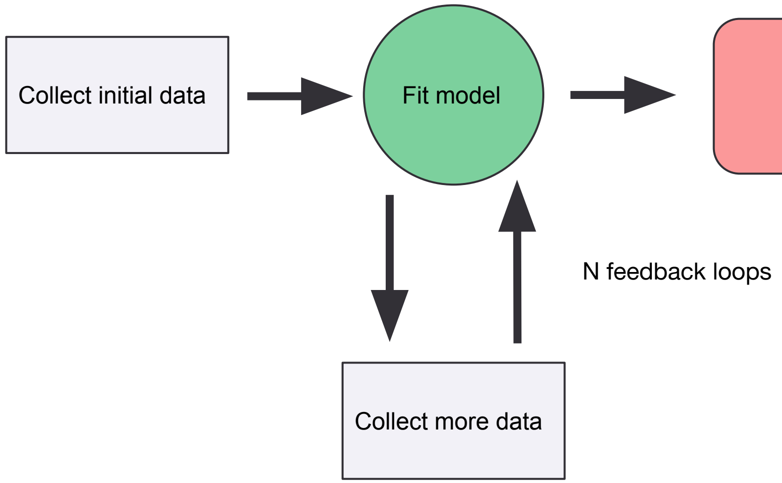

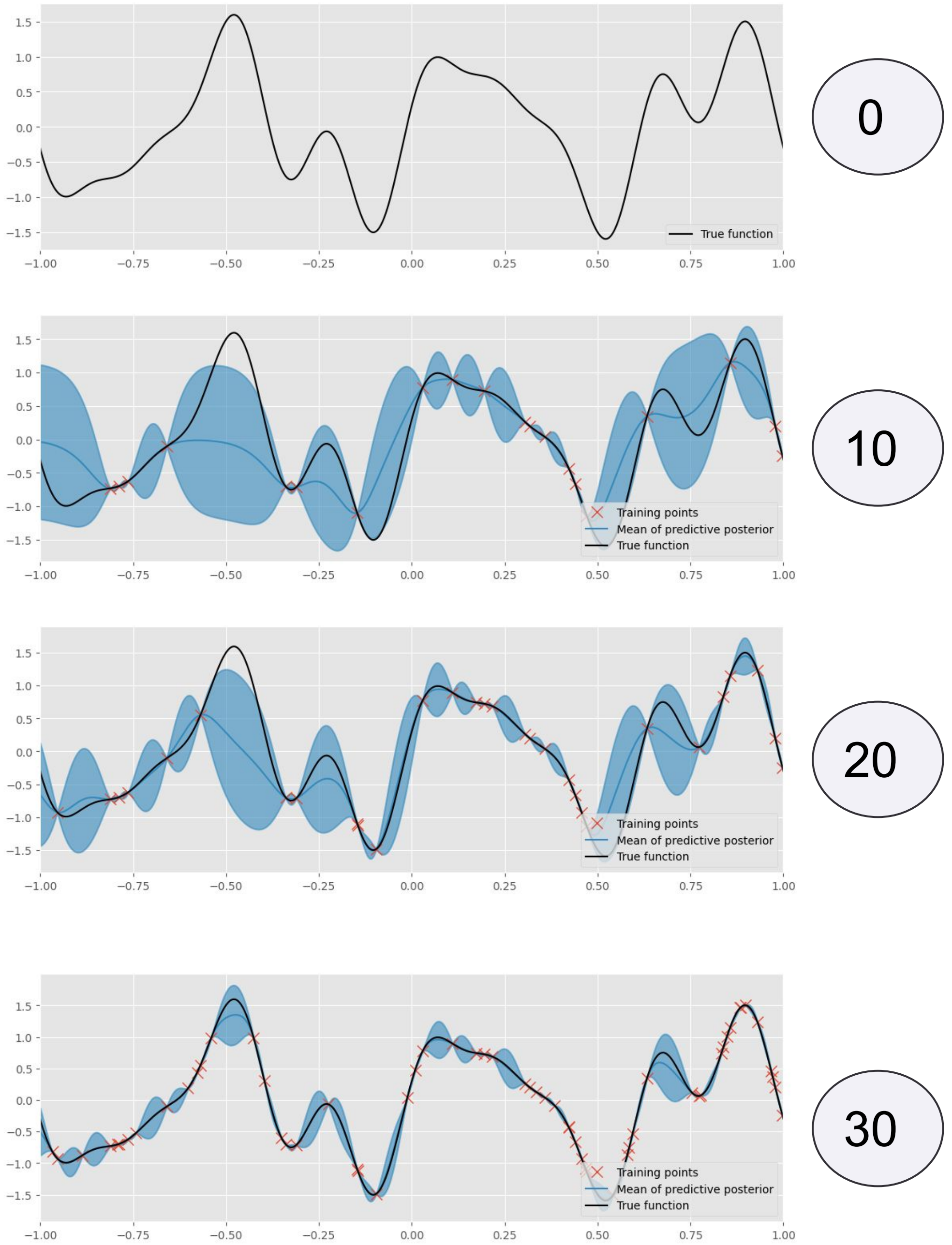

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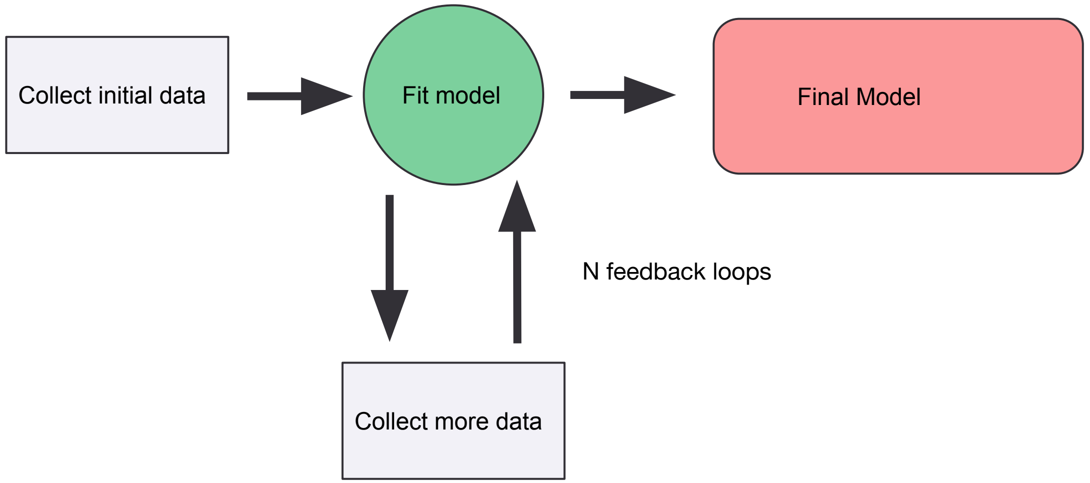

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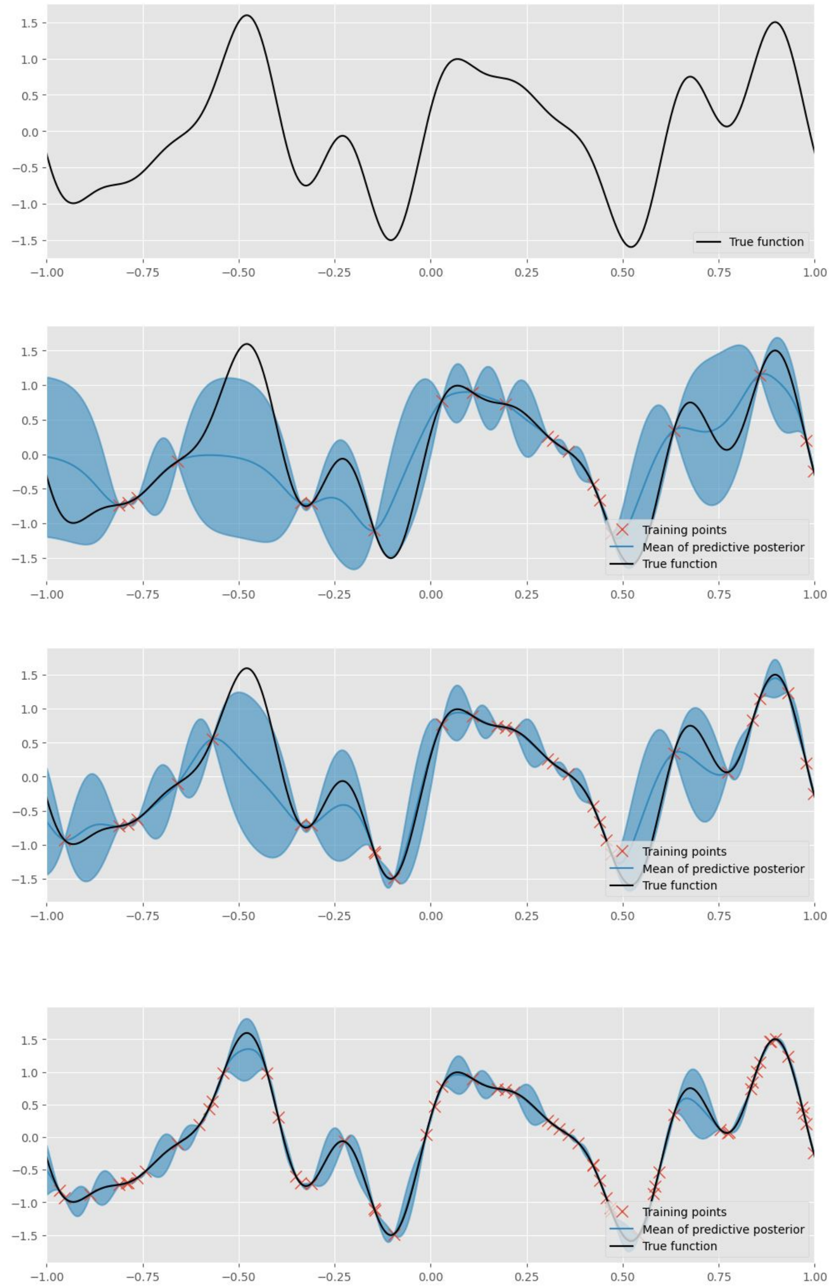

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Active learning

Sequentially collecting more data to improve your model for the task at hand

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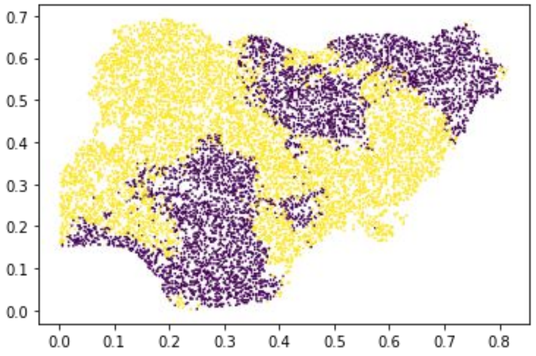

Malaria incidence in Nigeria

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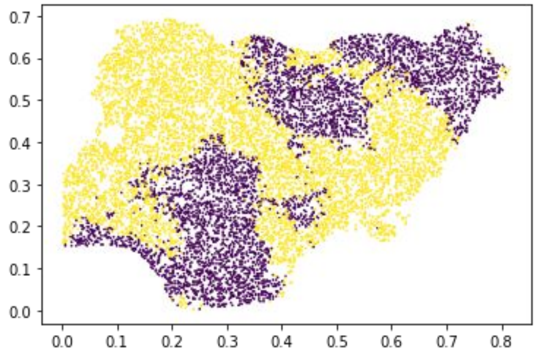

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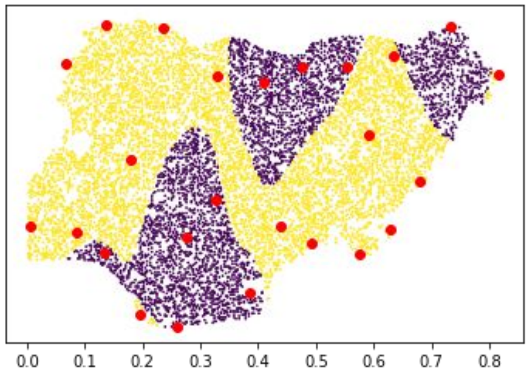

Model on Random data

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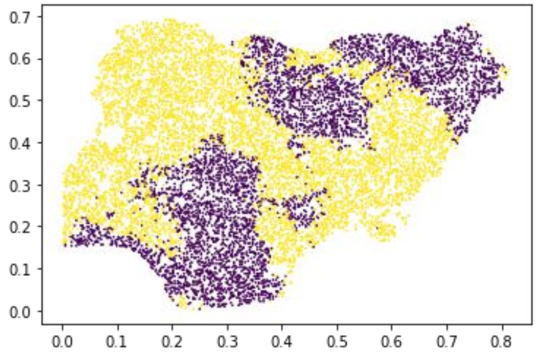

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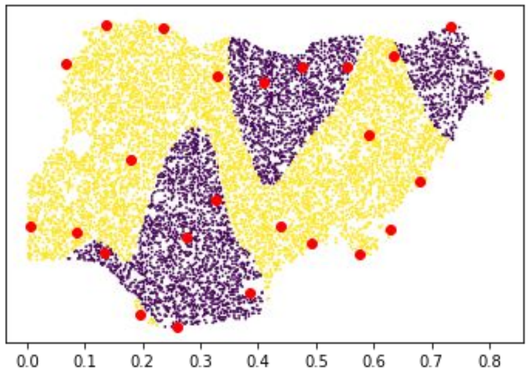

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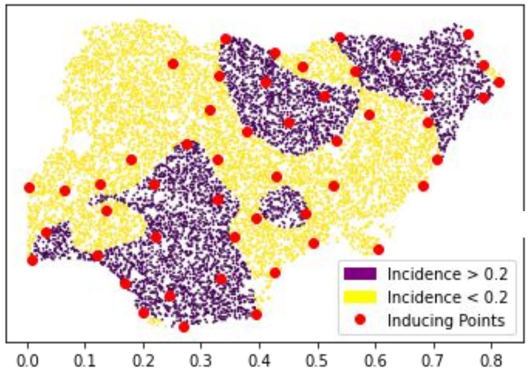


Model from data chosen by Active learning

So, Bayesian Optimisation?

i.e. Active learning for optimisation

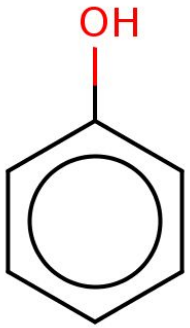
A molecular design pipeline

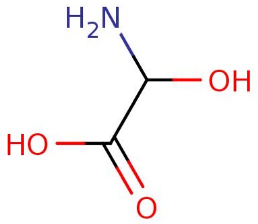
Efficiently explore molecule space

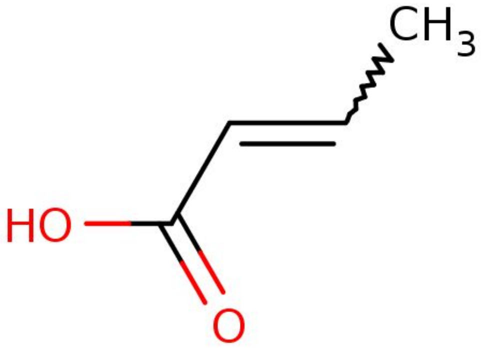
A molecular design pipeline

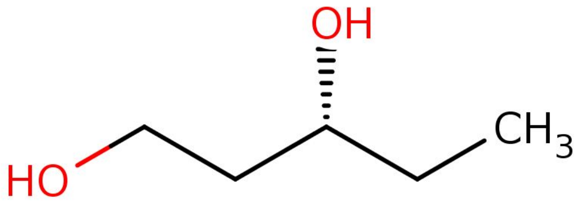
Efficiently explore molecule space

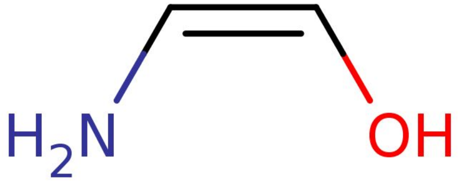
- **Large** library of candidates











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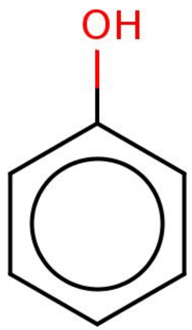
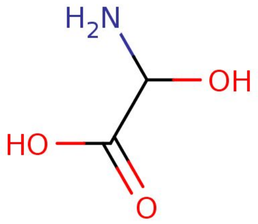
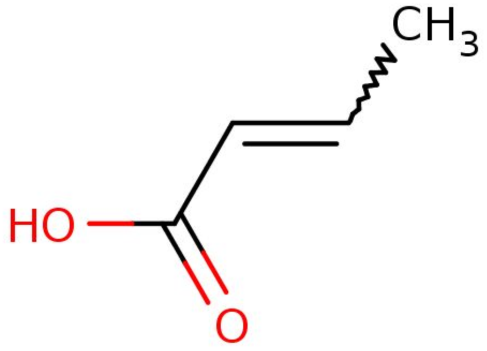
A molecular design pipeline

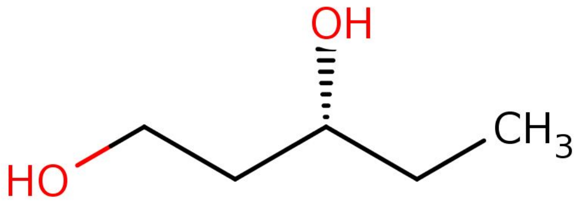
Efficiently explore molecule space

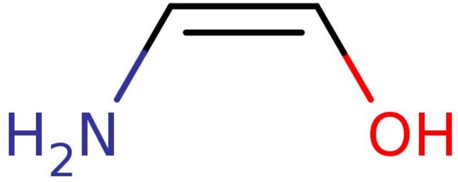
- **Large** library of candidates
- **Expensive** experiments (<10)











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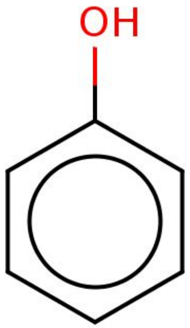

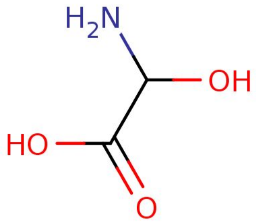

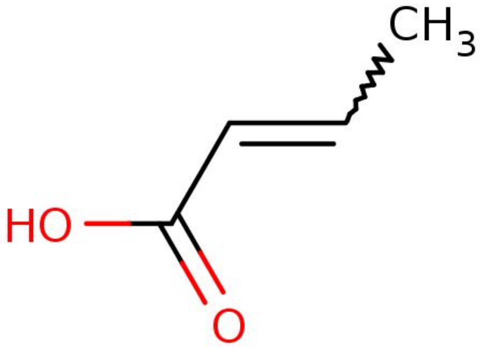

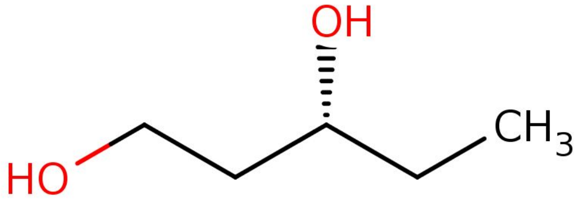

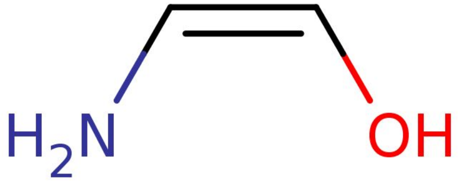

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A molecular design pipeline

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- **Large** library of candidates
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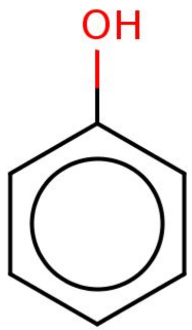
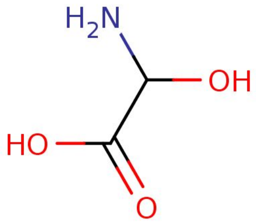
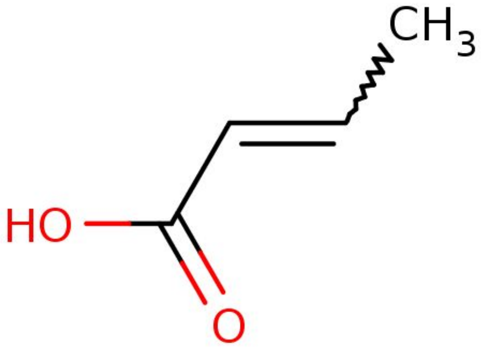
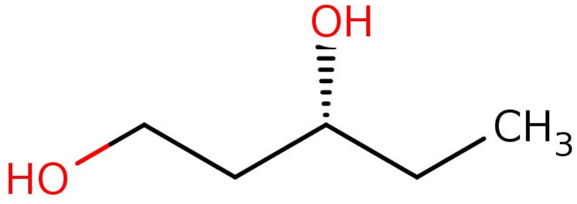
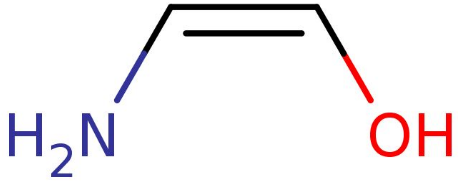
- High degree of **parallelism**











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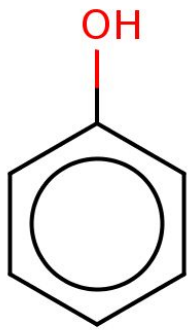
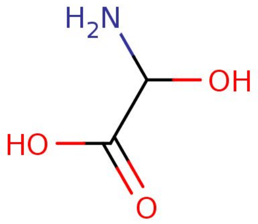
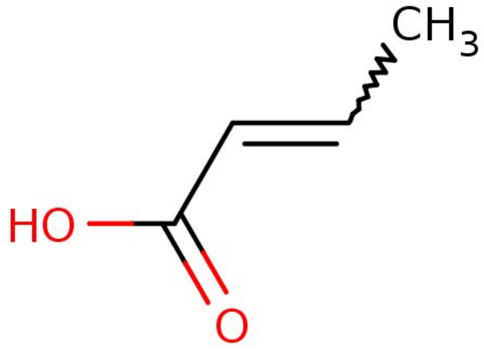
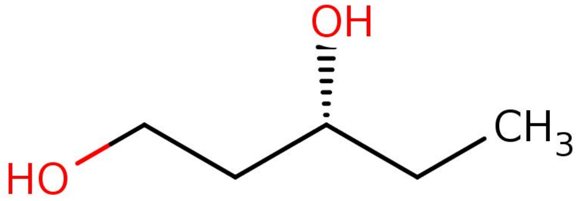
Efficiently explore molecule space

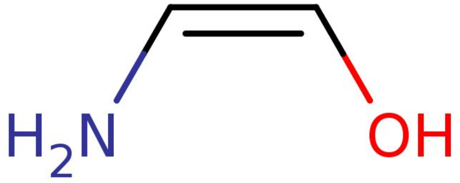
- **Large** library of candidates
- **Expensive** experiments (<10)
- High degree of **parallelism**
- Want molecules with high **affinity**











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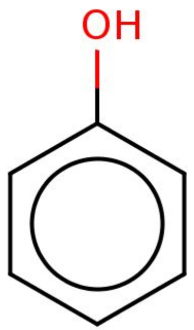
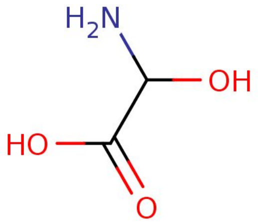
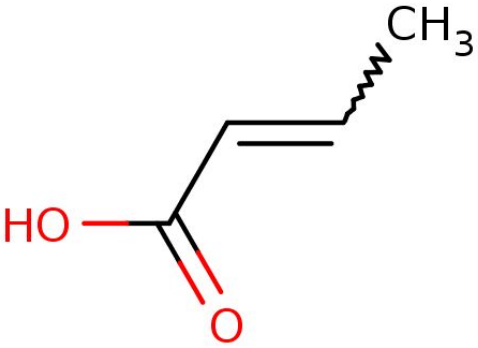
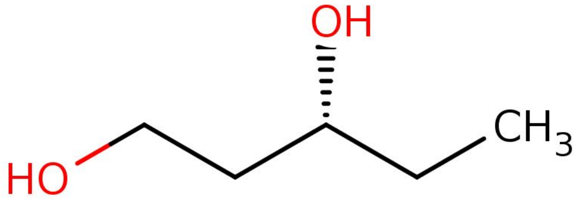
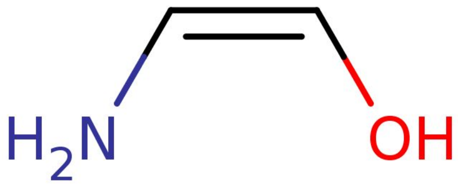
  - Also easy to make











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A molecular design pipeline

Efficiently explore molecule space

- **Large** library of candidates
- **Expensive** experiments (<10)
- High degree of **parallelism**
- Want molecules with high **affinity**
    - Also easy to make
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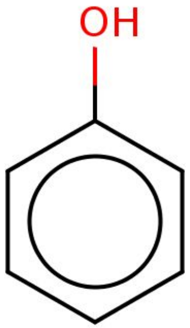

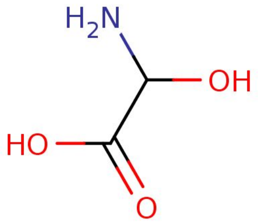

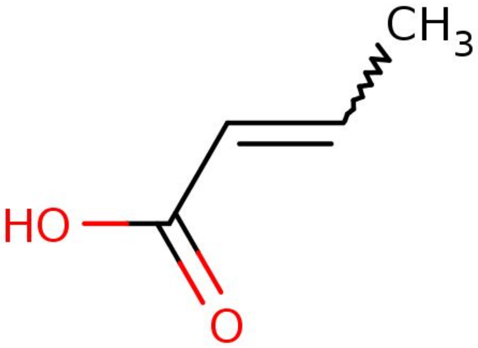

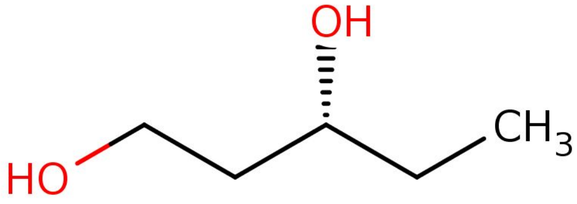

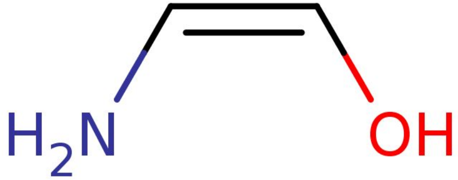

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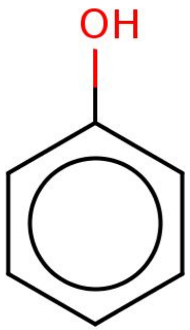

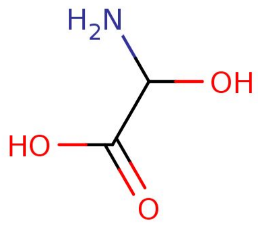

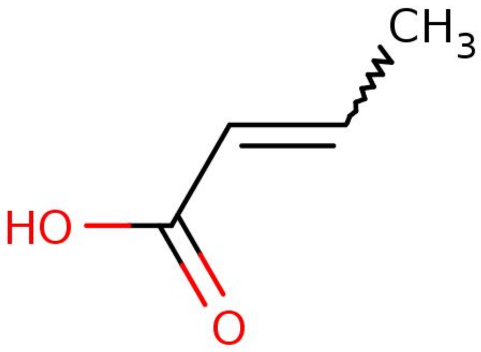

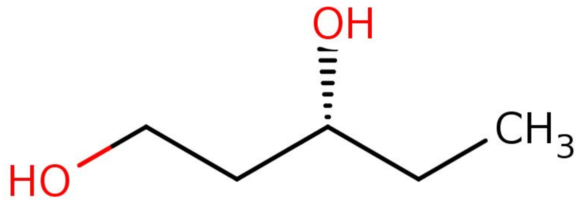

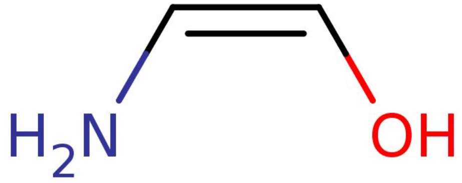

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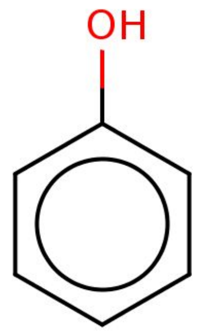
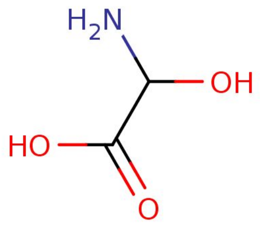
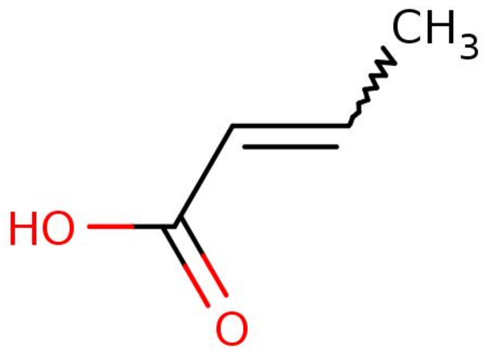
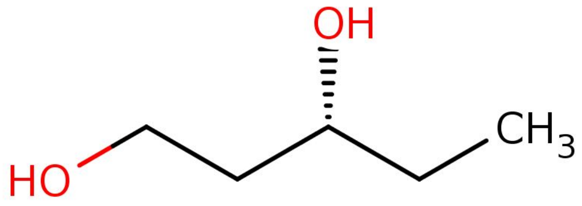
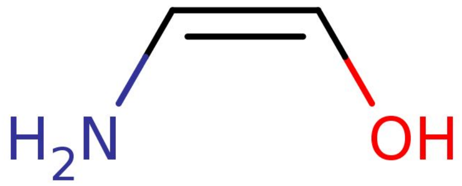
    - In a new area of "patent space"











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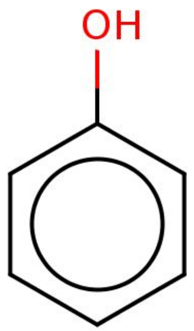

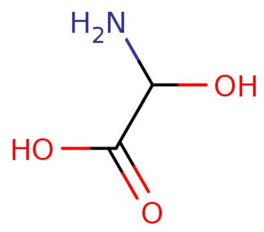

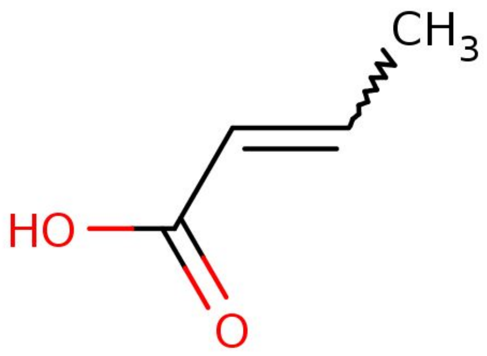

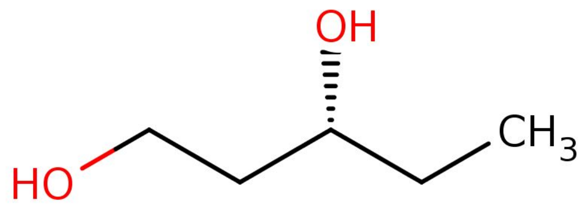

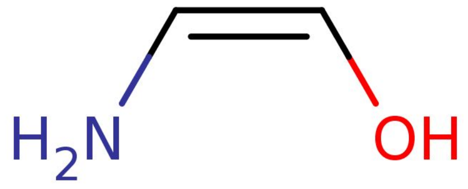

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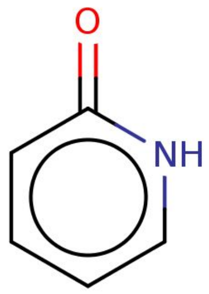
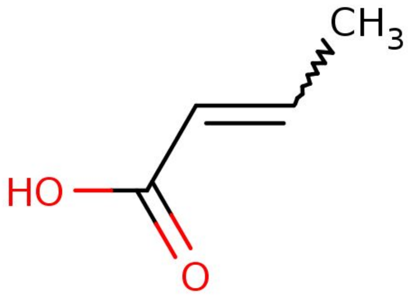
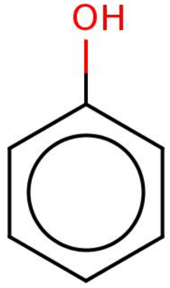
Any ideas?

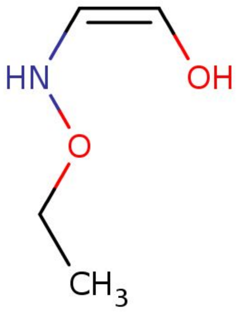
A Simpler Example

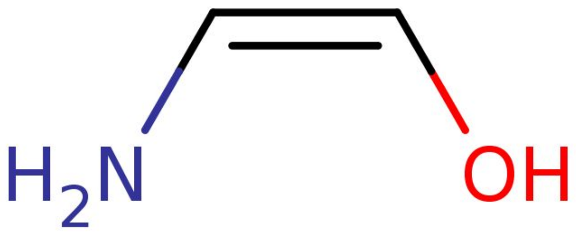
Can evaluate **at most** 4

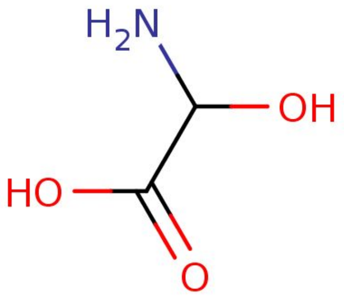






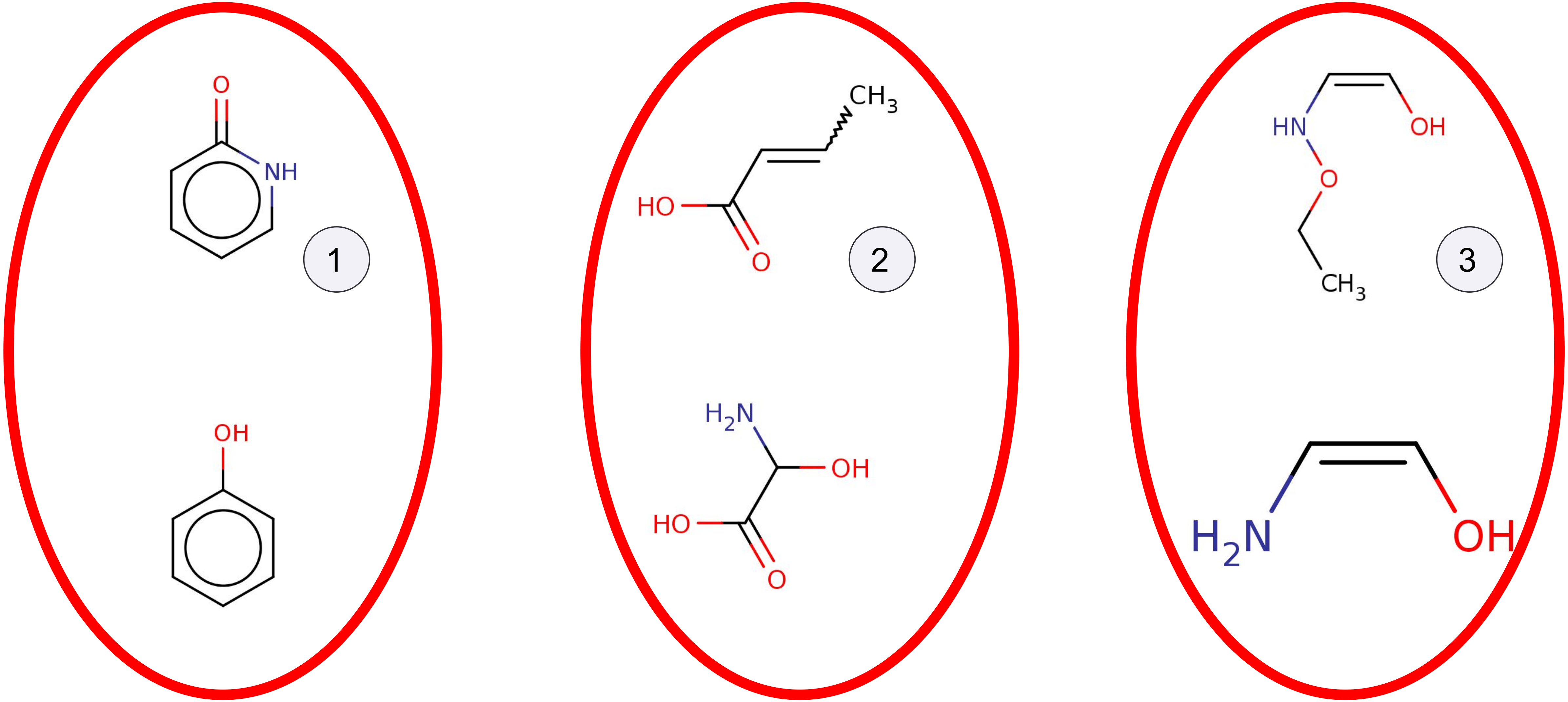






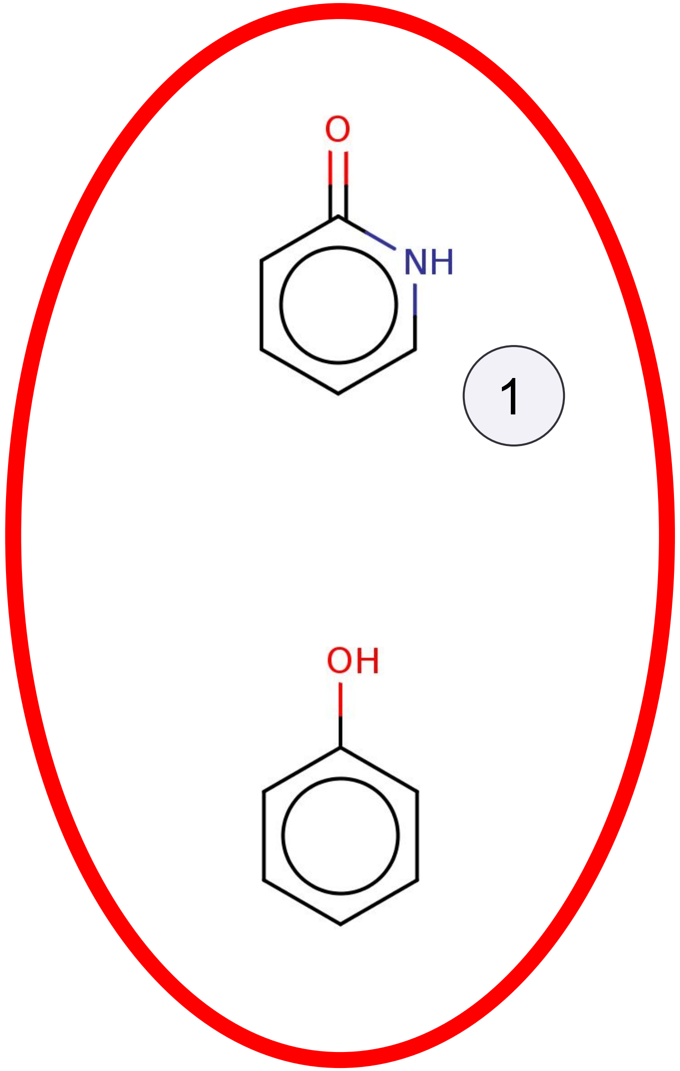
A Simpler Example (grouped)

Can evaluate **at most** 4



A Simpler Example (grouped)

Can evaluate **at most** 4



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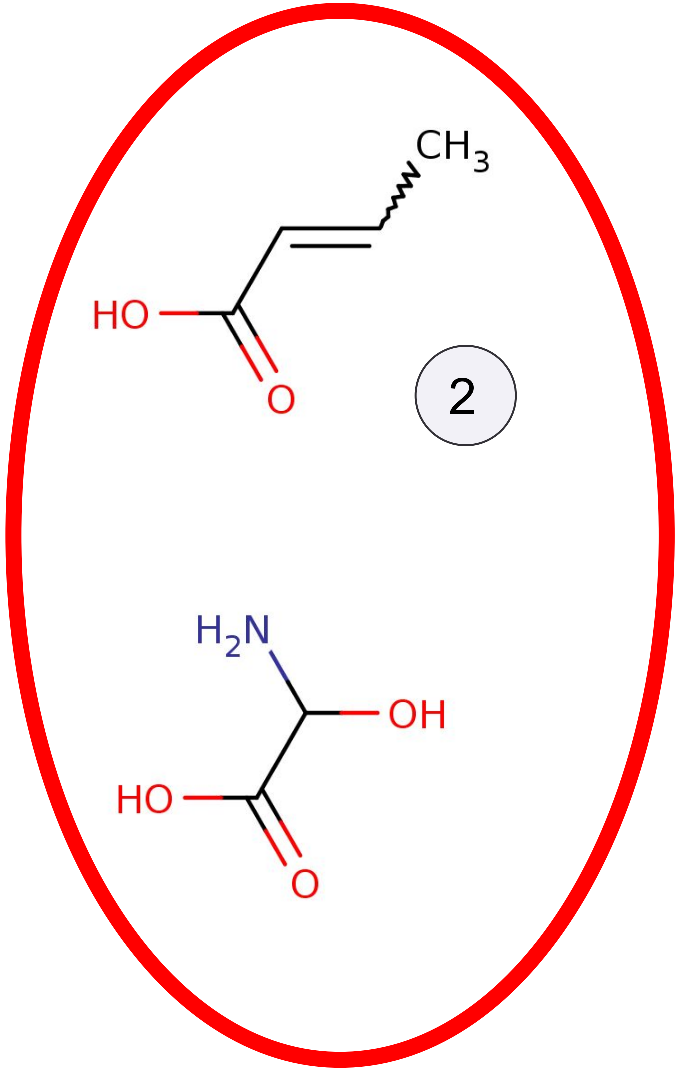

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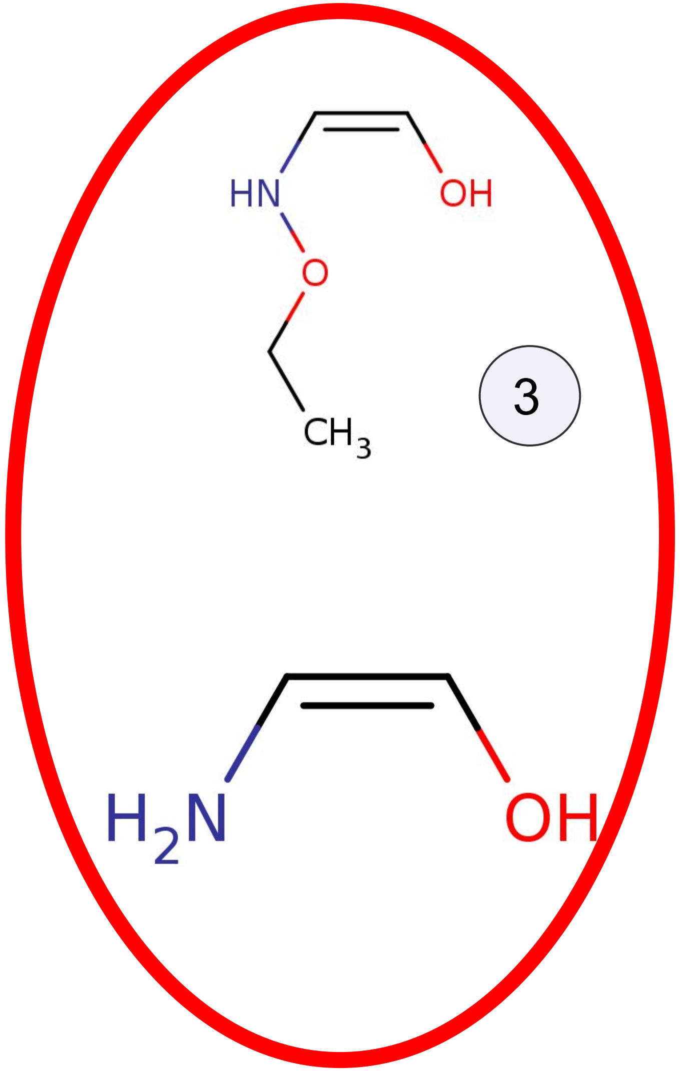
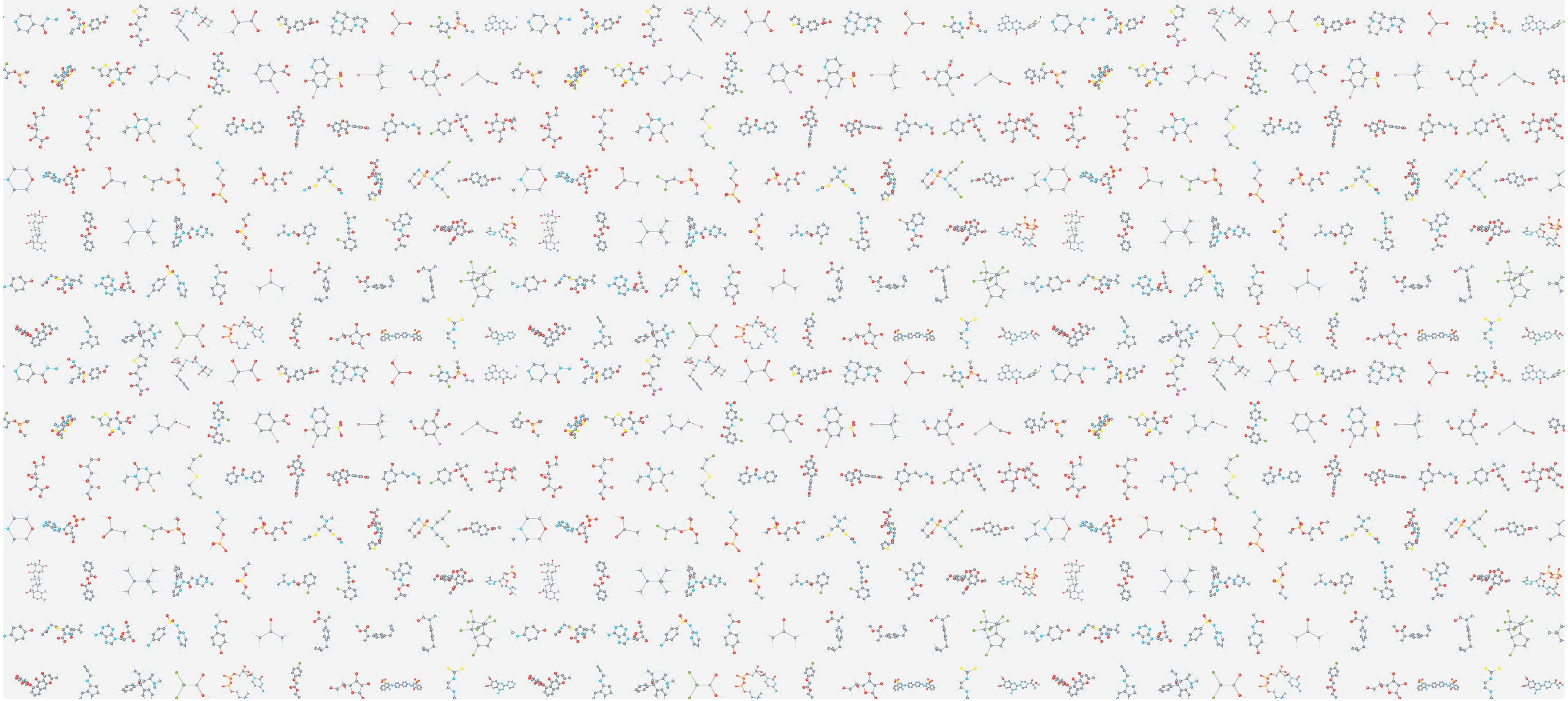


3

Explore v.s. **exploit**?

What about at scale?

eek



https://www.horizons-mag.ch/2018/09/06/the-universe-of-molecules/

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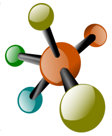
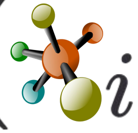
eek

https://www.horizons-mag.ch/2018/09/06/the-universe-of-molecules/

An Aside: GPs for Molecules

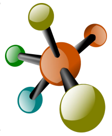
Structured Input Spaces

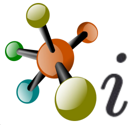
$y_i = f($  $_i) + \epsilon_i$

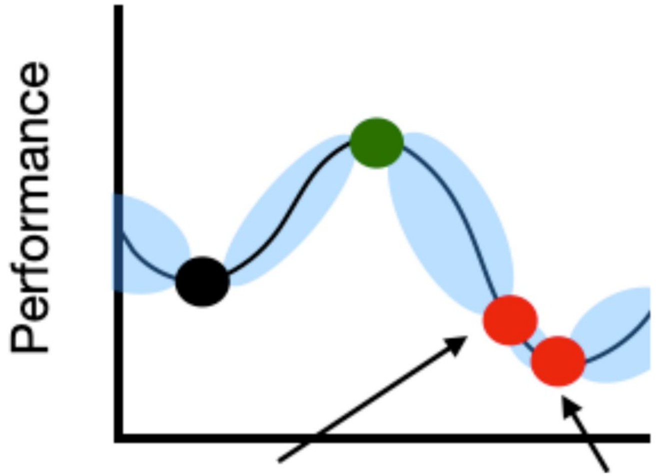
$D_N = \{($  $_i, y_i)\}_i^N$

An Aside: GPs for Molecules

Structured Input Spaces

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

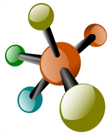
$D_N = \{($  $_i, y_i)\}_i^N$

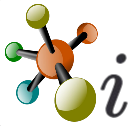


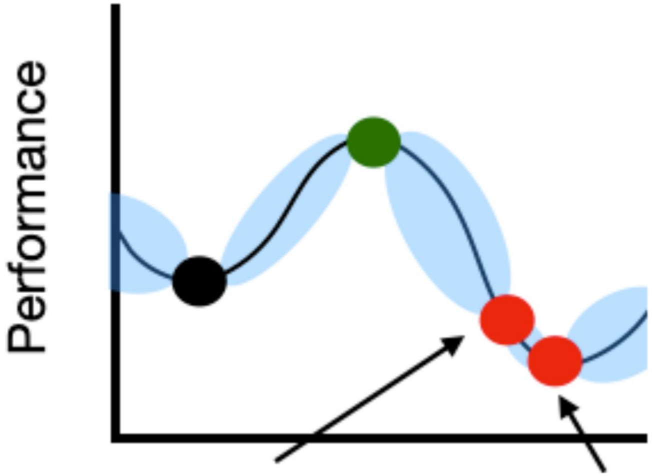
What do we require to define a GP?

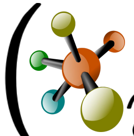
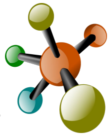
An Aside: GPs for Molecules

Structured Input Spaces

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

$D_N = \{($  $_i, y_i)\}_i^N$



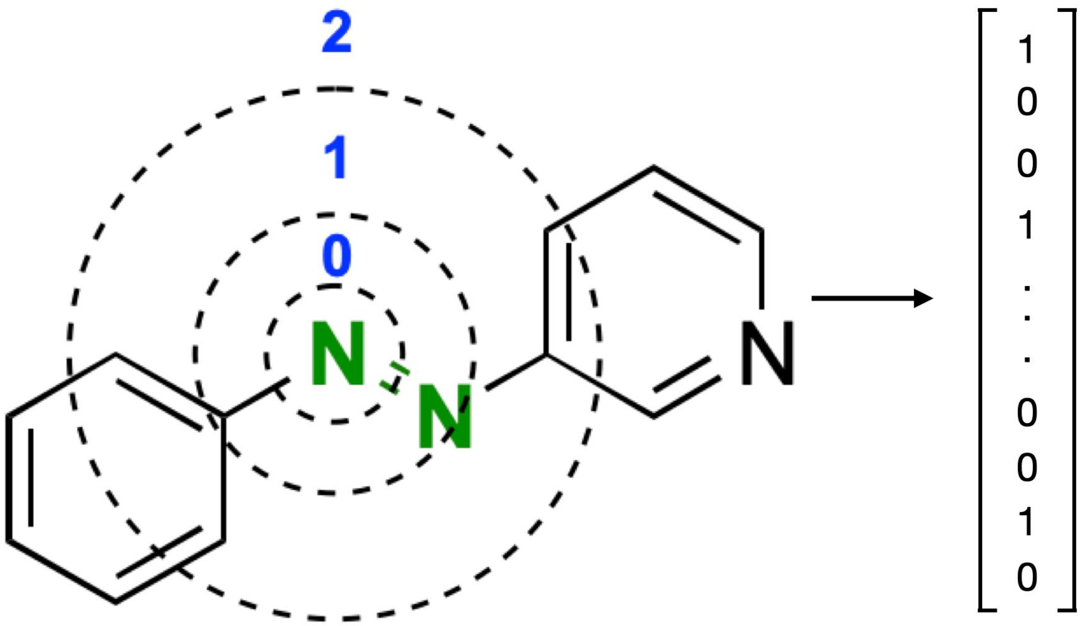
$k($  $_i,$  $_j) = ?$

What do we require to define a GP?

An Aside: GPs for Molecules

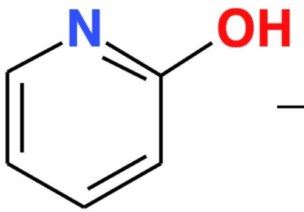
Fingerprint Kernels

$$k(\cdot_i, \cdot_j) = k_{\text{linear}}(\Phi(\cdot_i), \Phi(\cdot_j))$$

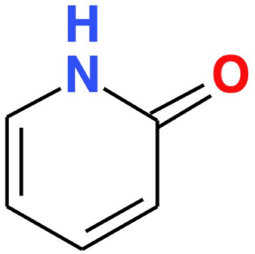


An Aside: GPs for Molecules

String kernels between SMILES strings



$\longrightarrow$ *Oc*1*ncccc*1



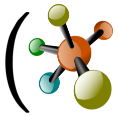
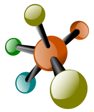
$\longrightarrow$ $O = c1[nH]cccc1$

Automatically choosing next molecules

Using GP posteriors and utility functions

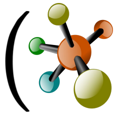
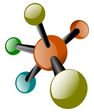
Automatically choosing next molecules

Using GP posteriors and utility functions

- $U_f($  $)$: what is the utility of evaluating  (if it will return f)

Automatically choosing next molecules

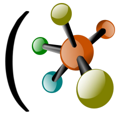
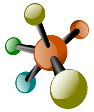
Using GP posteriors and utility functions

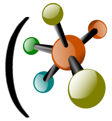
- $U_f($$)$: what is the utility of evaluating  (if it will return f)

    - $f^\star$ Is best so far

Automatically choosing next molecules

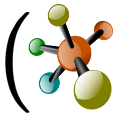
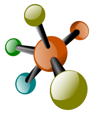
Using GP posteriors and utility functions

- $U_f($  $)$: what is the utility of evaluating  (if it will return f)

  - $f^{\star}$ Is best so far
  - Has there been an improvement? $U_f($  $) = \mathbb{1}_{(f > f^{\star})}$

Automatically choosing next molecules

Using GP posteriors and utility functions

- $U_f($$)$: what is the utility of evaluating  (if it will return f)

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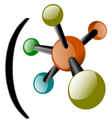
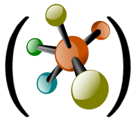
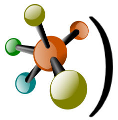
  - Has there been an improvement? $U_f($$) = \mathbb{1}_{(f > f^\star)}$
  - How big was the improvement? $U_f($$) = \max(f - f^\star, 0)$

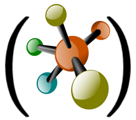
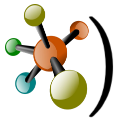
Automatically choosing next molecules

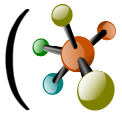
Using GP posteriors and utility functions

- $\alpha($  $) = \mathbb{E}_f[U_f($  $)]$: what utility is predicted by my model of f

Automatically choosing next molecules

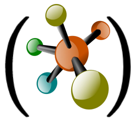
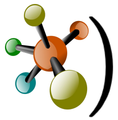
Using GP posteriors and utility functions

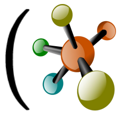
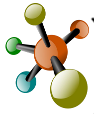
- $\alpha($  $) = \mathbb{E}_f[U_f($  $)]$: what utility is predicted by my model of f

- What the probability of improvement? $\alpha_{\mathrm{PI}}($  $) = \mathbb{E}_f\left[\mathbb{1}_{(f > f^\star)}\right]$

Automatically choosing next molecules

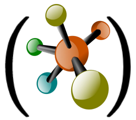
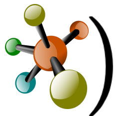
Using GP posteriors and utility functions

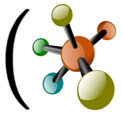
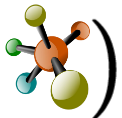
- $\alpha($  $) = \mathbb{E}_f[U_f($  $)]$: what utility is predicted by my model of f

  - What the probability of improvement? $\alpha_{\mathrm{PI}}($  $) = \mathbb{E}_f\left[\mathbb{1}_{(f > f^\star)}\right]$
  - How much improvement do we expect? $\alpha_{\mathrm{EI}}($  $) = \mathbb{E}_f[\max(f - f^\star, 0)]$

Automatically choosing next molecules

Using GP posteriors and utility functions

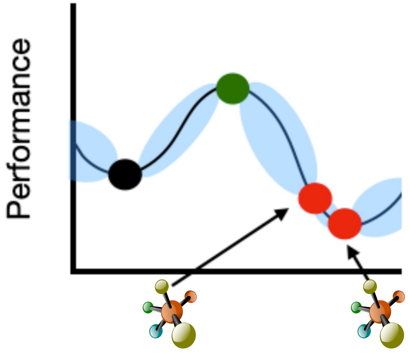
- $\alpha($  $) = \mathbb{E}_f[U_f($  $)]$: what utility is predicted by my model of f

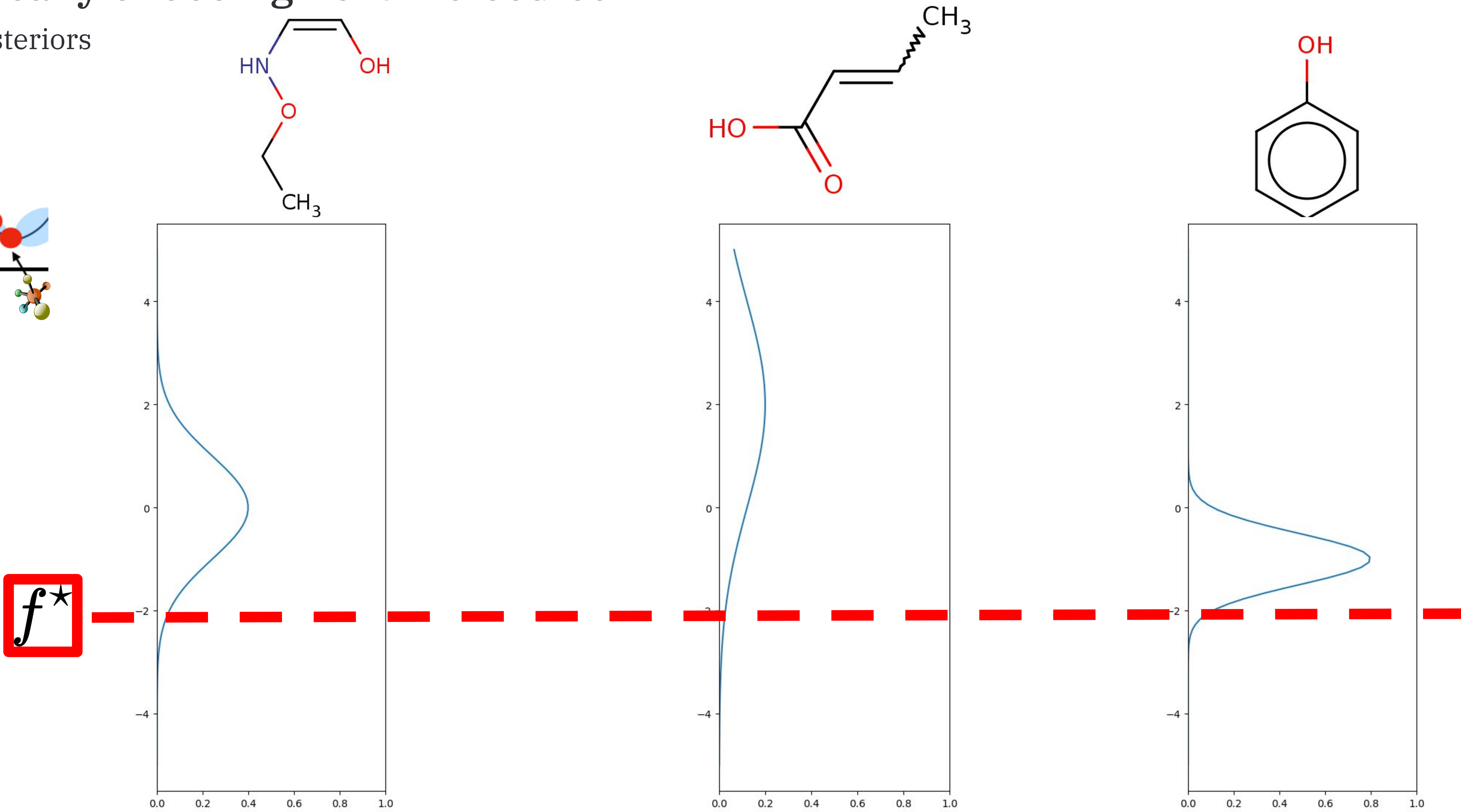
  - What the probability of improvement? $\alpha_{\mathrm{PI}}($  $) = \mathbb{E}_f\left[\mathbb{1}_{(f > f^\star)}\right]$
  - How much improvement do we expect? $\alpha_{\mathrm{EI}}($  $) = \mathbb{E}_f[\max(f - f^\star, 0)]$

$$f \sim \mathcal{N}\left(\mu,\, \sigma^2\right)$$

Automatically choosing next molecules

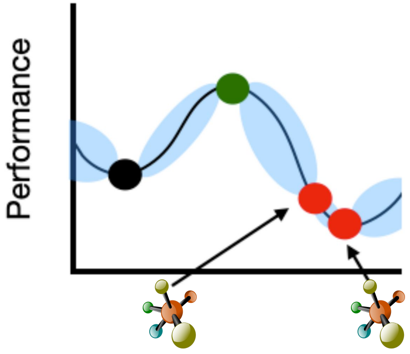
Using GP posteriors

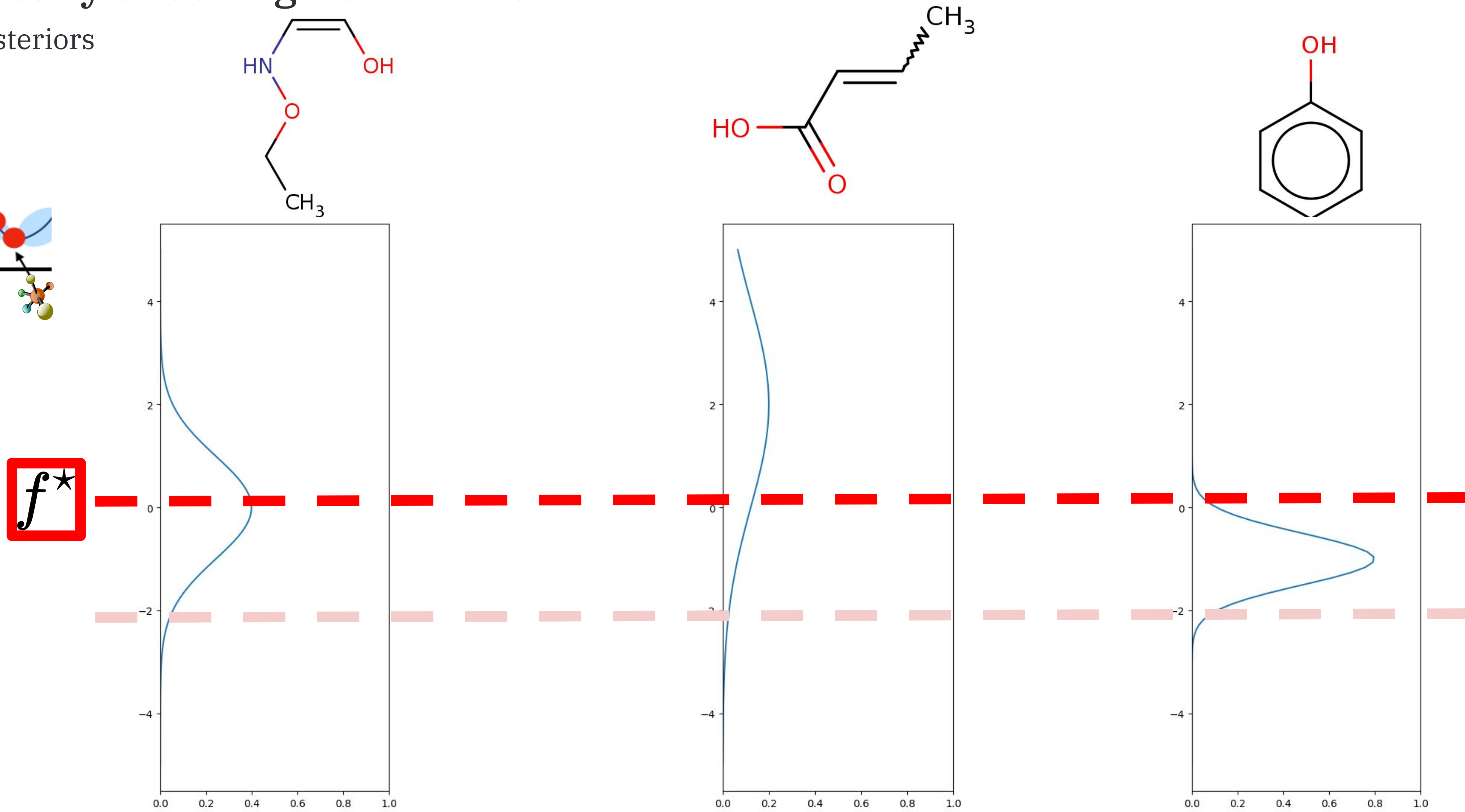




Automatically choosing next molecules

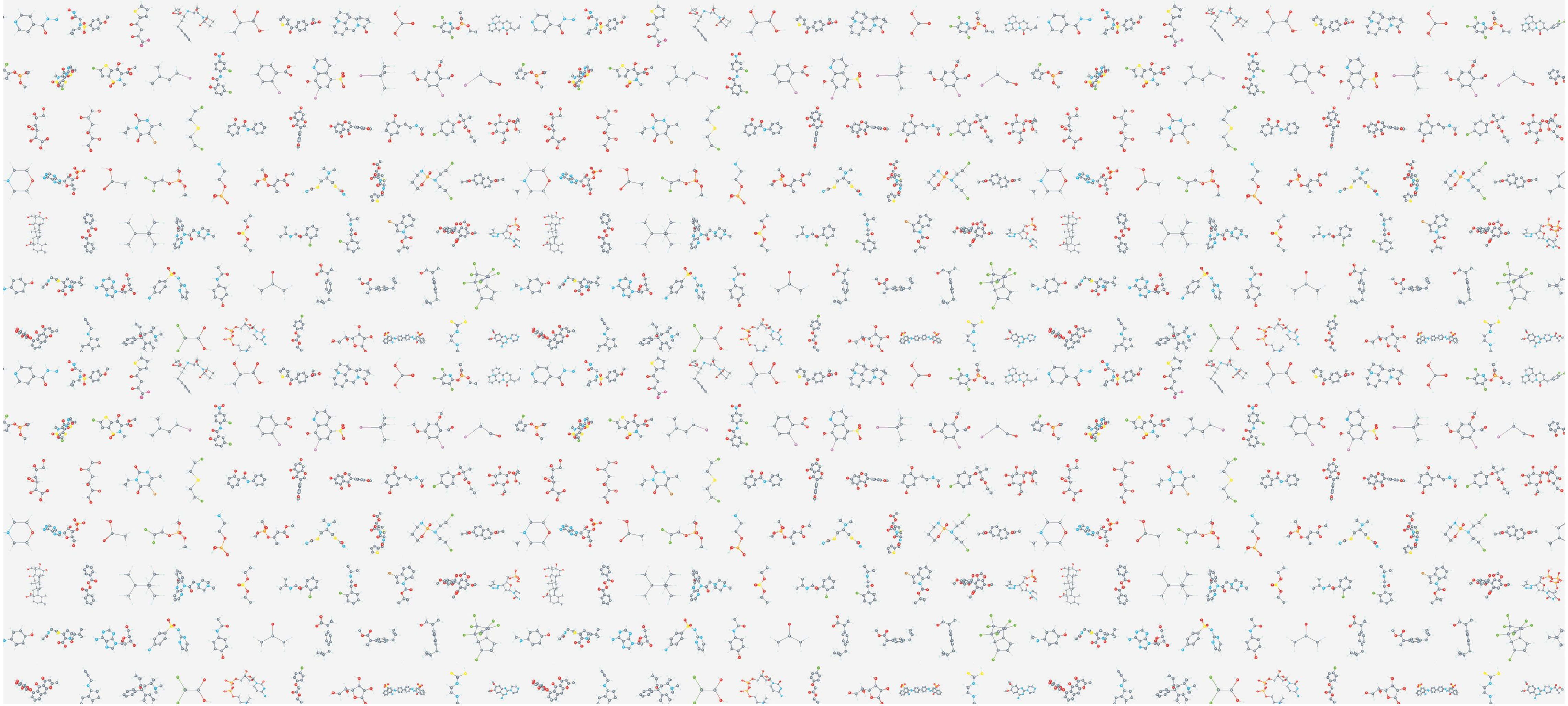
Using GP posteriors





Automatically choosing next molecules

Calc acquisition function and pick best



https://www.horizons-mag.ch/2018/09/06/the-universe-of-molecules/

Automatically choosing next molecules

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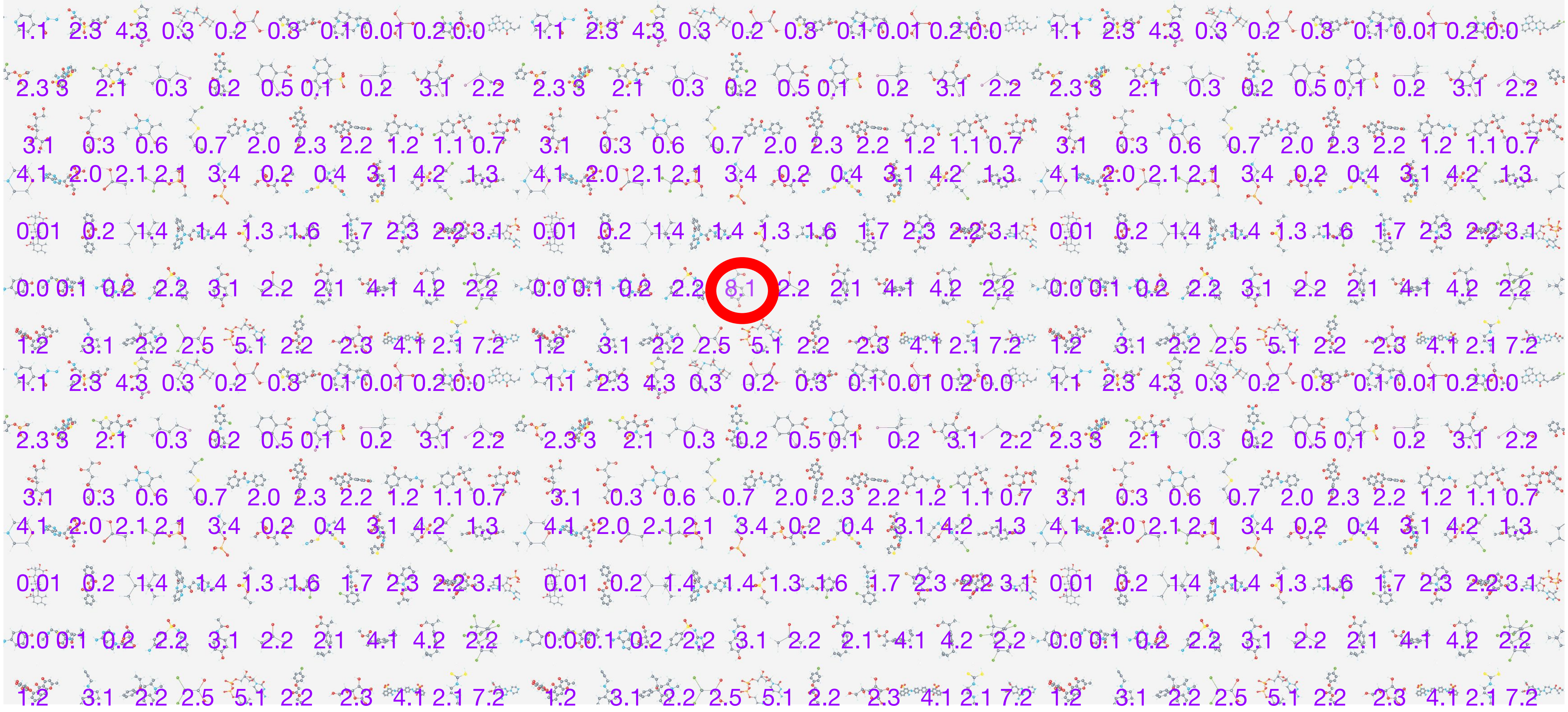

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Automatically choosing next molecules

Full Bayesian optimisation loop

1. Evaluate 2 random molecules

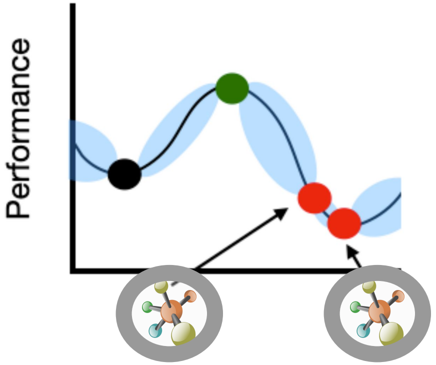
https://www.horizons-mag.ch/2018/09/06/the-universe-of-molecules/

Automatically choosing next molecules

Full Bayesian optimisation loop

1. Evaluate 2 random molecules

2. Fit GP model to measurements



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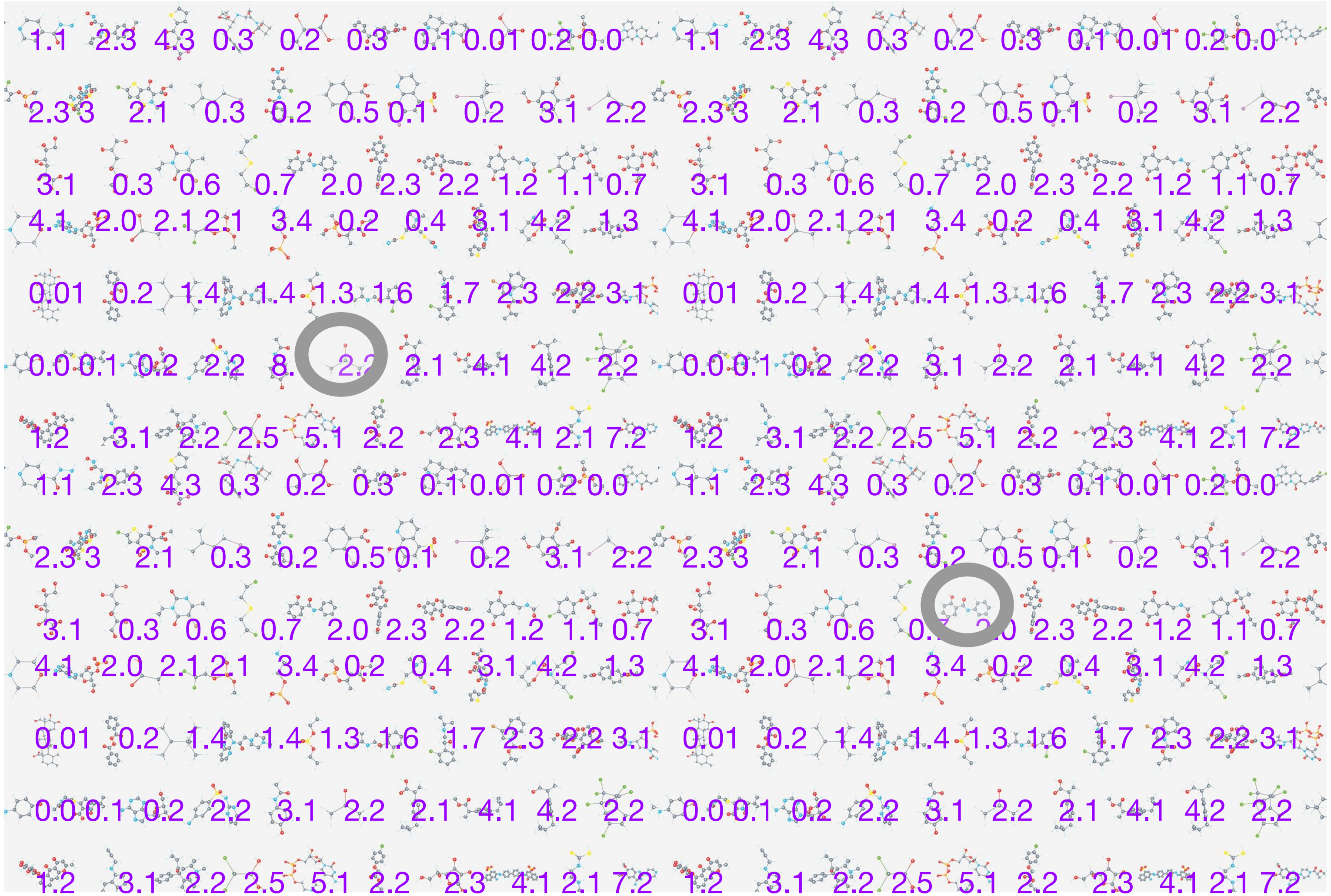

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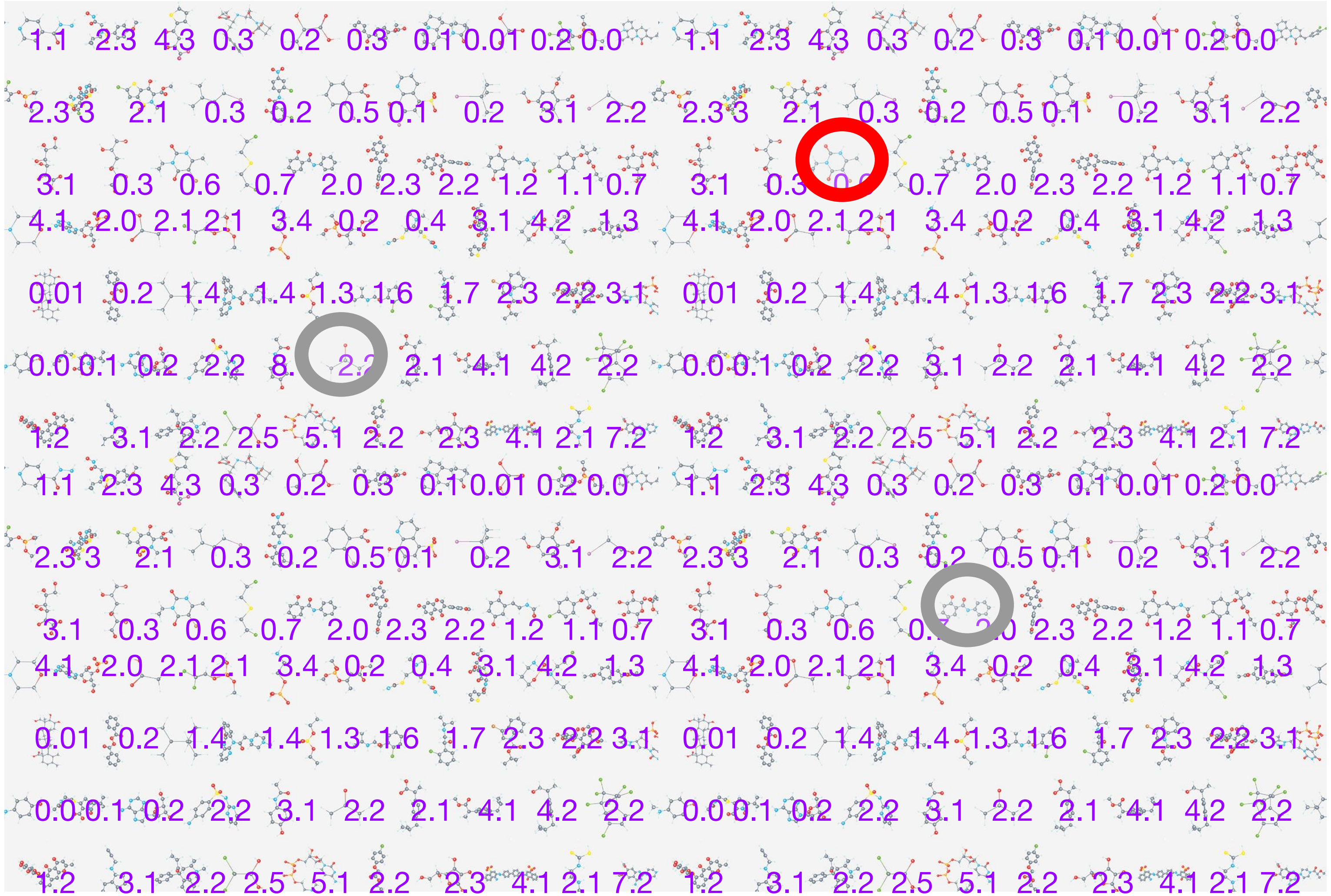

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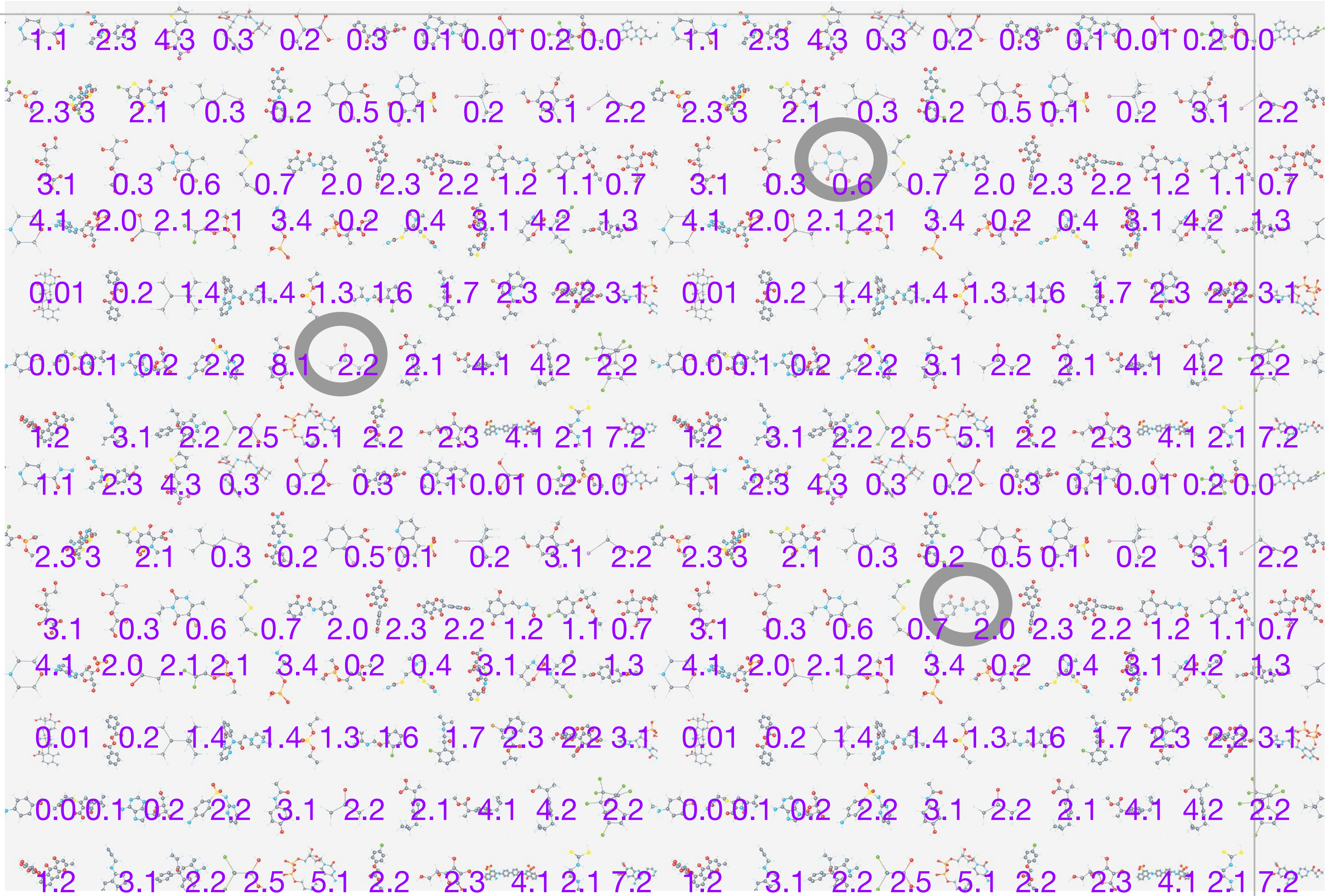

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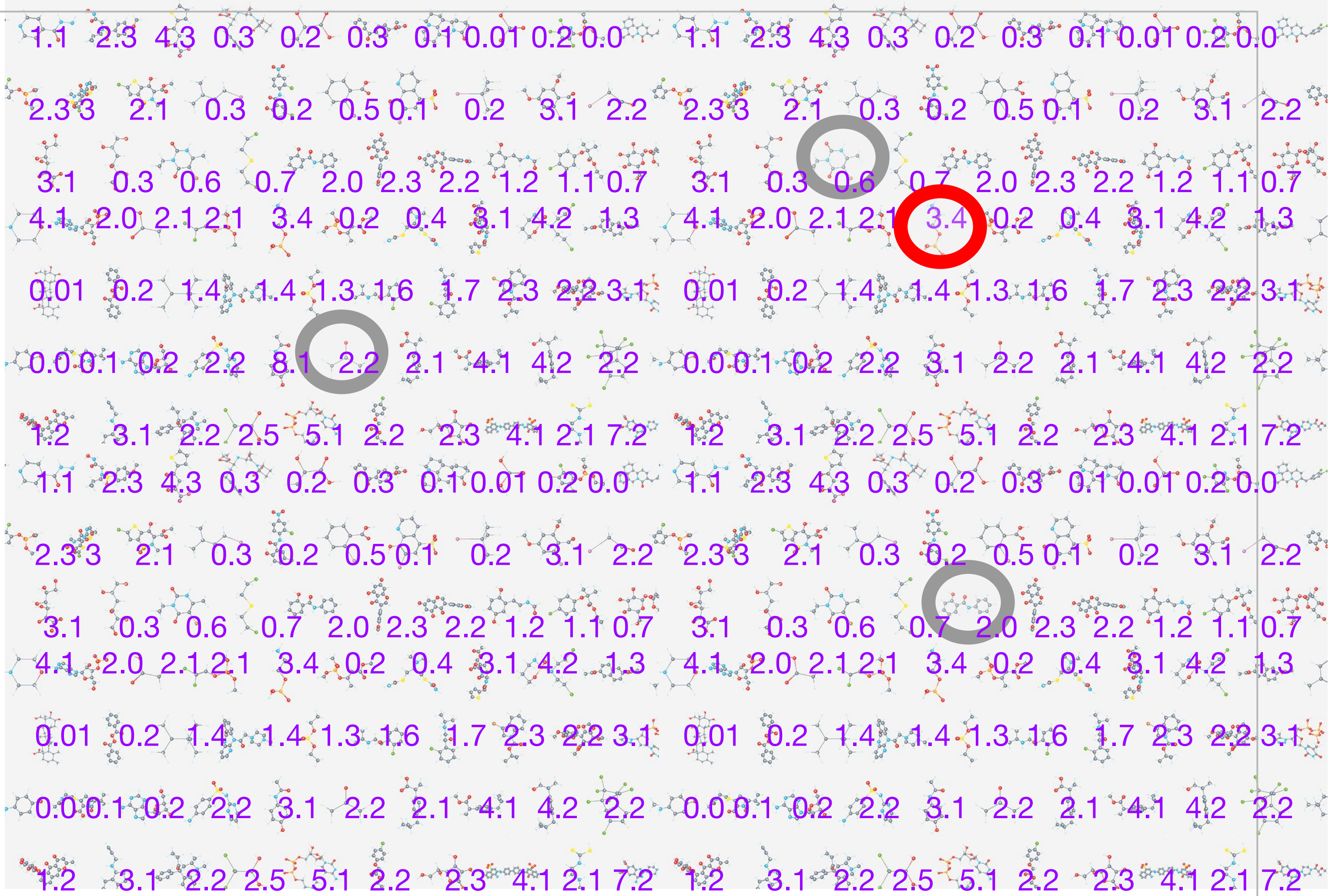

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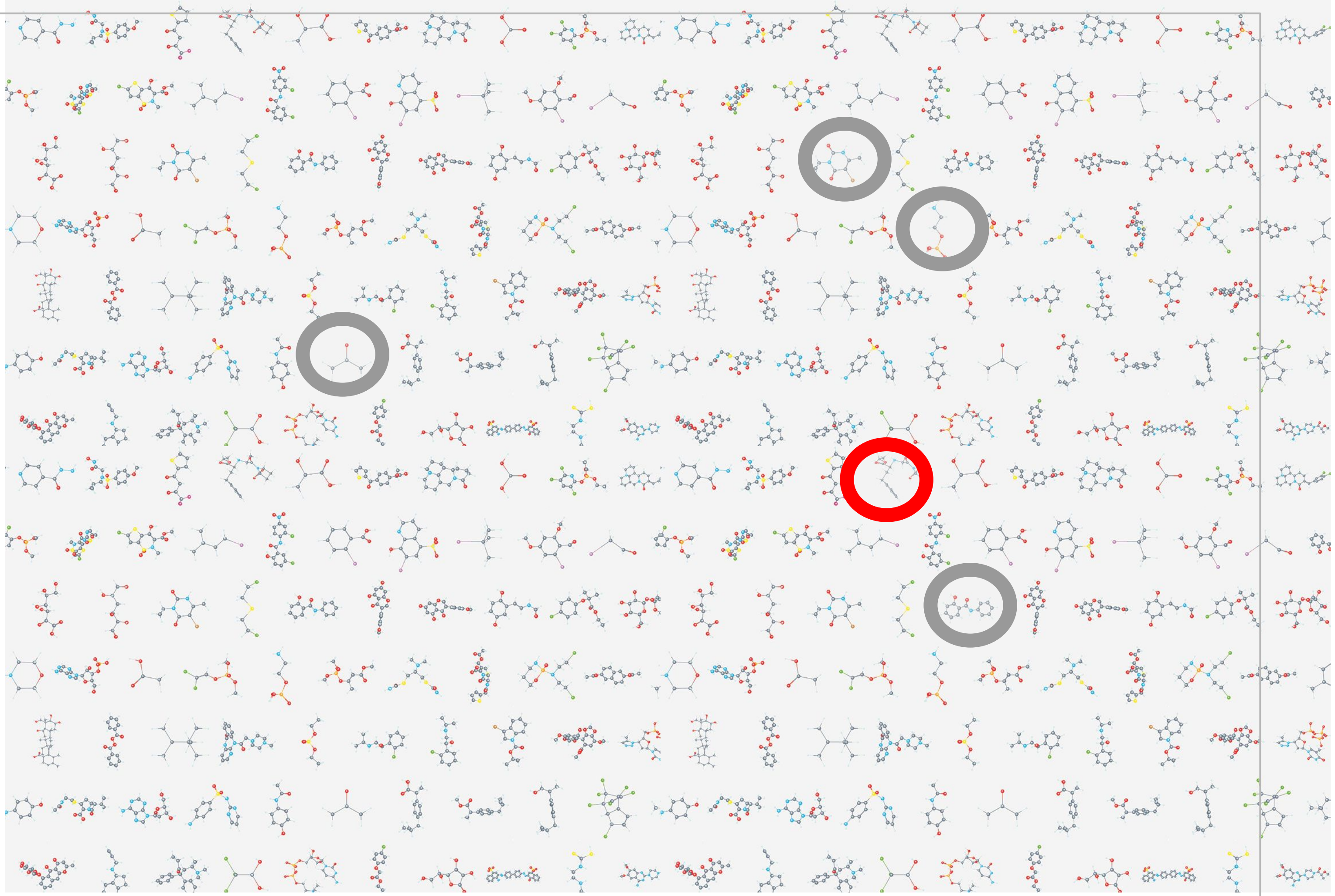

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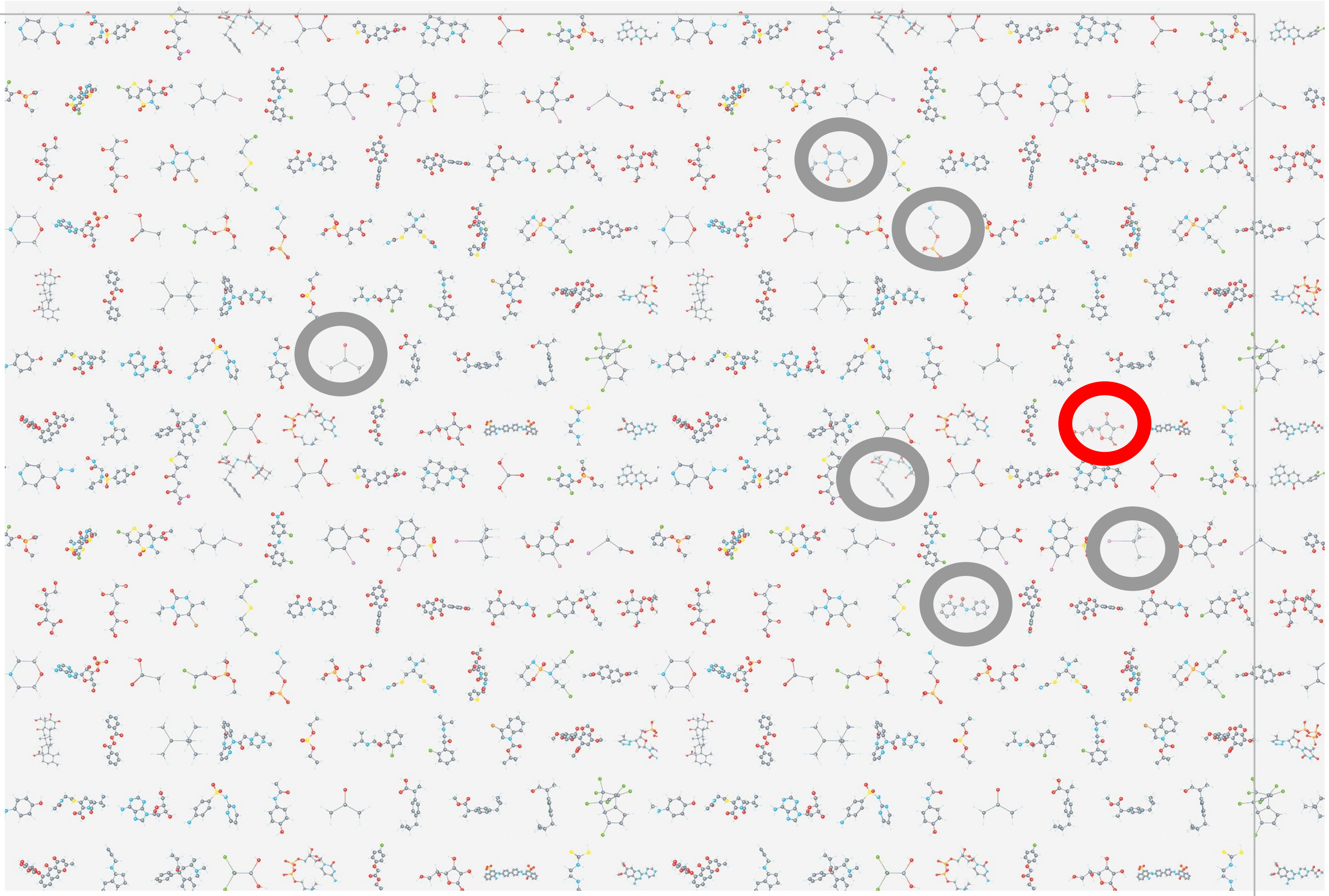

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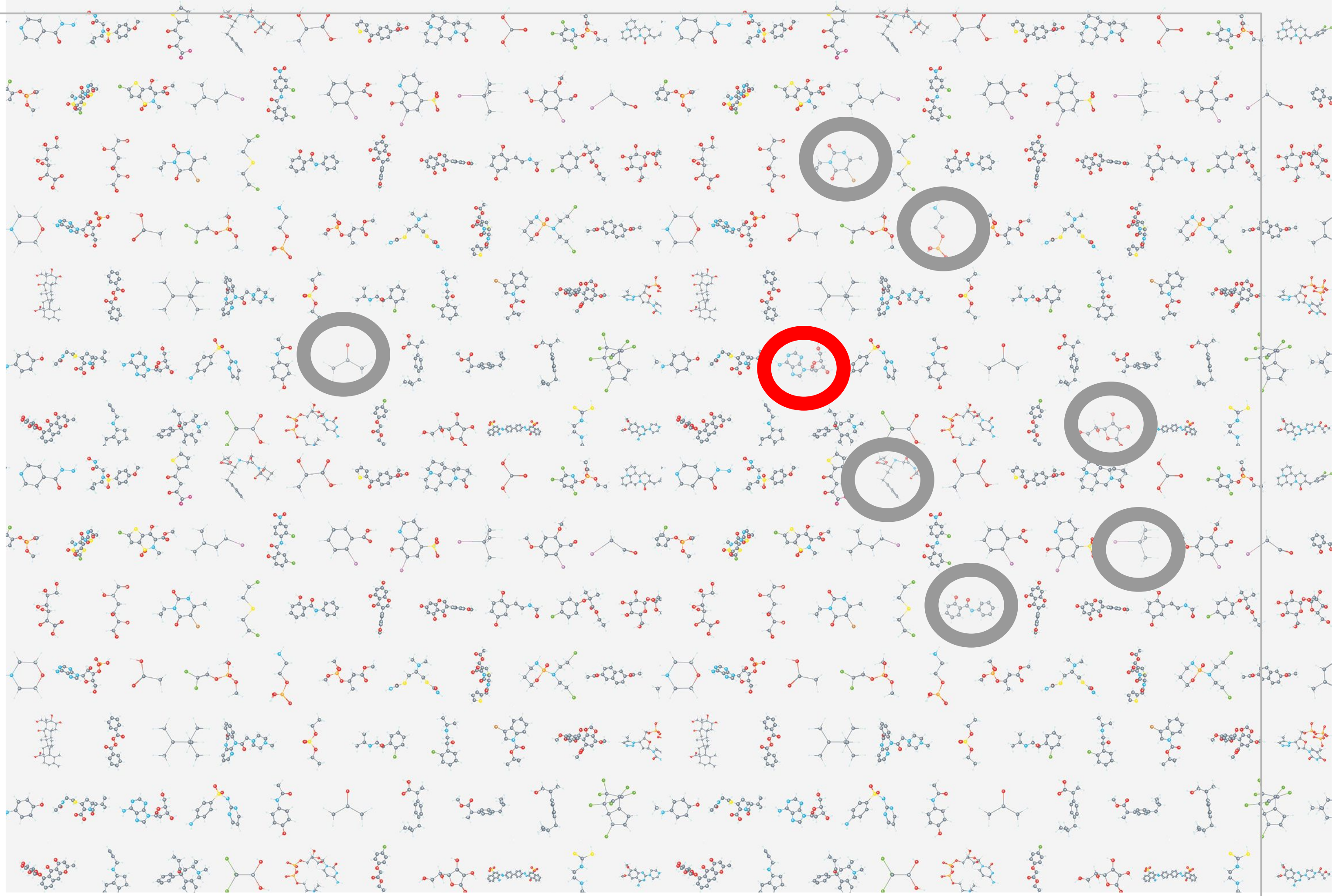

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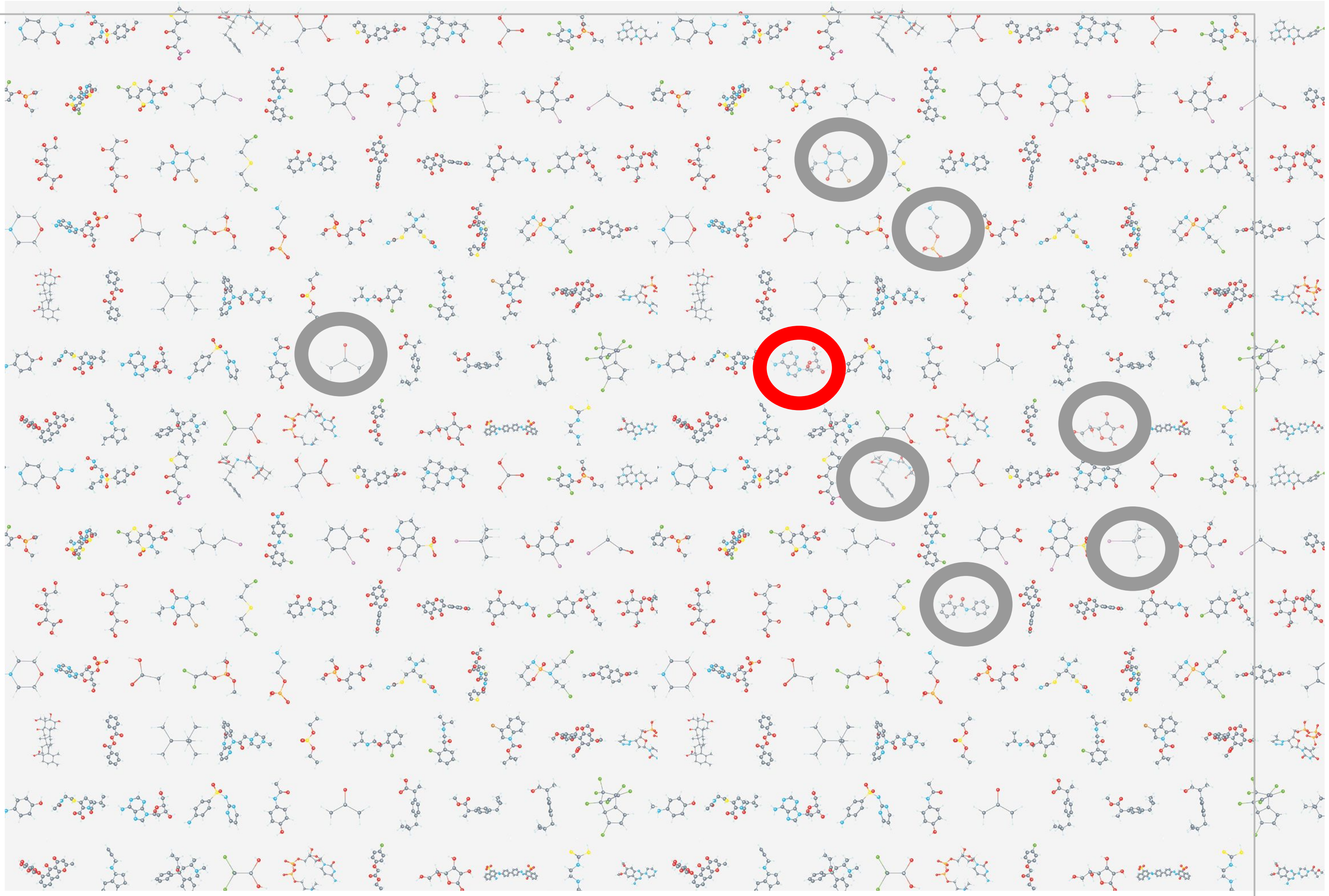
And so on ....



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What about standard optimisation problems?

i.e. infinite candidates

BO Demo

Let's find the maximum of a 1D function:

BO Demo

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Using as **few** function evaluations as possible!

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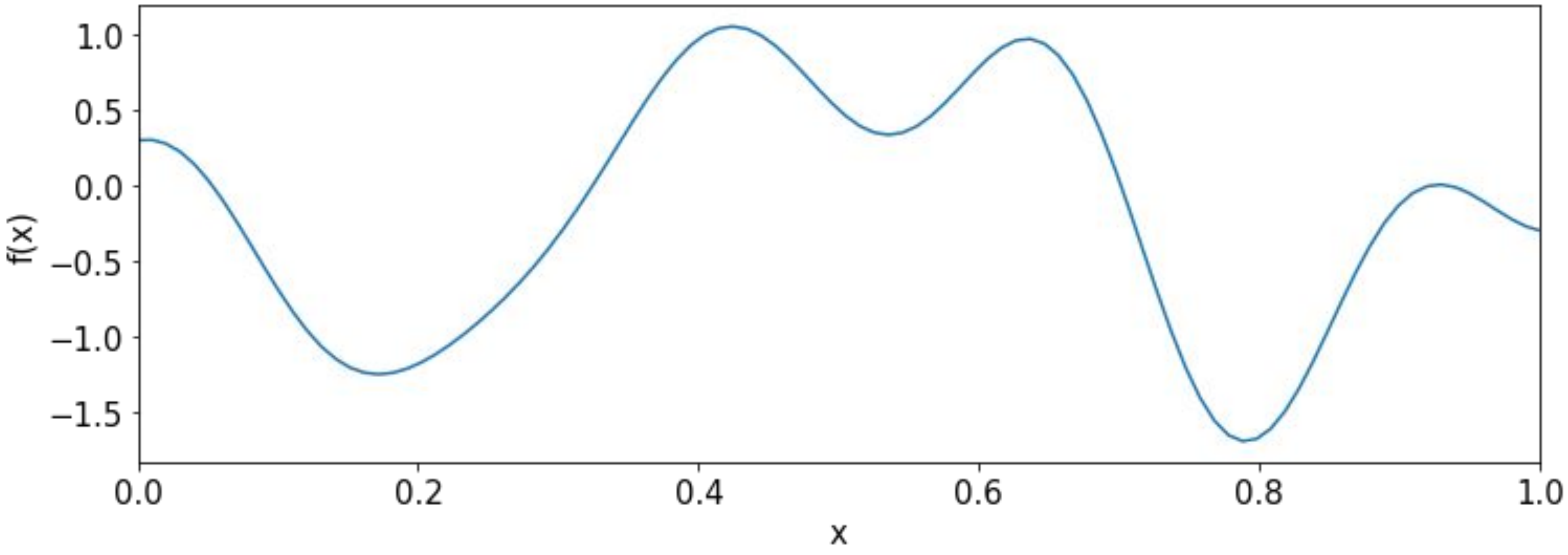

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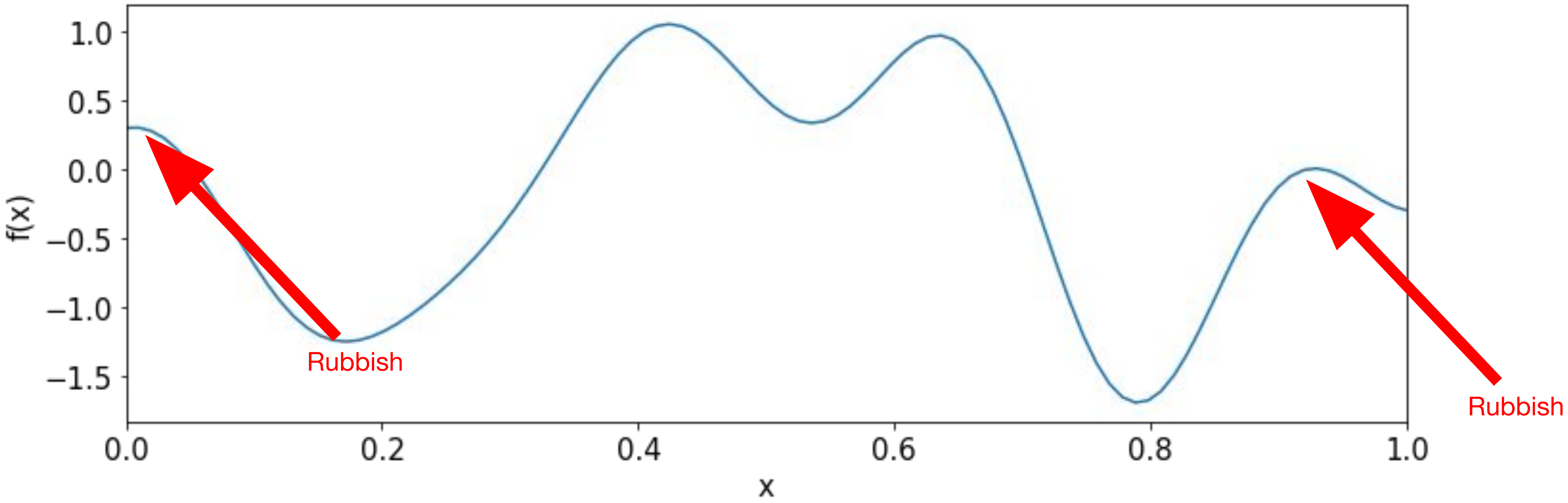

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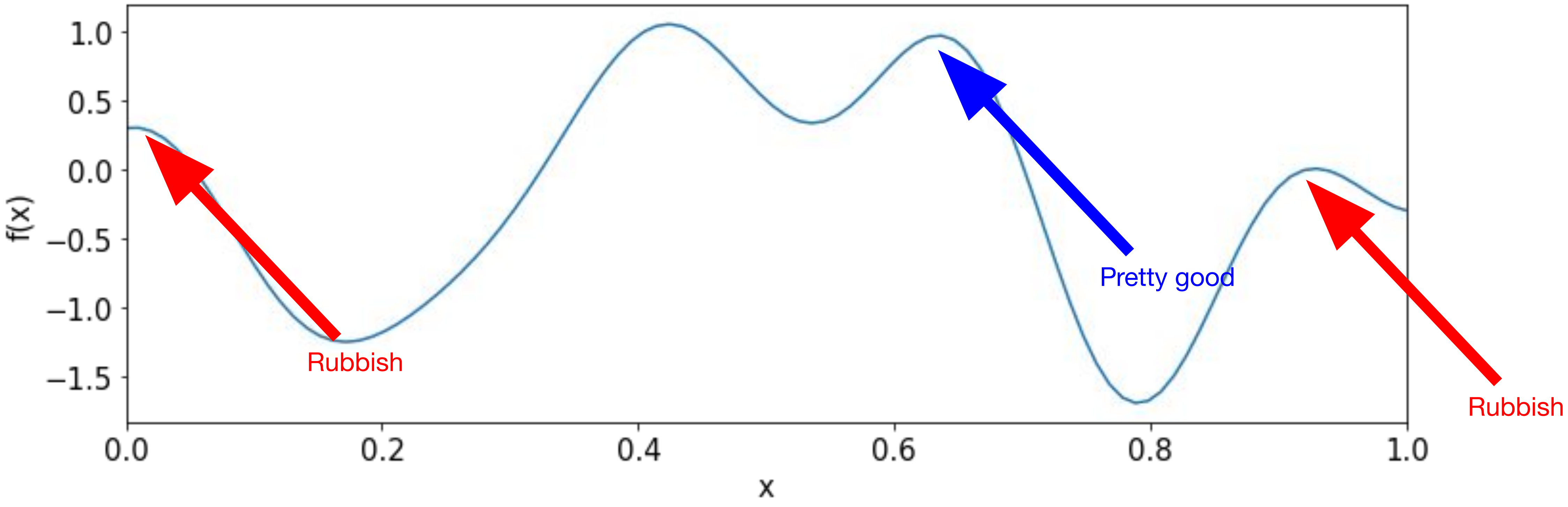

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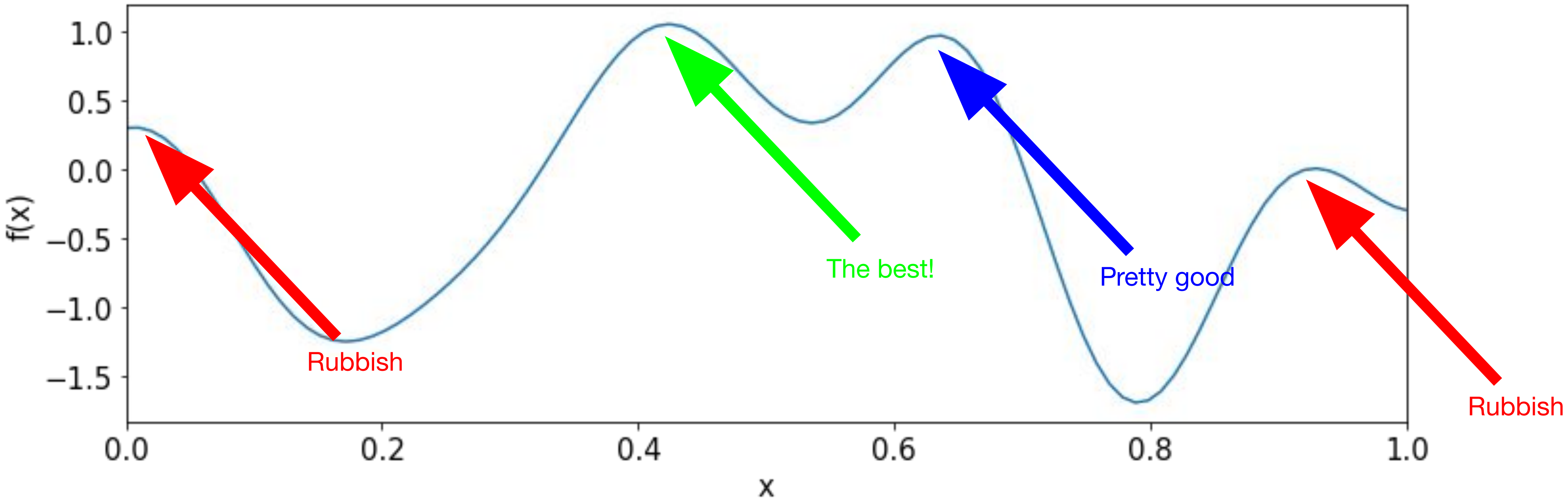
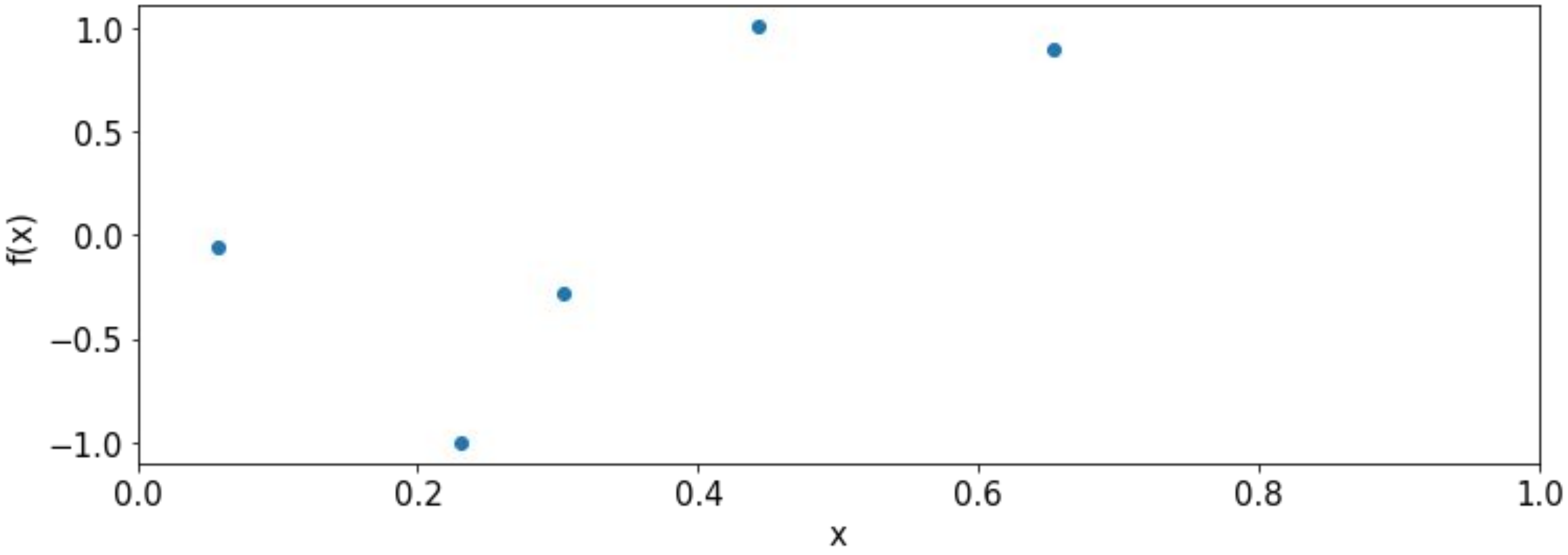


BO Demo

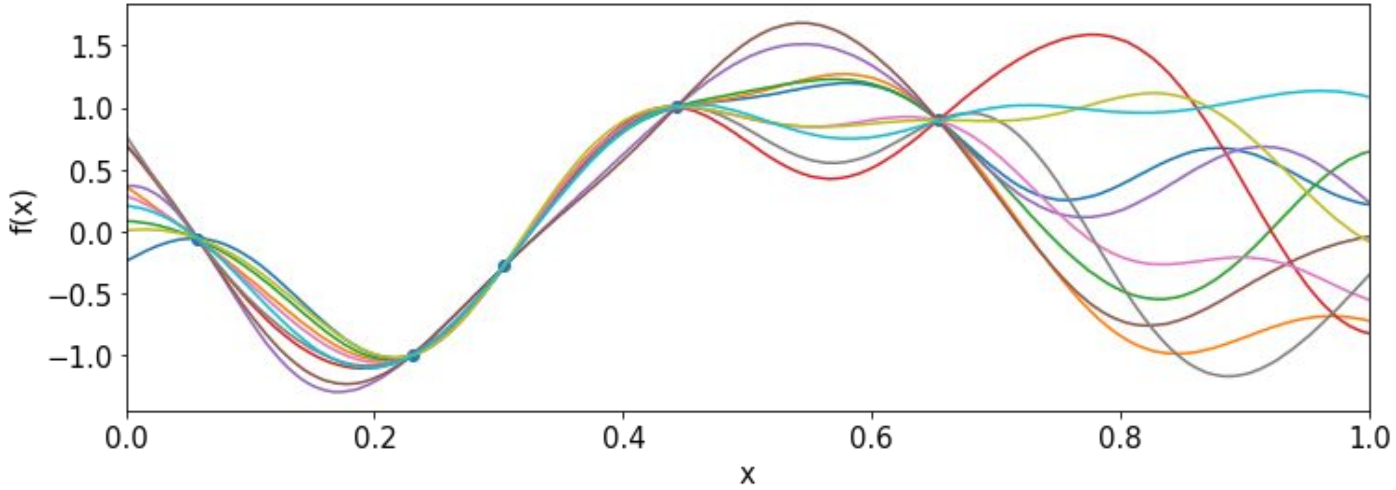
Suppose we make 5 evaluations

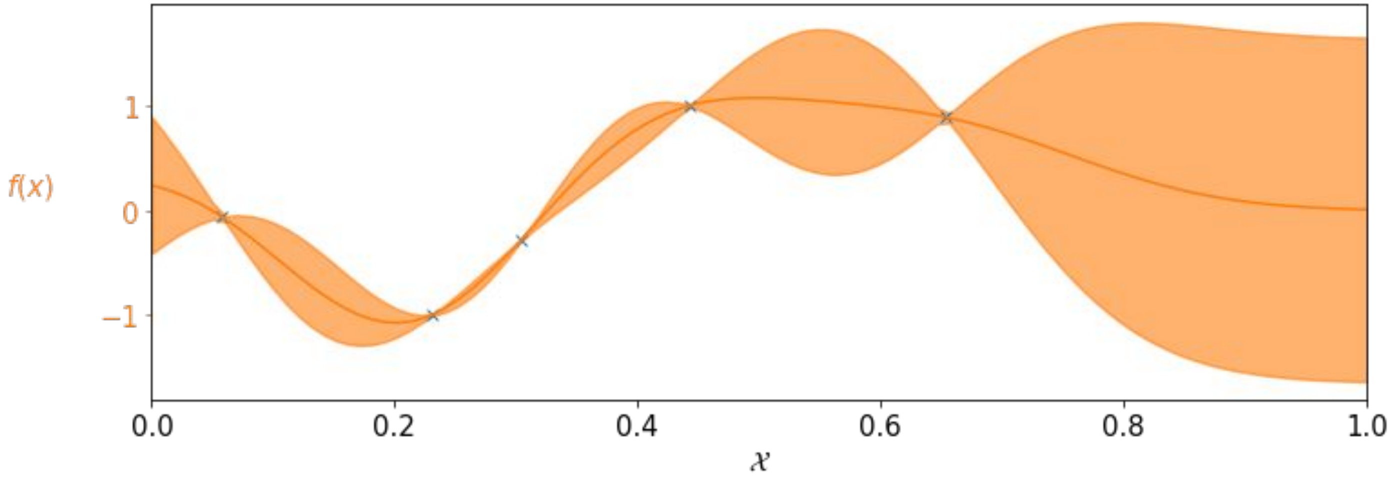


Where should we next evaluate? Explore/Exploit?

How to automate BO: step 1

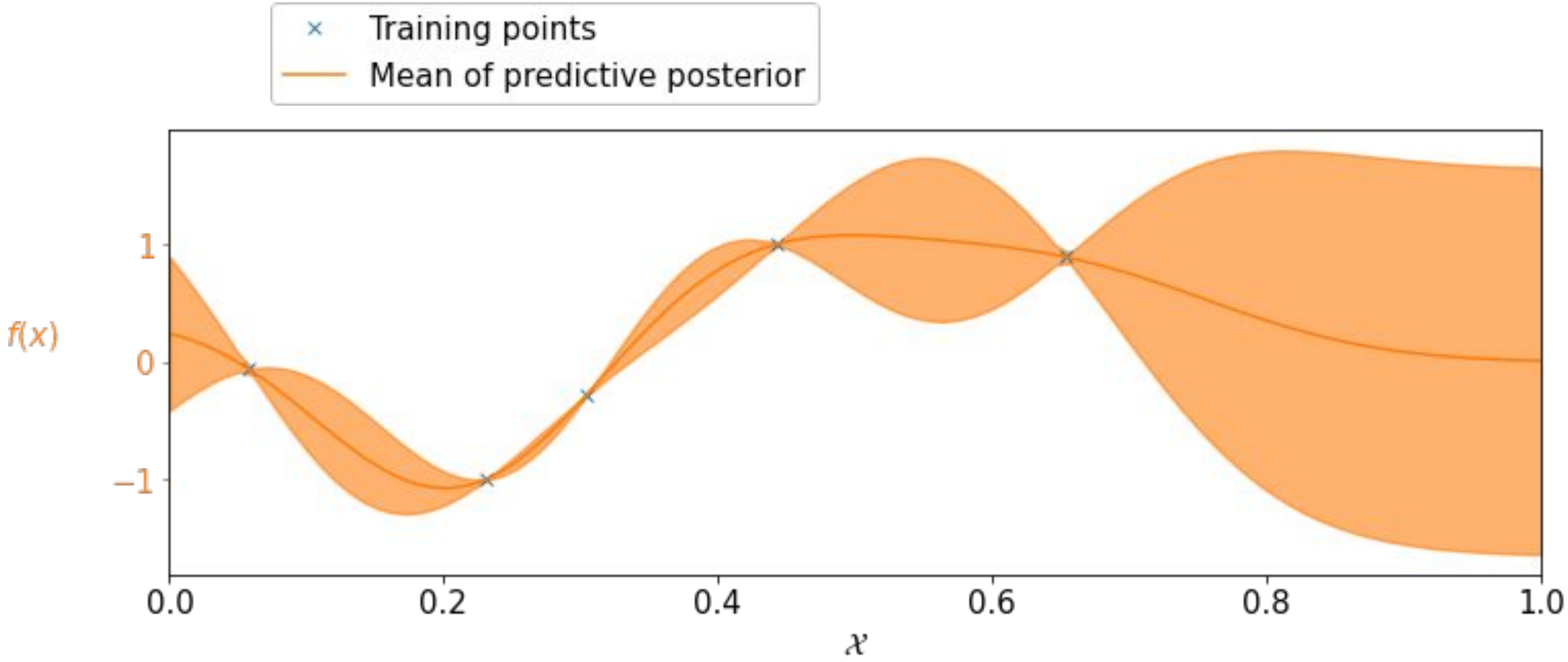
Use a statistical model like a Gaussian process





How to automate BO: step 2

Automated decision making via an acquisition function like expected improvement



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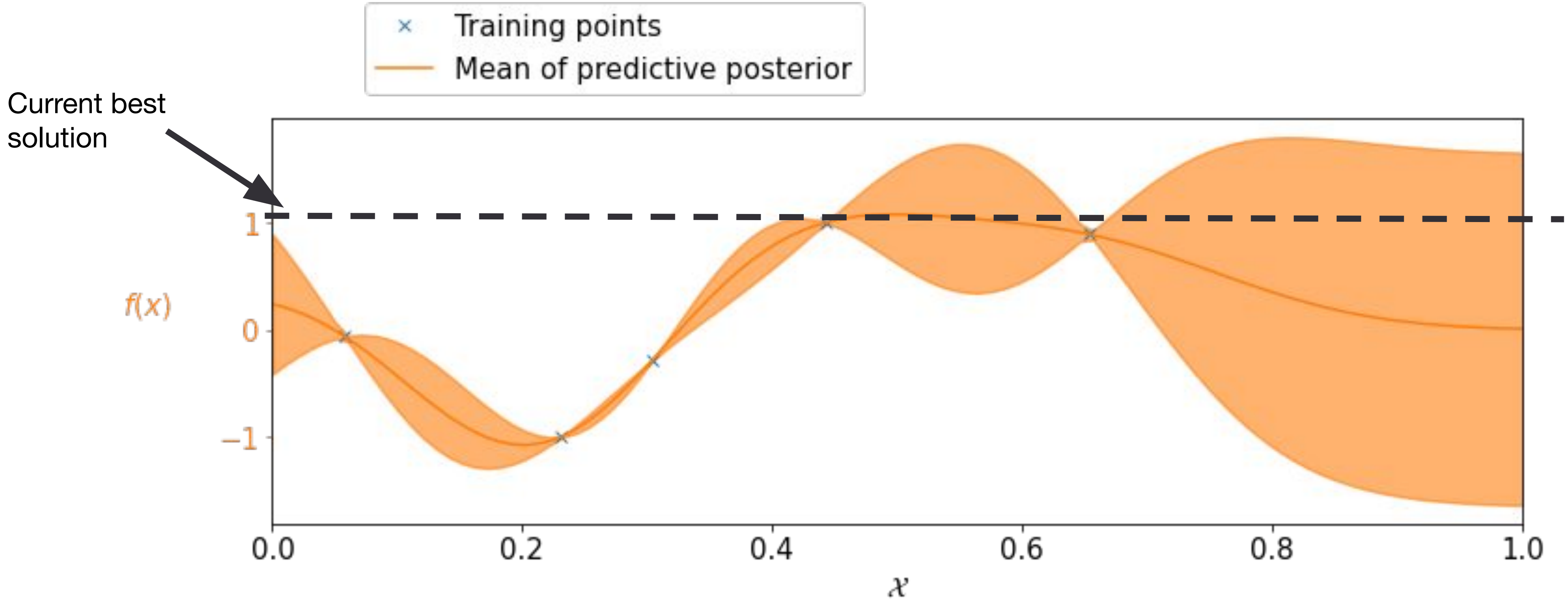

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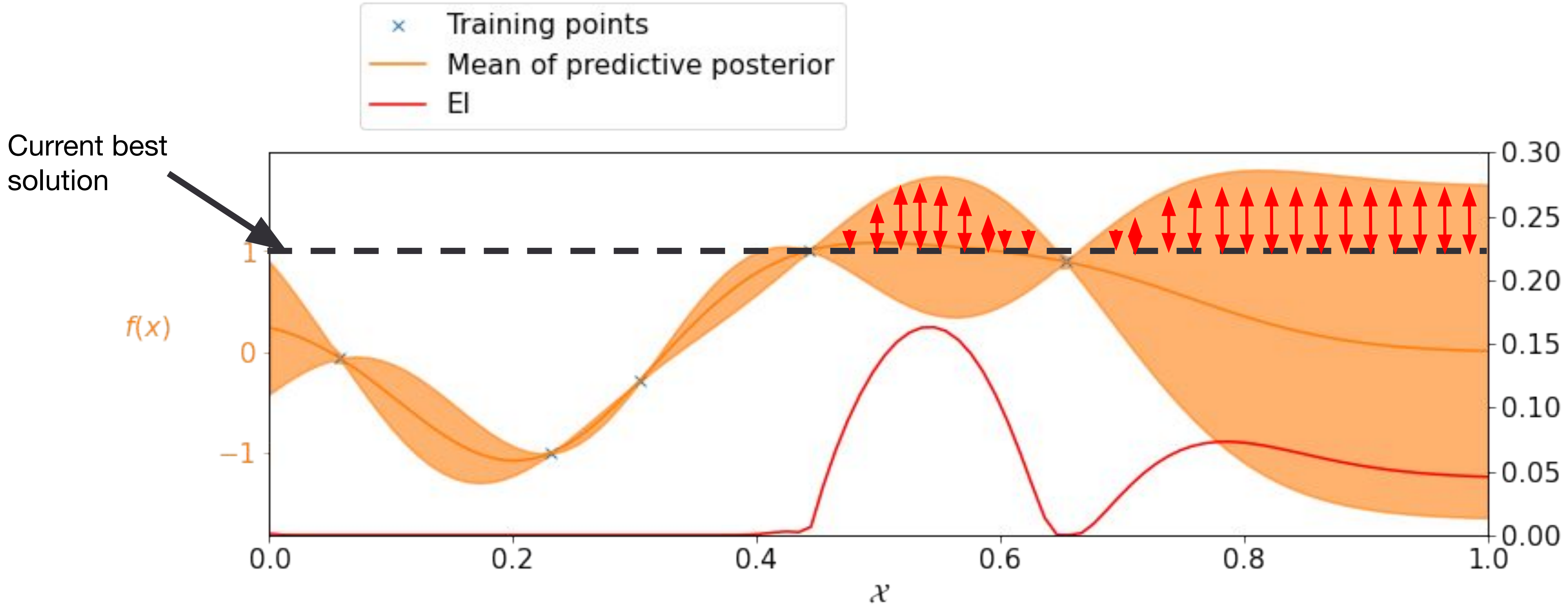

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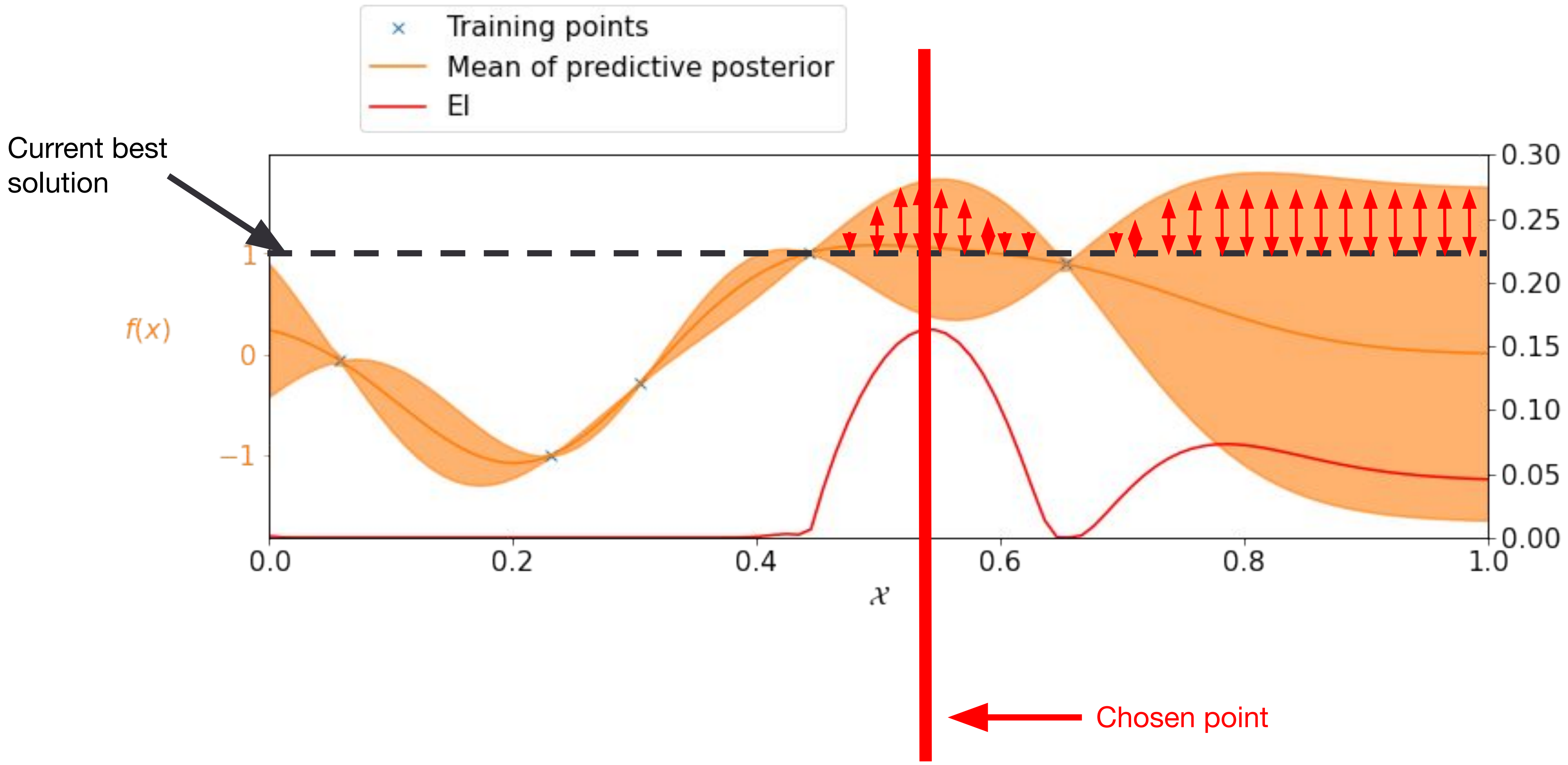
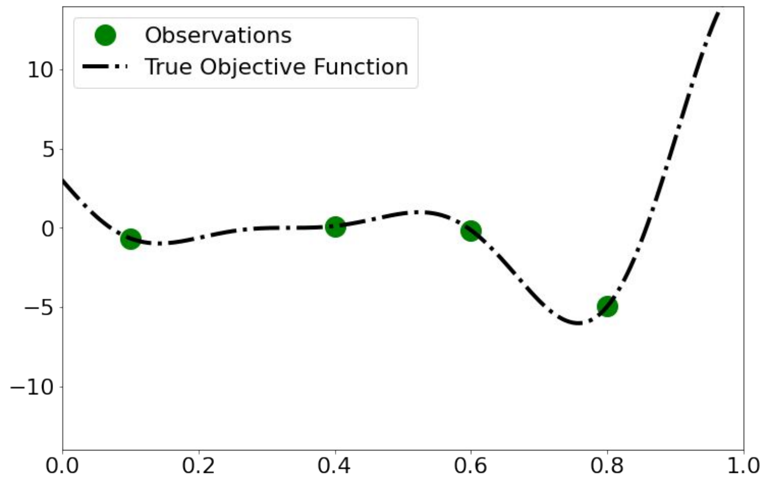


Expected Improvement

Demo BO loop



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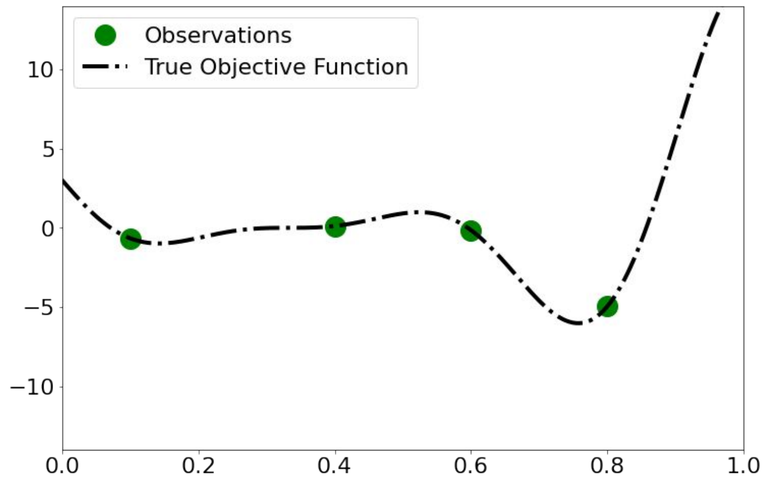

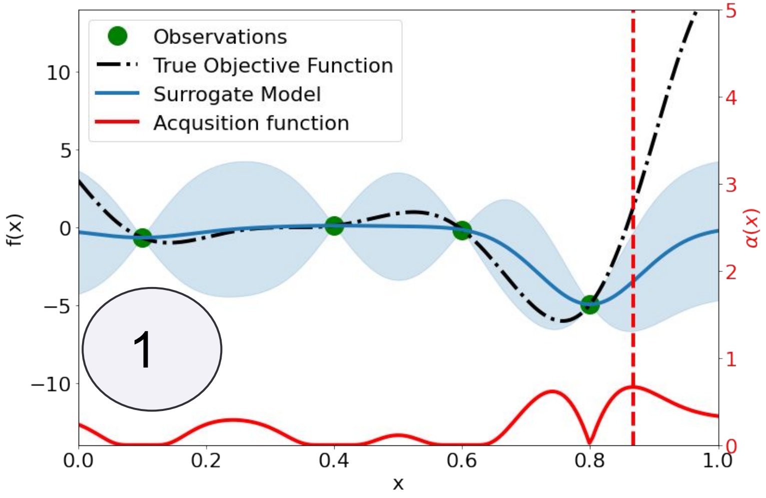

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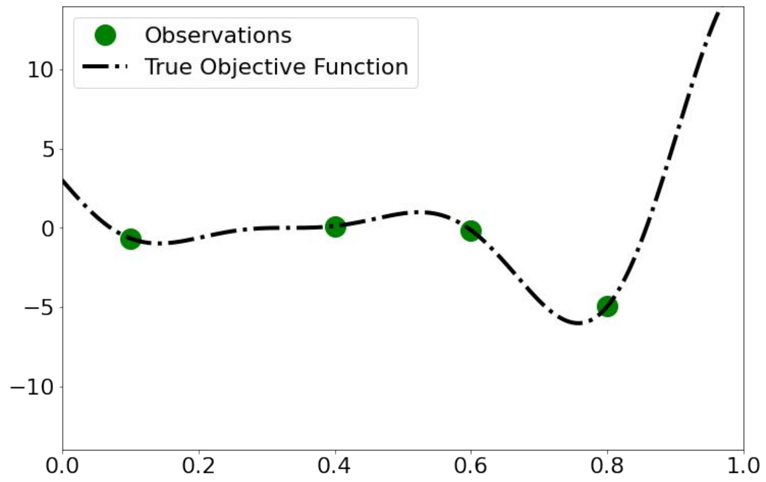

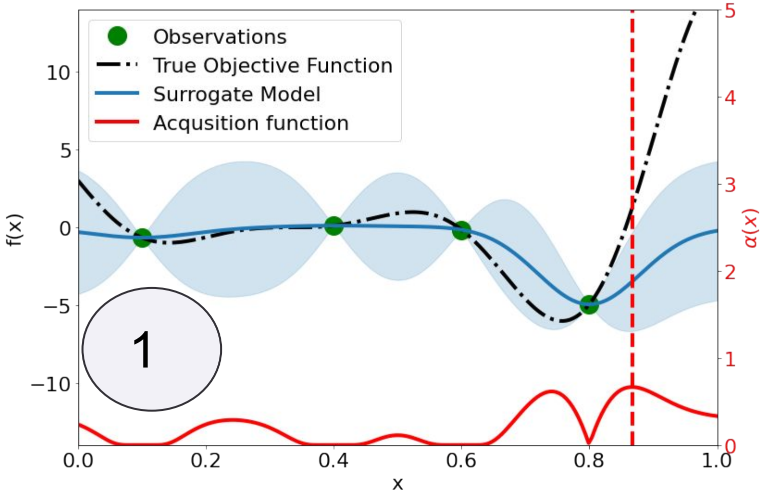

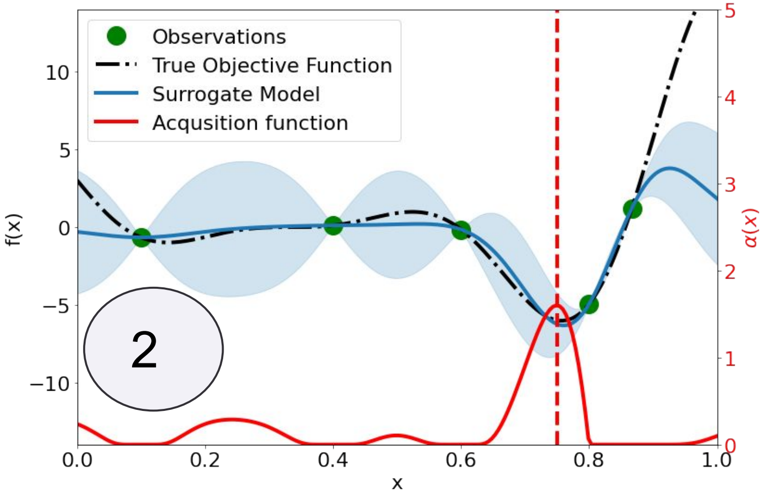

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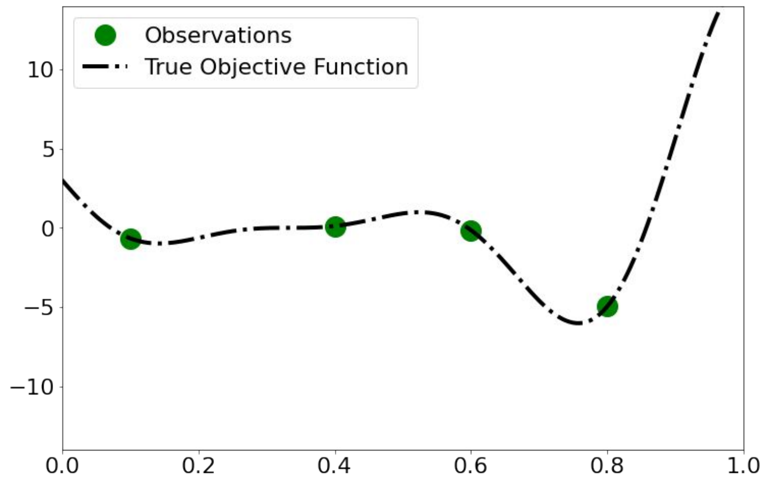

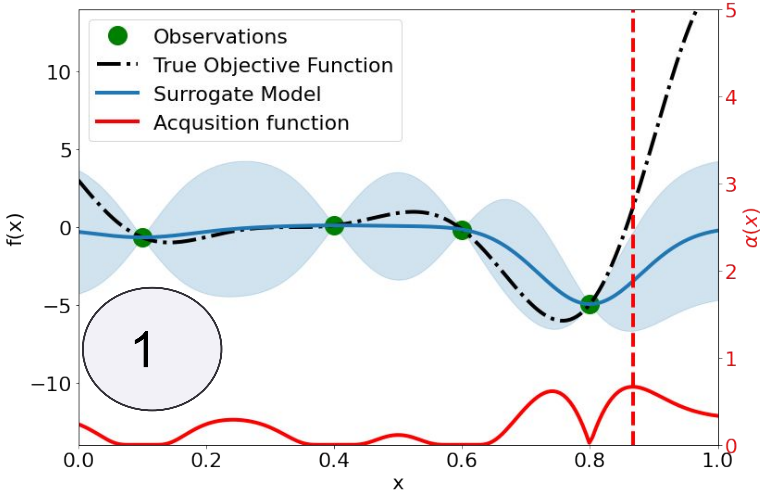

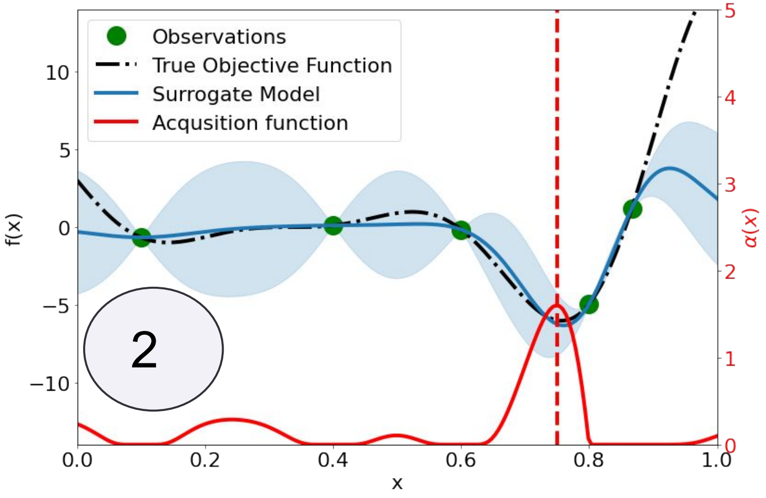

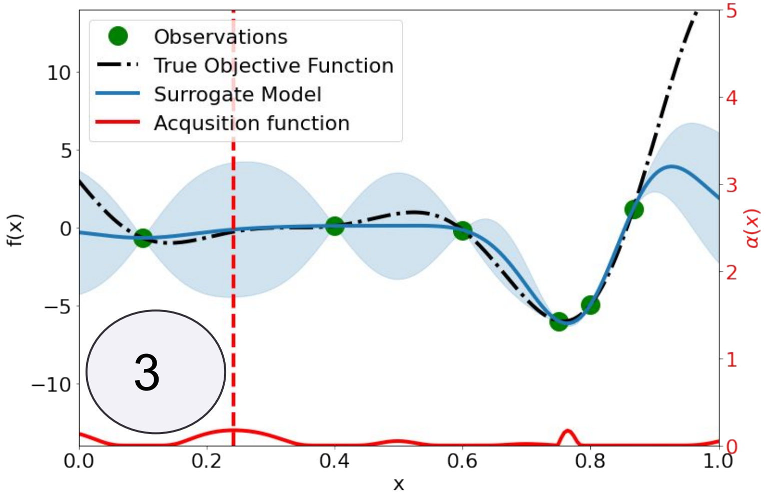

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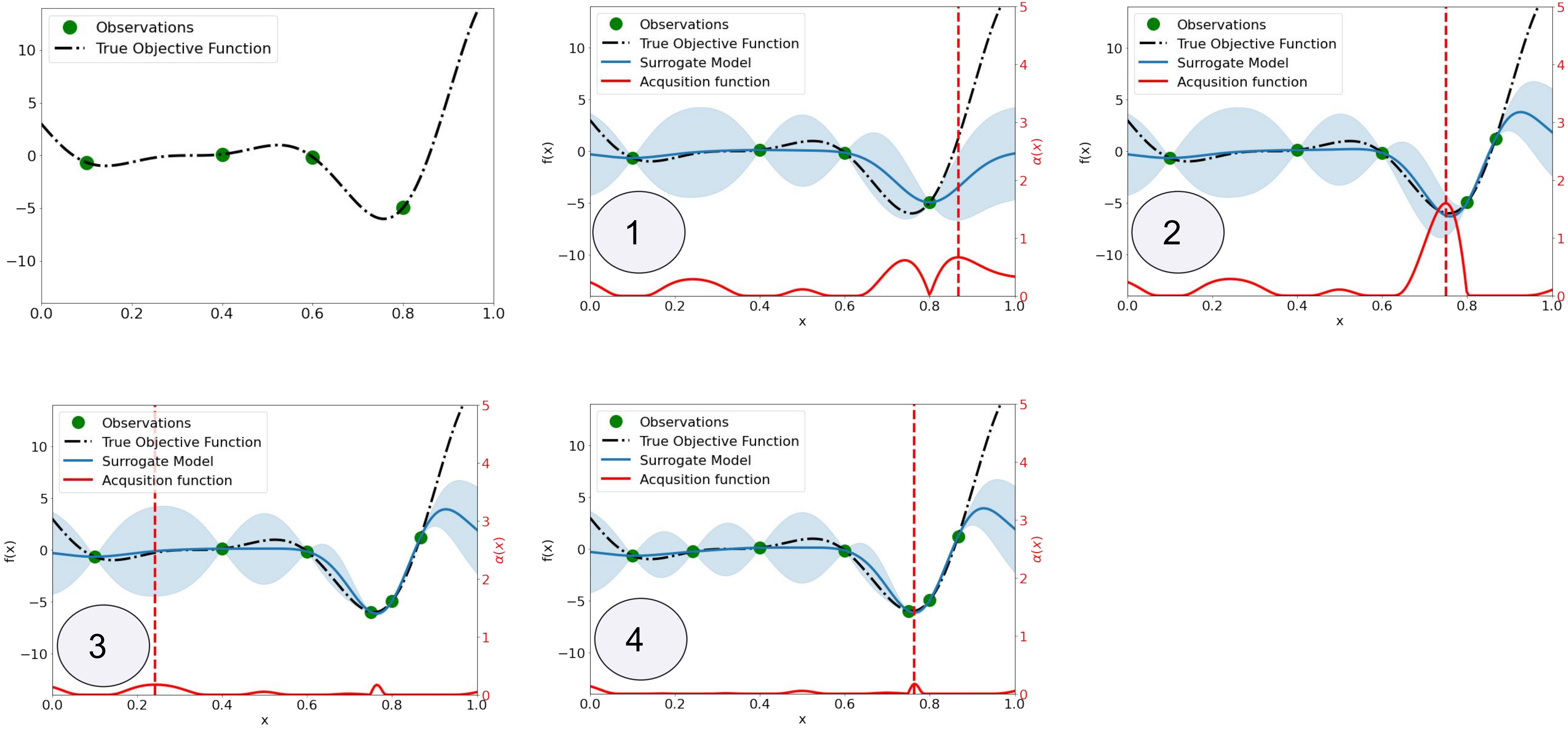

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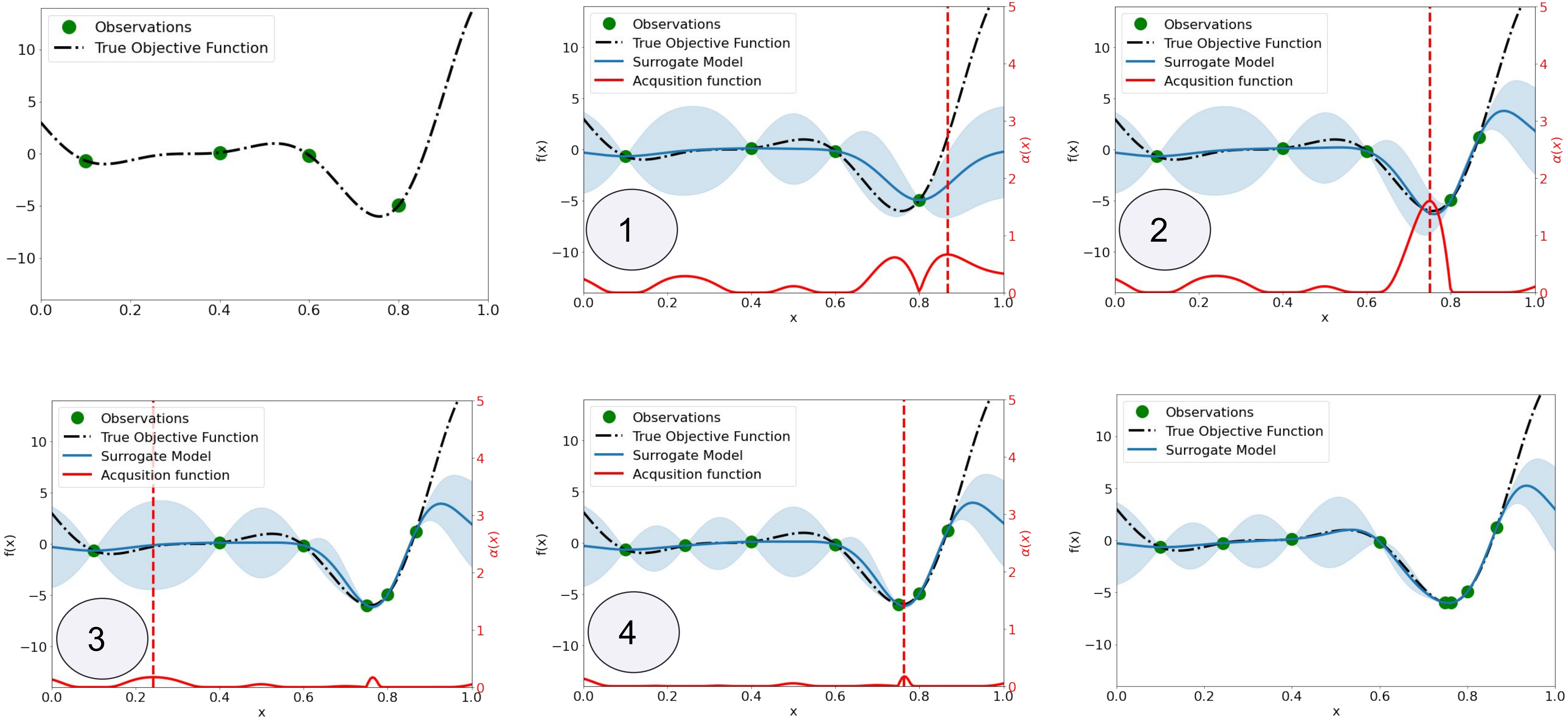

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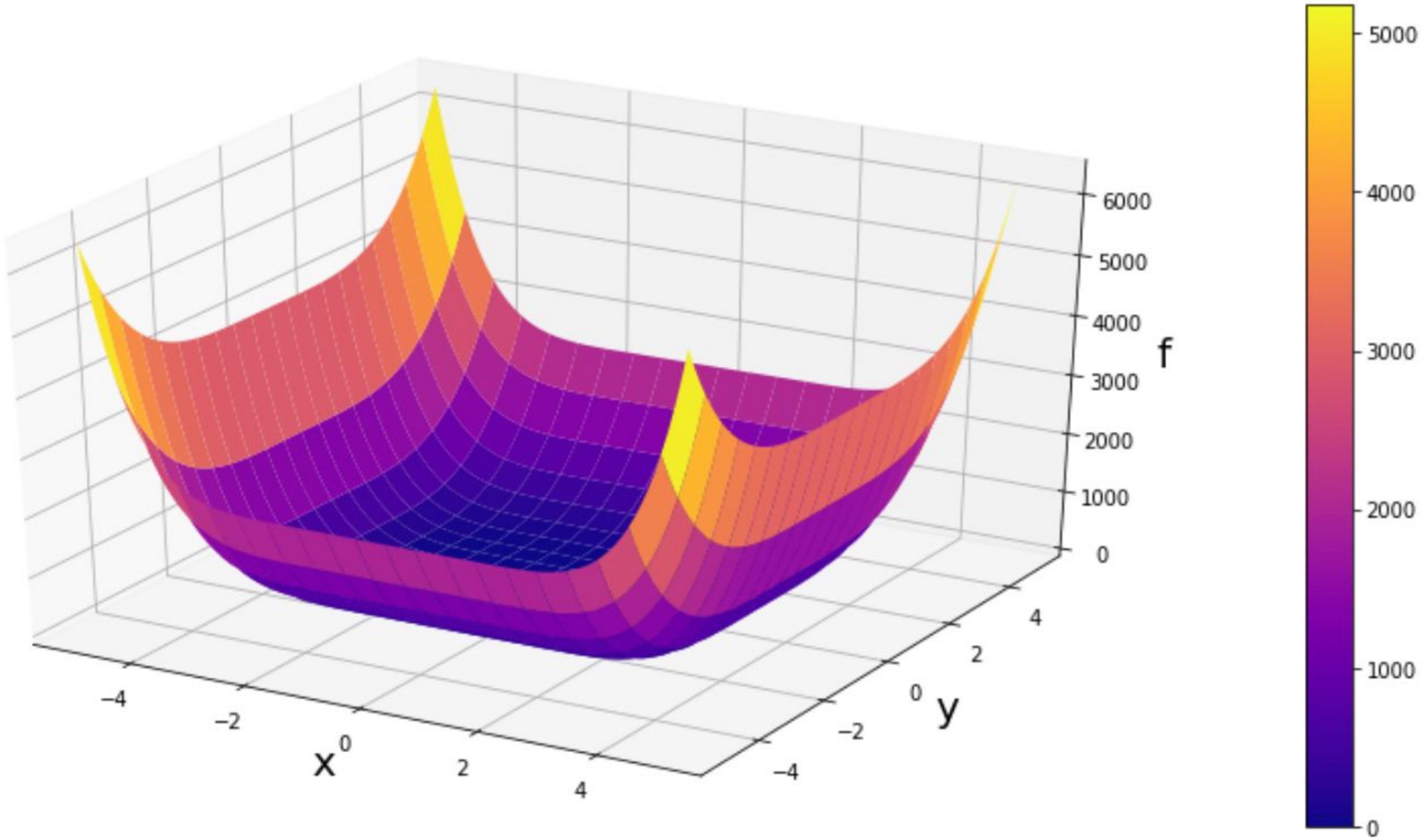
BO Demo 2

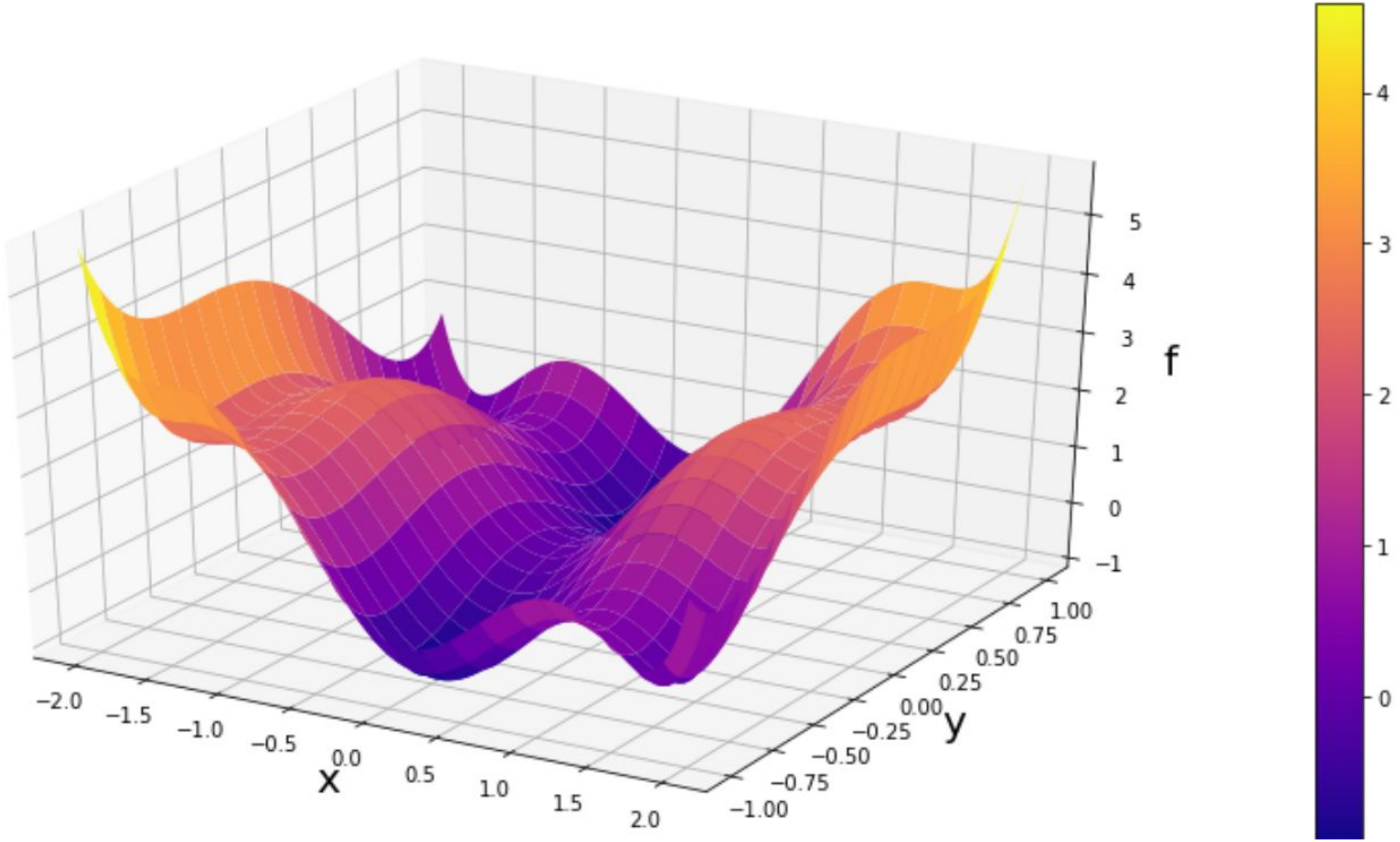
Let minimize the 6 Hump Camel function



Looks like we **can** use a local optimizer!

BO Demo 2

Zoom in: Perhaps not quite as easy?



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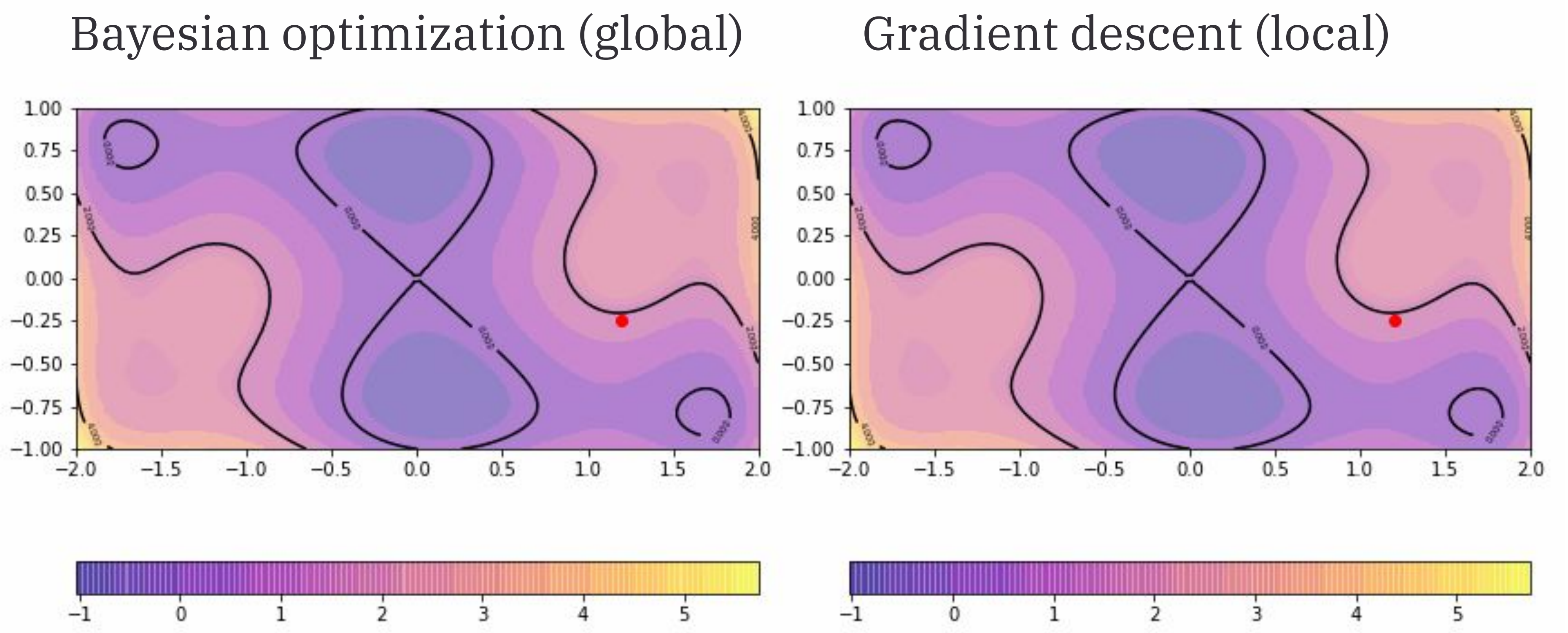
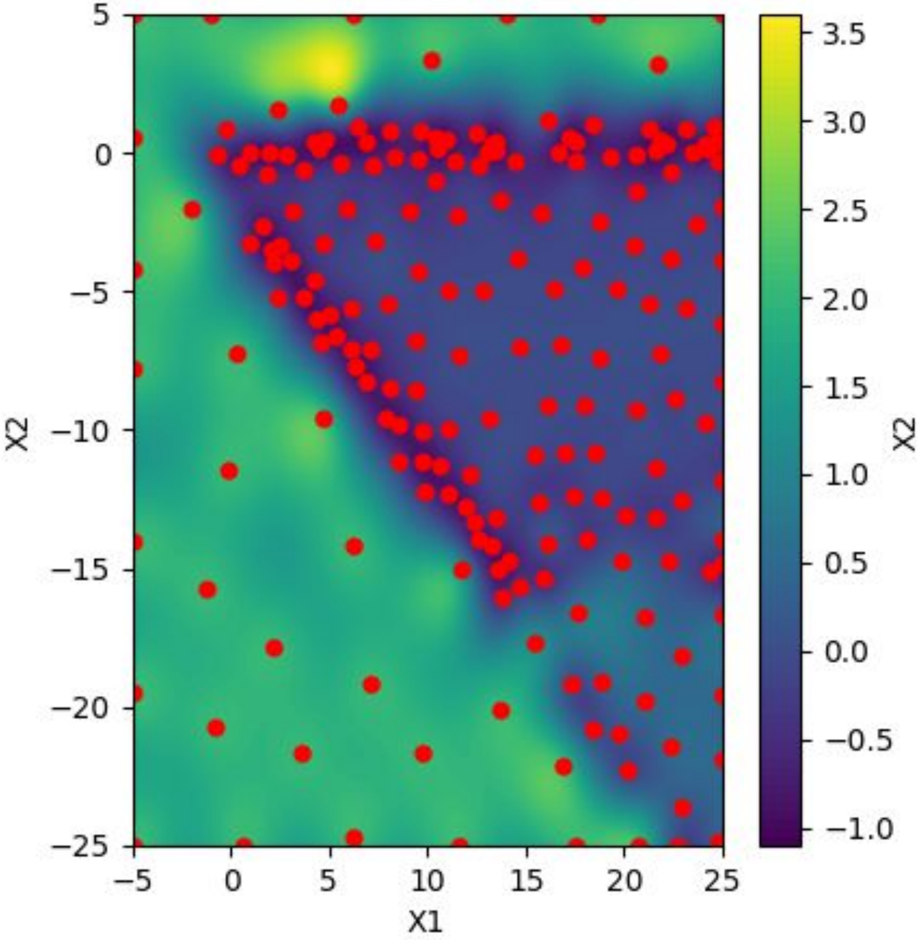
BO Demo 2

Bayesian optimization is a global optimizer



BO Demo 3

Efficient coverage of the search space



So why do we care about Bayesian Optimization?

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- We do not need gradients or noiseless observations (i.e. **black-box** optimization)

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Increasing cost

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BO: clever modelling rather than brute force!

Cool things that you can do with BO

- Fine-tune the performance of AlphaGO (https://arxiv.org/abs/1812.06855)
- Allow Amazon Alexa learn how to speak with new voices (https://arxiv.org/abs/2002.01953)
- Efficiently find new molecules / genes (https://arxiv.org/abs/2010.00979)
- Fine-tune electric car engines
- Optimize large climate models

A great new reference for BO: **https://bayesoptbook.com/**

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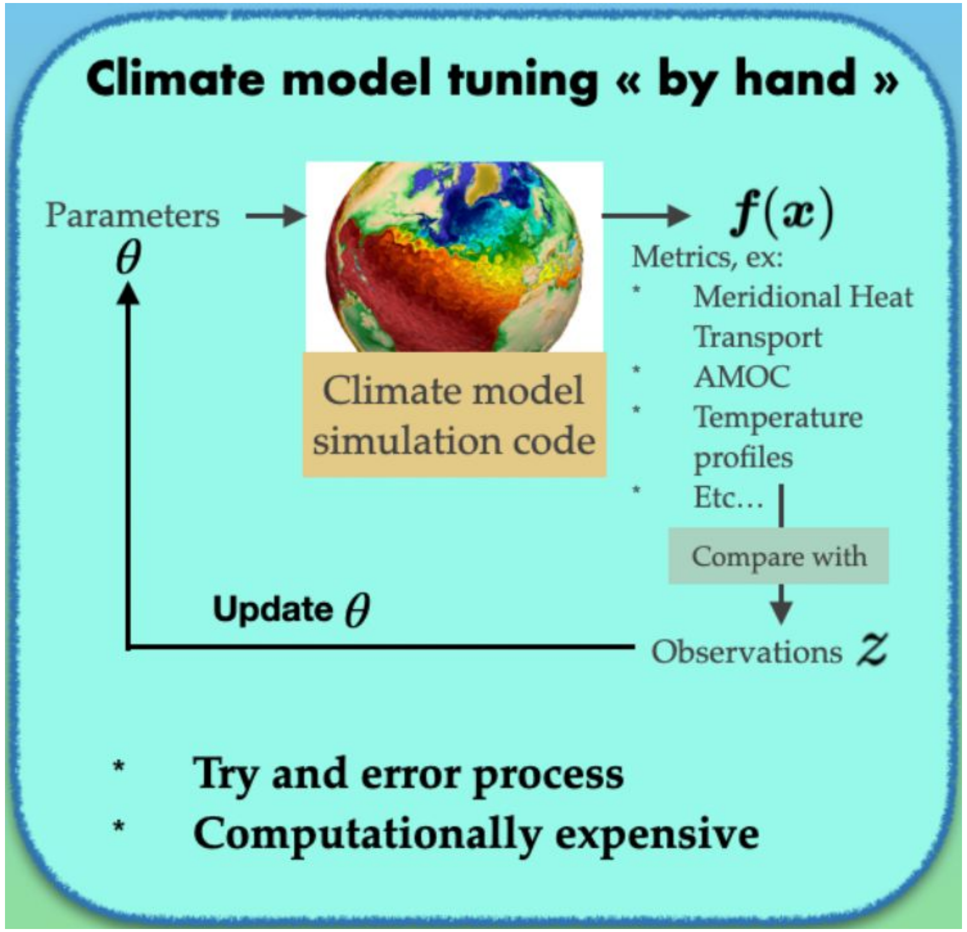
So, Climate model calibration?

Climate model calibration

Identifying reasonable values for model parameters



Lguensat et al. 2022.

Climate model calibration

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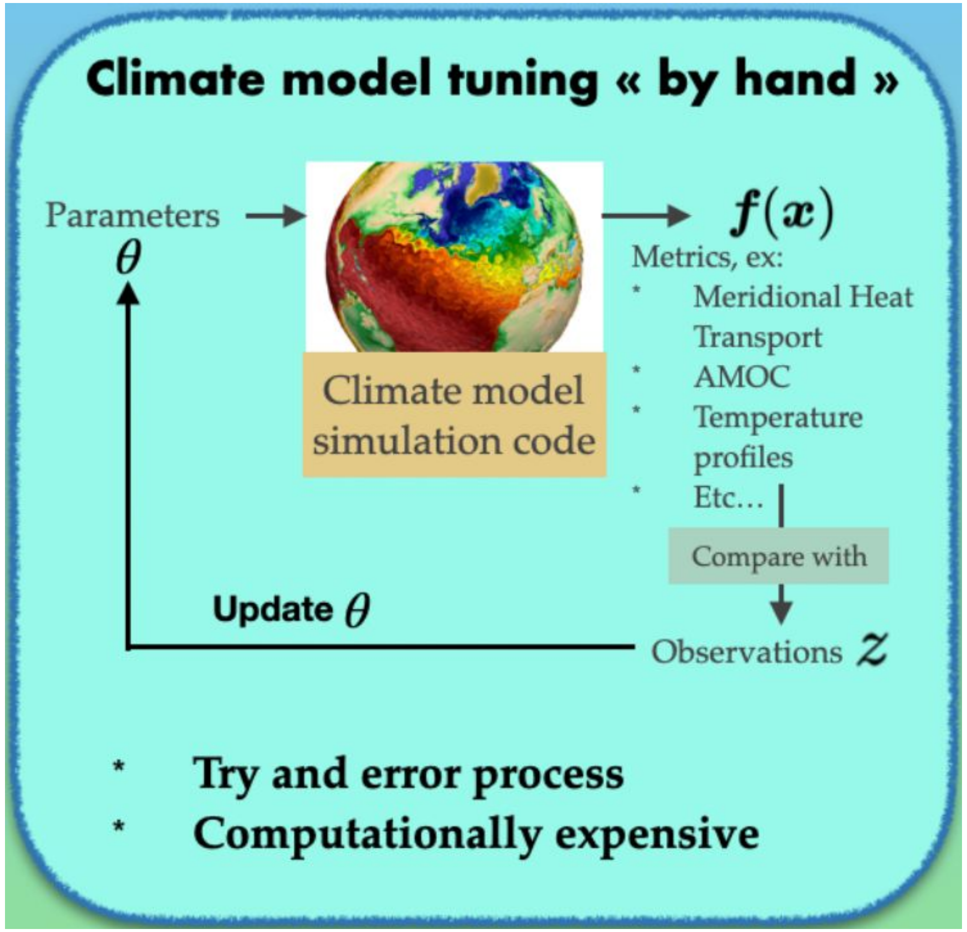

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- Need to find parameters that give high plausibility to historical data —----------> a **function maximisation** problem

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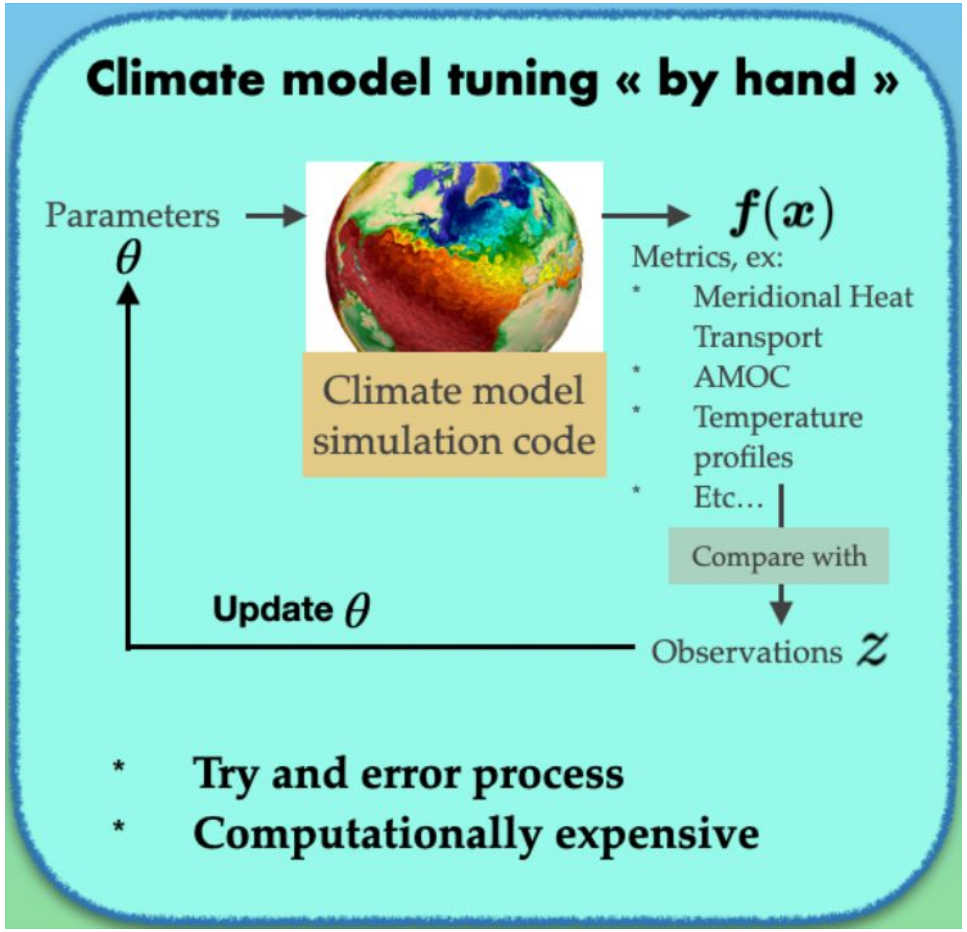


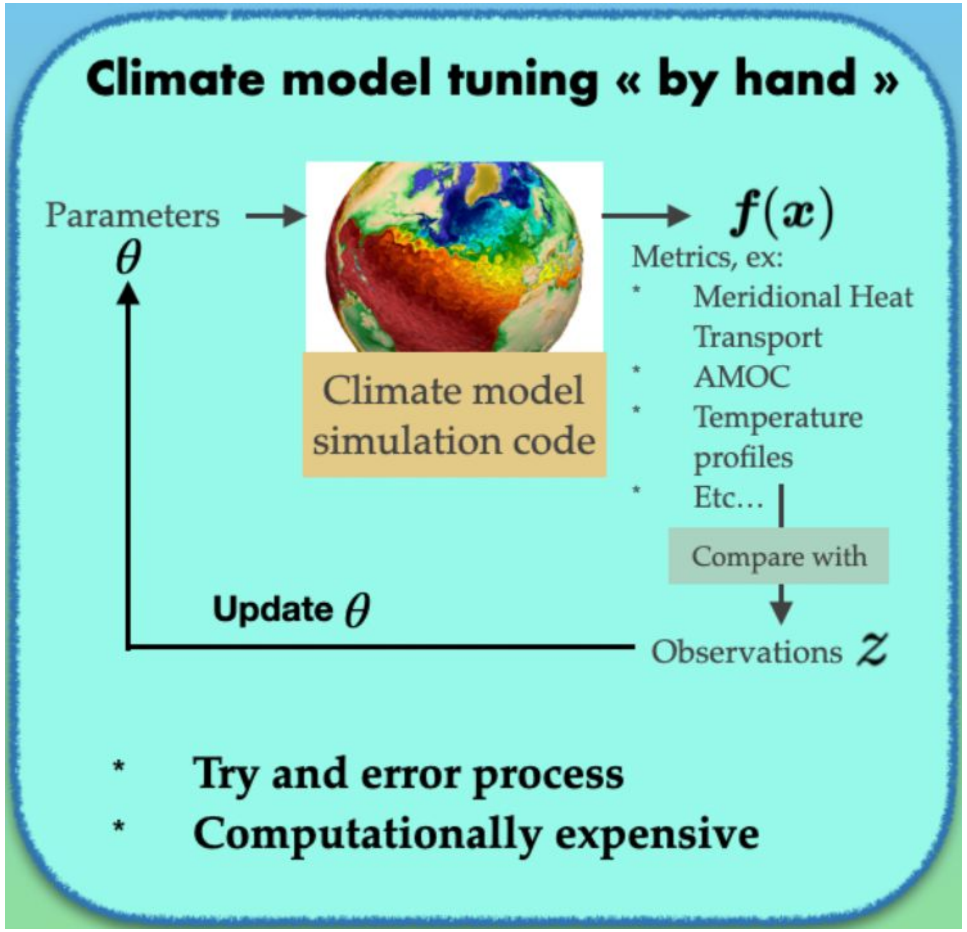
Lguensat et al. 2022.

- Need to find parameters that give high plausibility to historical data —----------> a **function maximisation** problem

- Climate models are expensive —-----------------> can only afford a **limited number of evaluations** (no grid!)

Climate model calibration

Identifying reasonable values for model parameters



Lguensat et al. 2022.

- Need to find parameters that give high plausibility to historical data —---------> a **function maximisation** problem
- Climate models are expensive —----------------> can only afford a **limited number of evaluations** (no grid!)
- We do not have gradients (easily) and limited prior knowledge —----------------> a **black-box** objective function

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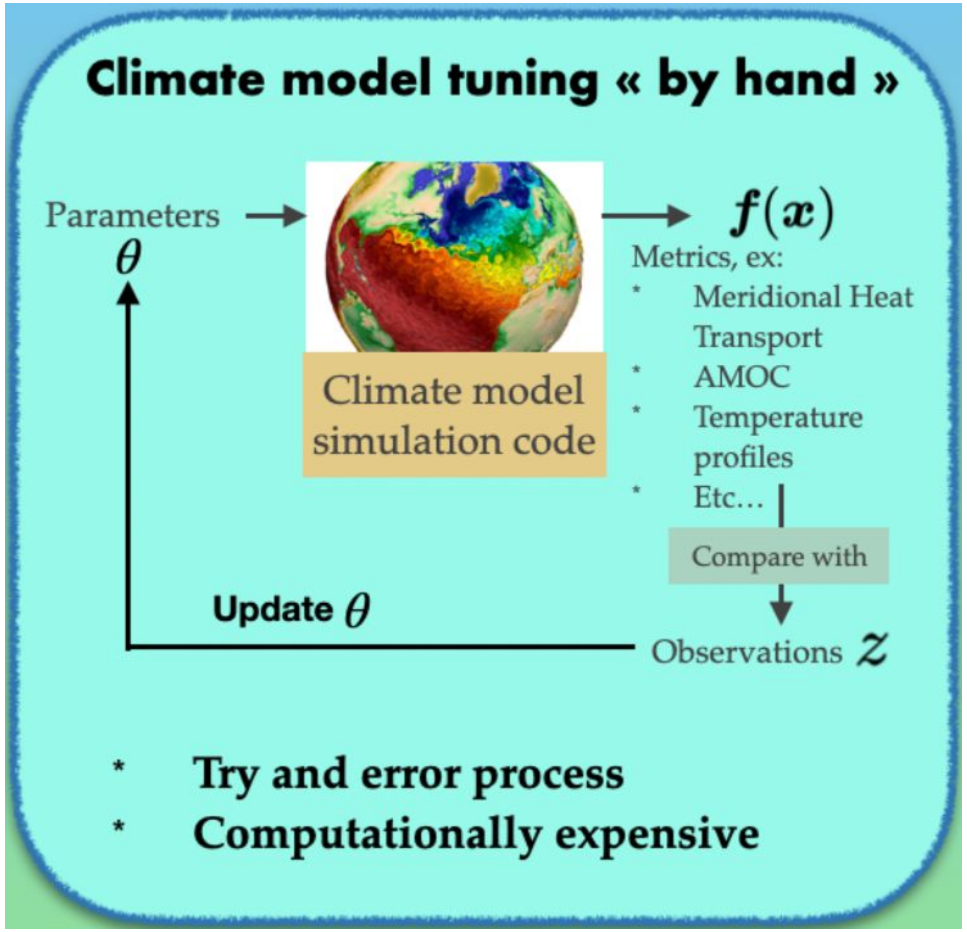
Climate model calibration

Identifying reasonable values for model parameters

So we have a resource-constrained black-box function optimisation!



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Climate model calibration by iteratively refocusing

sequentially whittle down the plausible region

Based on Lguensat et al. 2022.

Climate model calibration by iteratively refocusing

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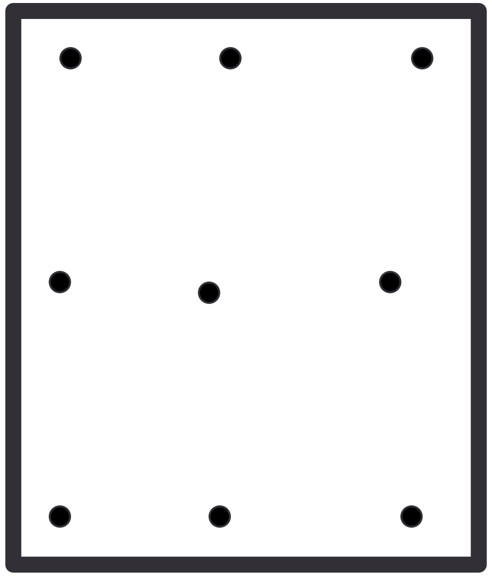

Initial Design

Based on Lguensat et al. 2022.

Climate model calibration by iteratively refocusing

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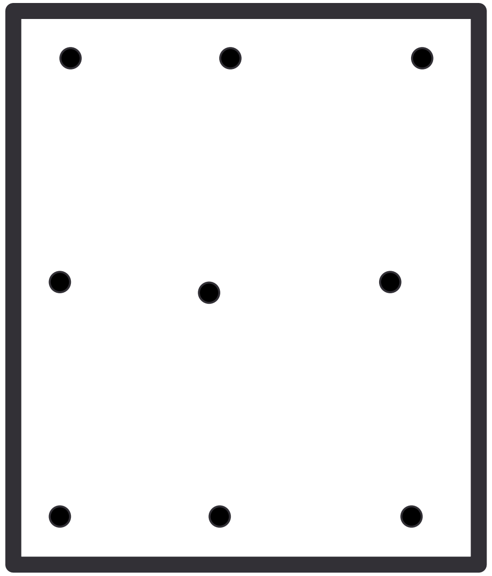
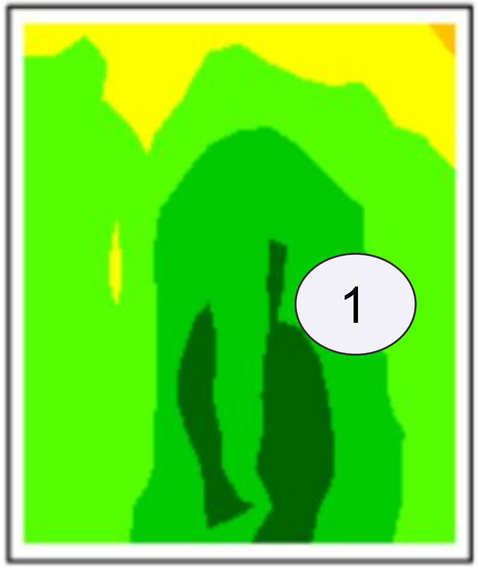


Initial Design



Predicted implausibility

Based on Lguensat et al. 2022.

Climate model calibration by iteratively refocusing

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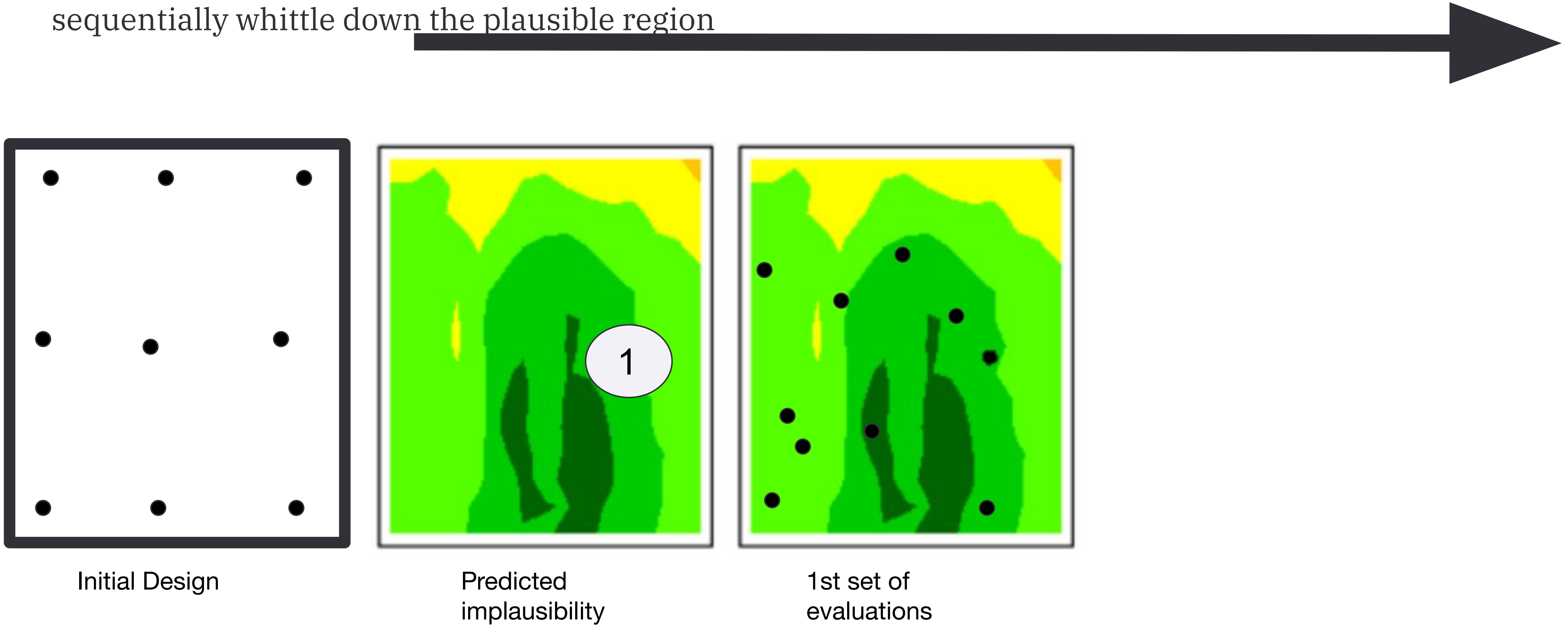

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Climate model calibration by iteratively refocusing

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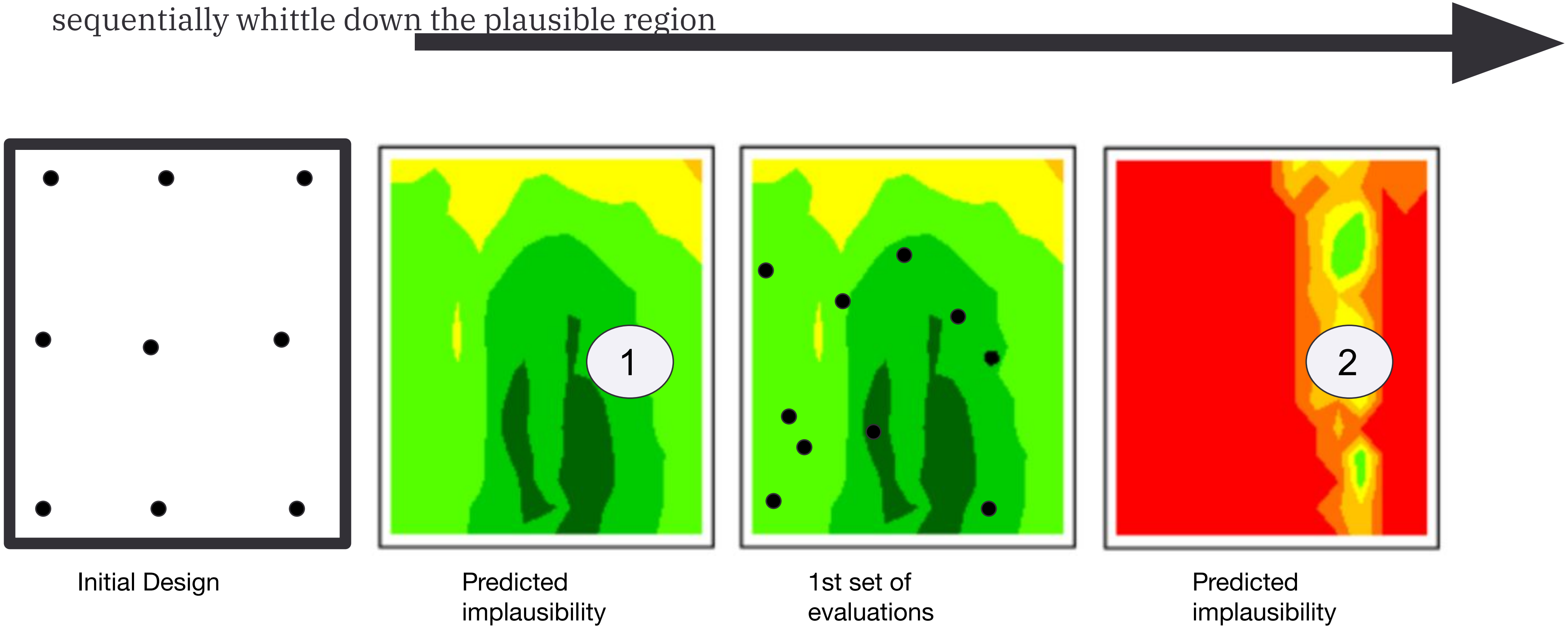

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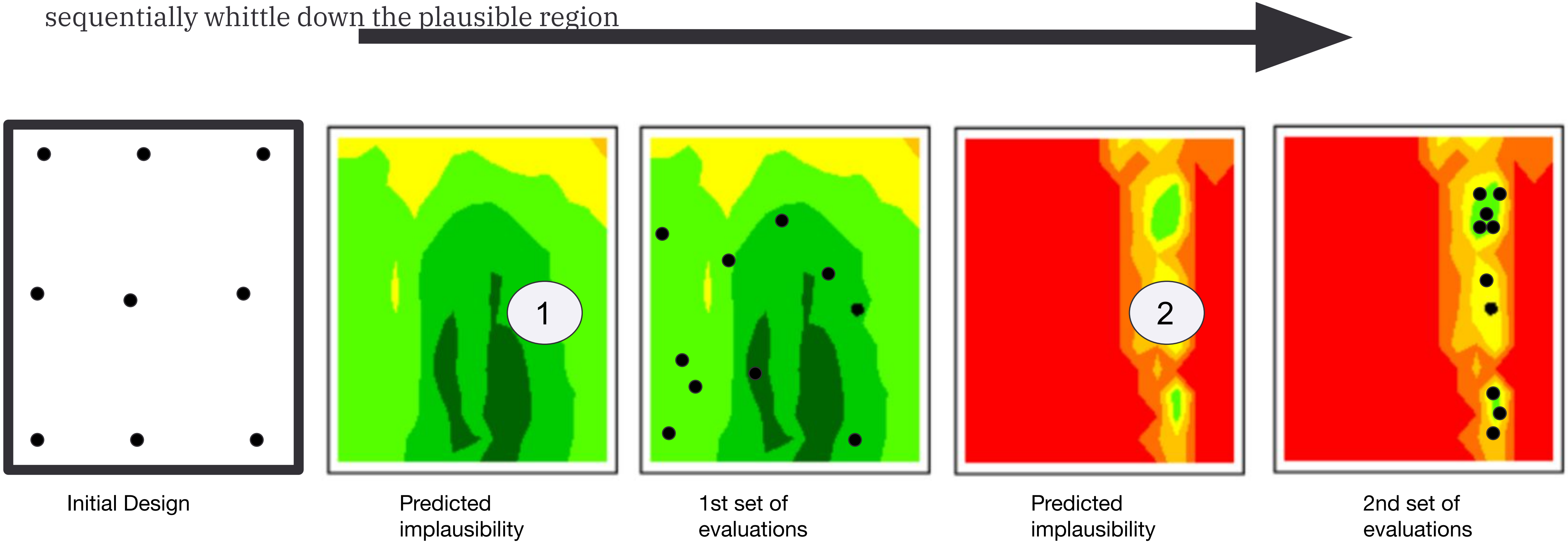

Based on Lguensat et al. 2022.

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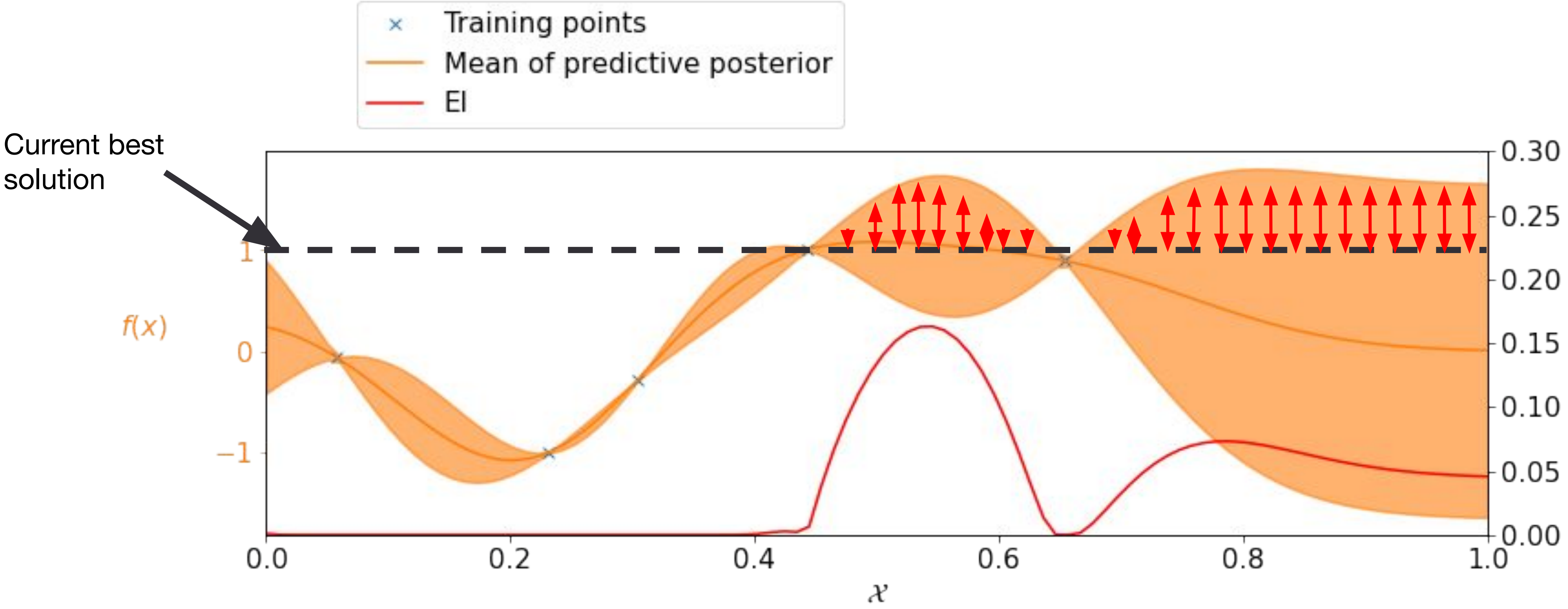
Back to molecular design

Large batches

Automatically choosing batches of points

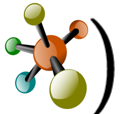
Using GP posteriors and utility functions



How to pick **3** points ?

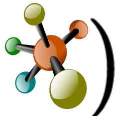
Automatically choosing batches of molecules

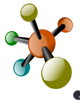
Using GP posteriors and utility functions

- $\alpha_{\mathrm{EI}}($  $) = \mathbb{E}_f[\max(f - f^\star, 0)]$ $\qquad f \sim \mathcal{N}(\mu, \sigma^2)$

Automatically choosing batches of molecules

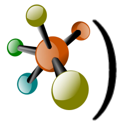
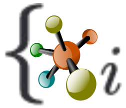
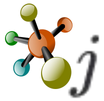
Using GP posteriors and utility functions

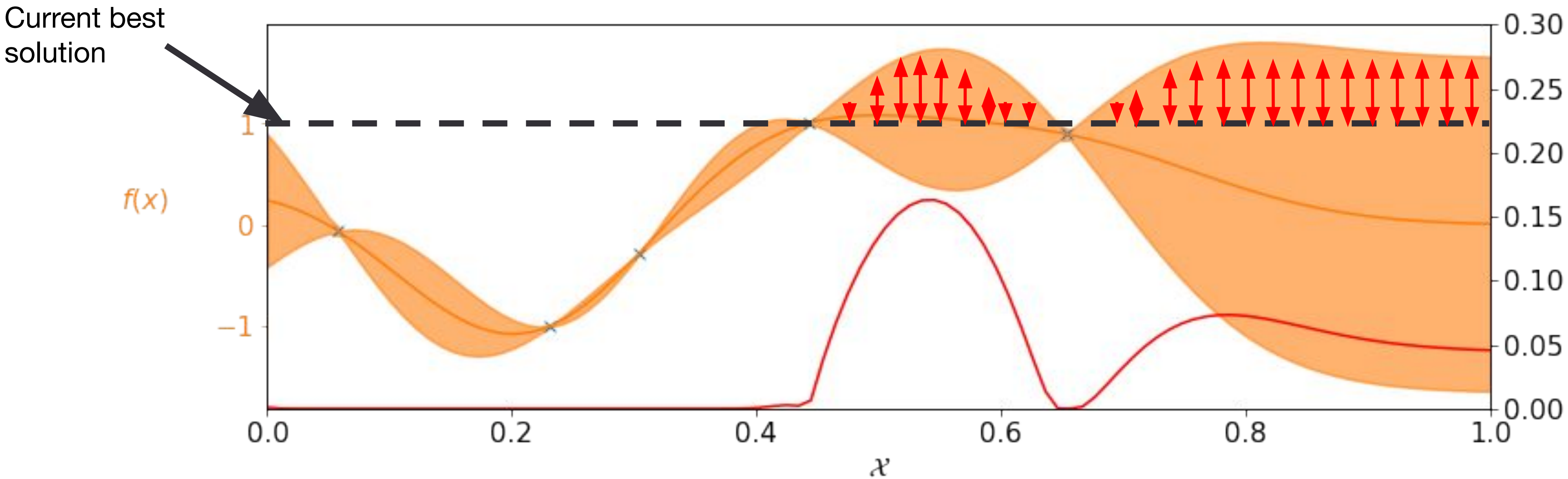
- $\alpha_{\mathrm{EI}}($  $) = \mathbb{E}_f[\max(f - f^\star, 0)]$

- $\alpha_{\mathrm{EI}}(\{$  $_i,$  $_j\}) = \, ???$

Automatically choosing batches of molecules

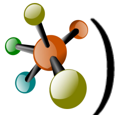
Using GP posteriors and utility functions

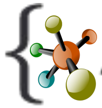
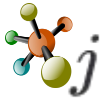
- $\alpha_{\mathrm{EI}}($  $) = \mathbb{E}_f[\max(f - f^\star, 0)]$
- $\alpha_{\mathrm{EI}}(\{$  $_i,$  $_j\}) = \mathbb{E}_{f_i, f_j}[\max(f_i - f^\star, f_j - f^\star, 0)]$



Automatically choosing batches of molecules

Using GP posteriors and utility functions

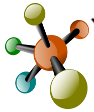
- $\alpha_{\mathrm{EI}}($  $) = \mathbb{E}_f[\max(f - f^\star, 0)]$

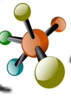
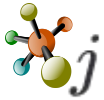
- $\alpha_{\mathrm{EI}}(\{$  $_i,$  $_j\}) = \mathbb{E}_{f_i,\, f_j}[\max(f_i - f^\star, f_j - f^\star, 0)]$

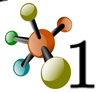
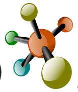
$$\begin{pmatrix} f_i \\ f_j \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} \mu_i \\ \mu_j \end{pmatrix}, \begin{pmatrix} \Sigma_{i,i} & \Sigma_{i,j} \\ \Sigma_{j,i} & \Sigma_{j,j} \end{pmatrix} \right)$$

Automatically choosing batches of molecules

Using GP posteriors and utility functions

- $\alpha_{\mathrm{EI}}($  $) = \mathbb{E}_f[\max(f - f^\star, 0)]$

- $\alpha_{\mathrm{EI}}(\{$  $_i,$  $_j\}) = \mathbb{E}_{f_i, f_j}[\max(f_i - f^\star, f_j - f^\star, 0)]$

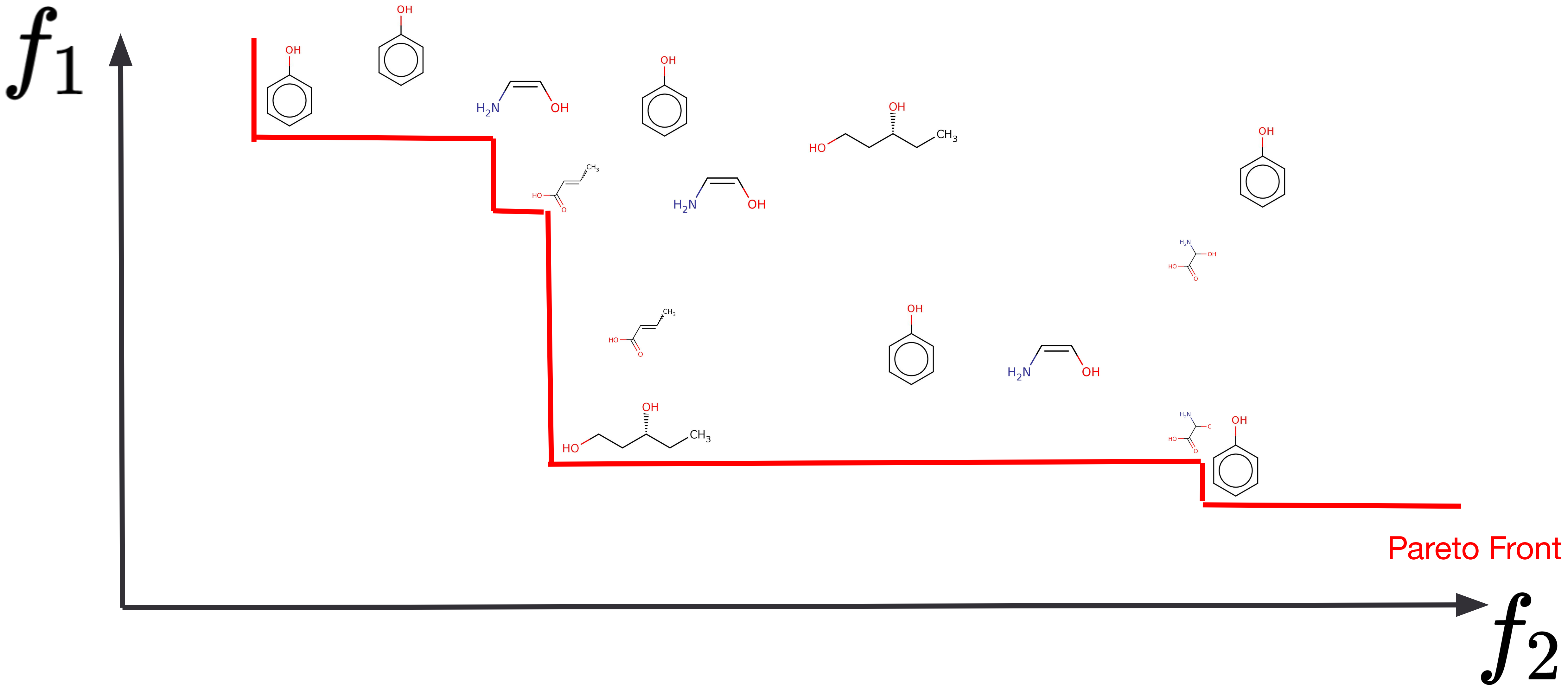
- $\alpha_{\mathrm{EI}}(\{$  $_1, \ldots,$  $_B\}) = ???$

Back to molecular design

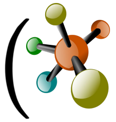
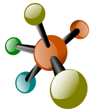
Multiple objectives

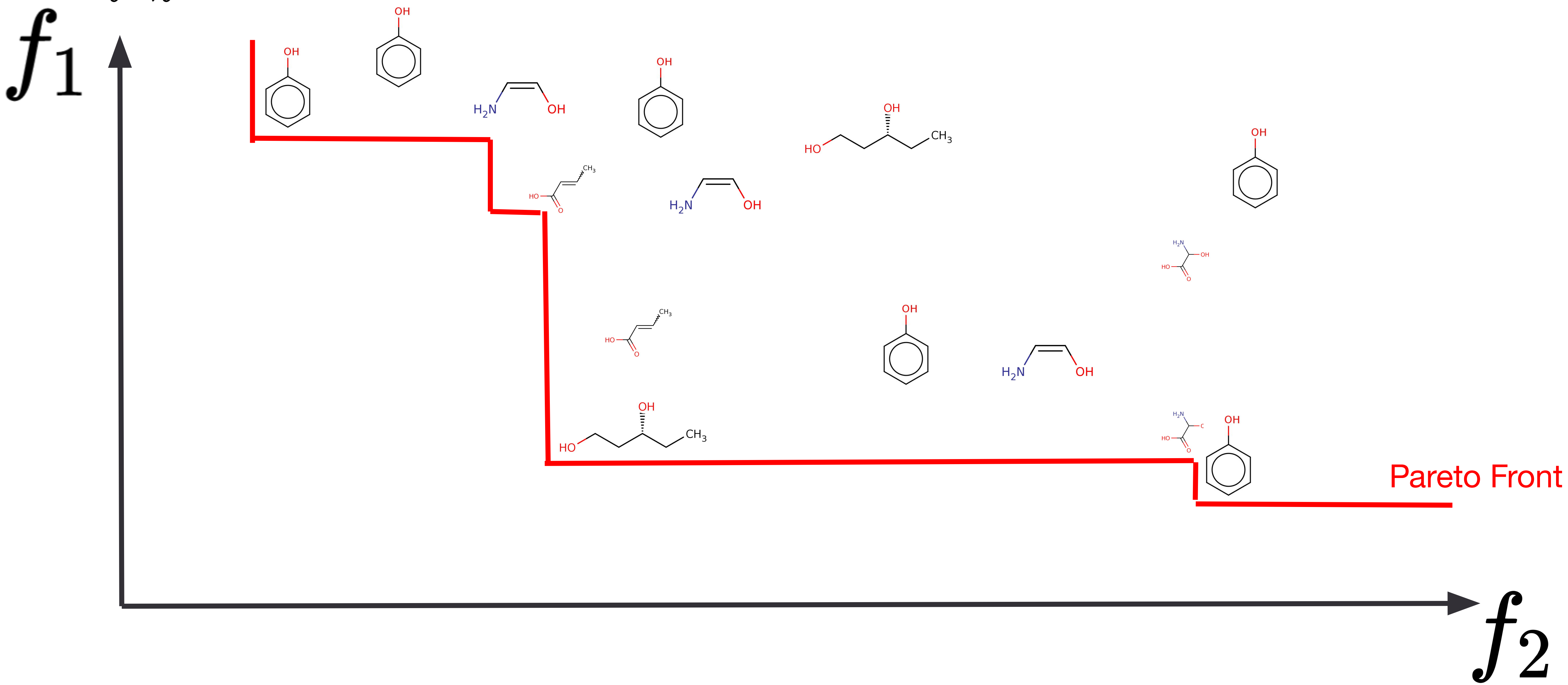
Multi-objective Optimisation

>1 competing objectives



Multi-objective Optimisation

$U_{f_1,f_2}($  $)$: what is the utility of evaluating  if it will return (f_1, f_2)



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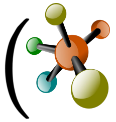
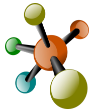
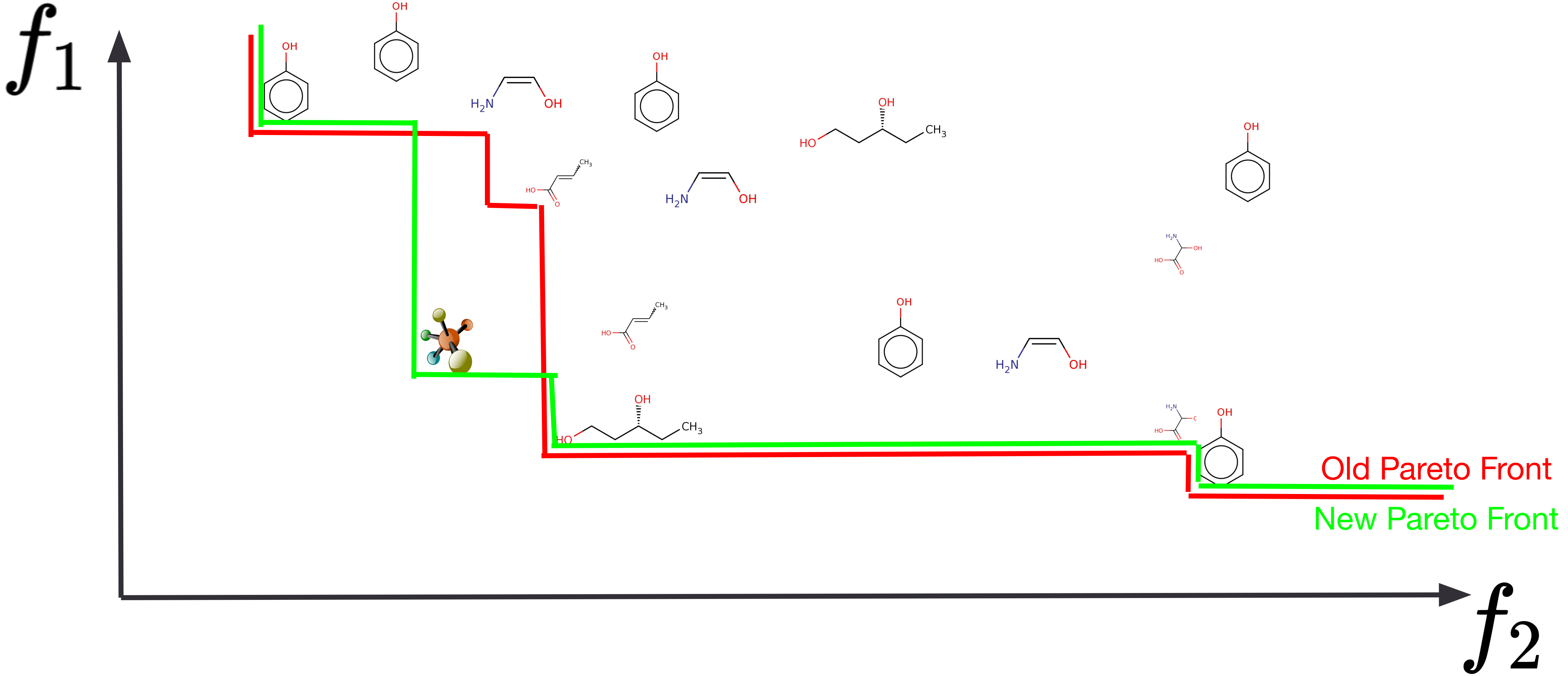
Multi-objective Optimisation

U_{f_1,f_2}(): what is the utility of evaluating  if it will return (f_1, f_2)



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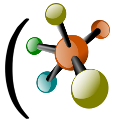
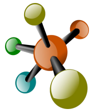
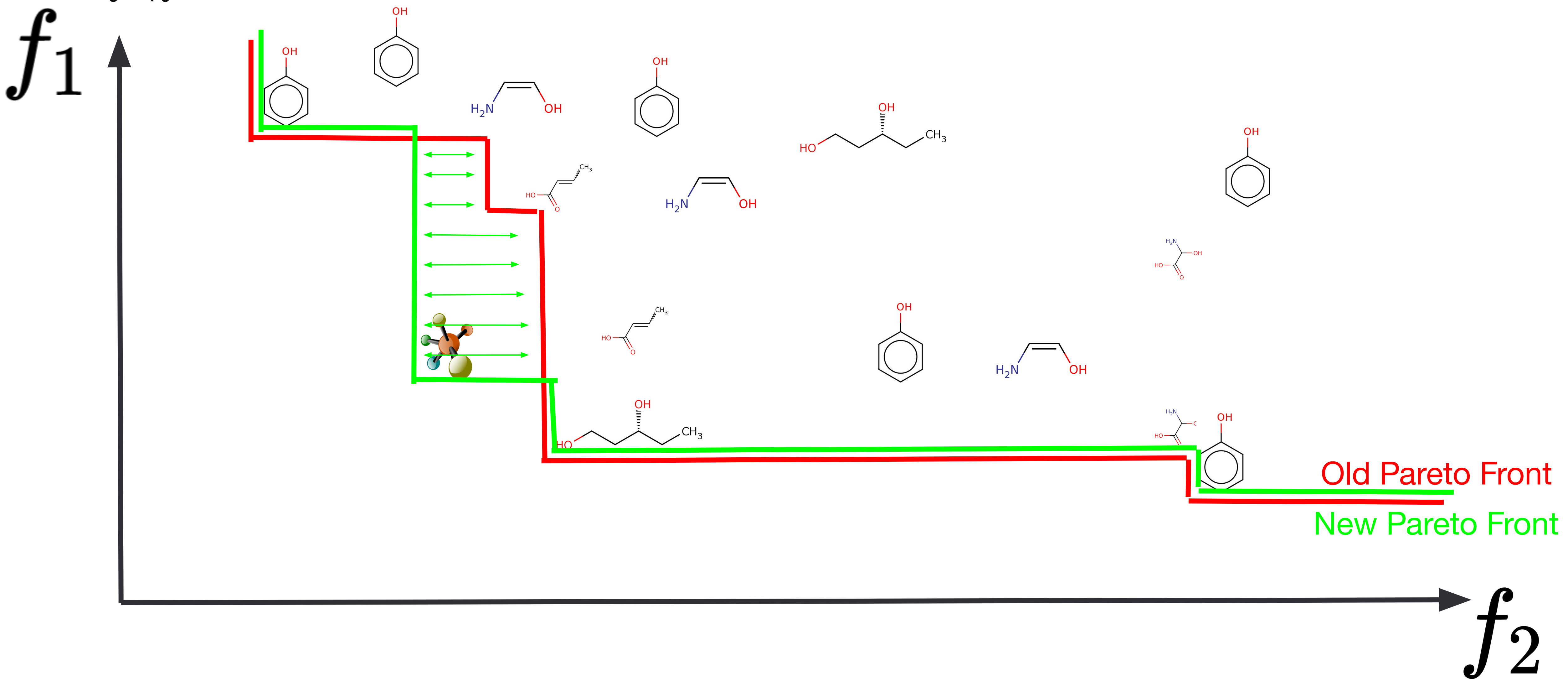
$U_{f_1,f_2}($  $)$: what is the utility of evaluating  if it will return (f_1, f_2)



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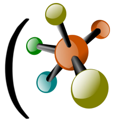
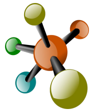
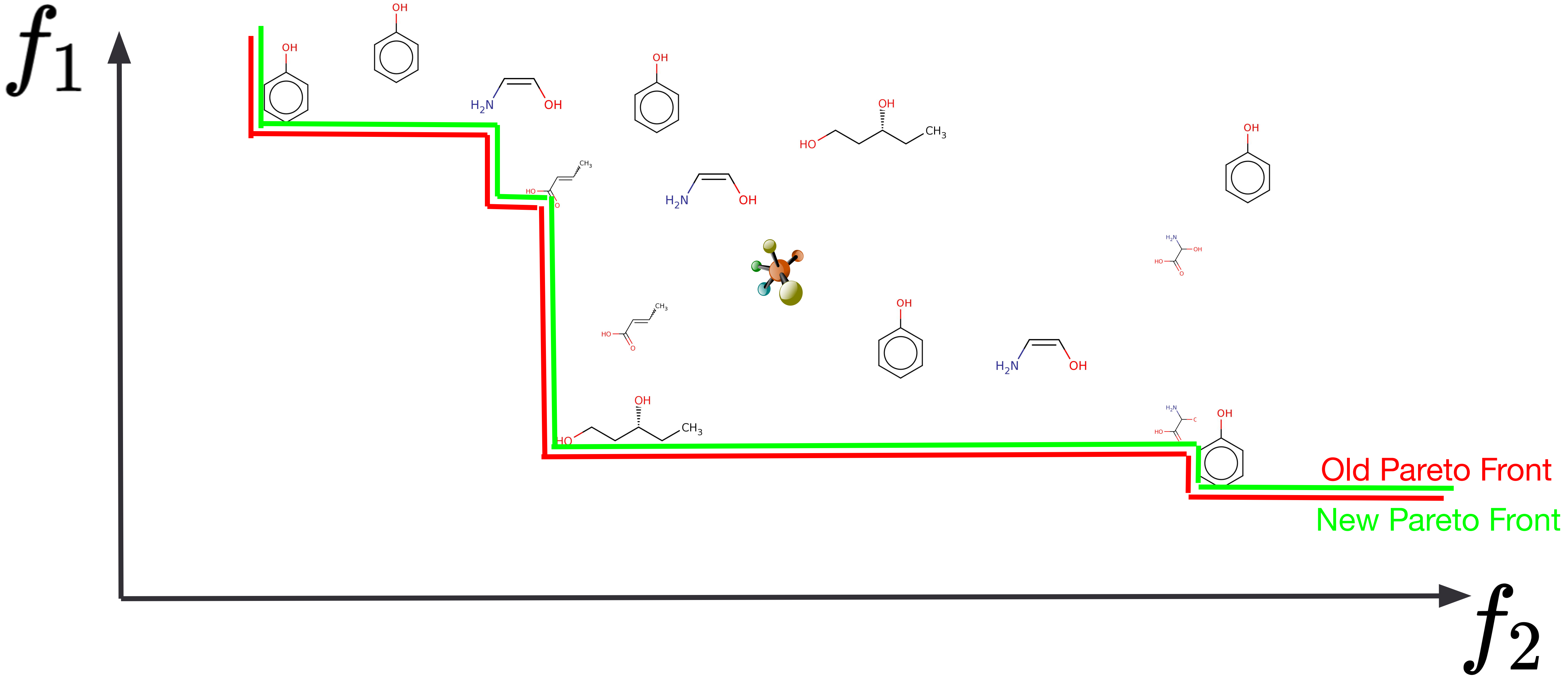
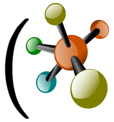
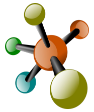
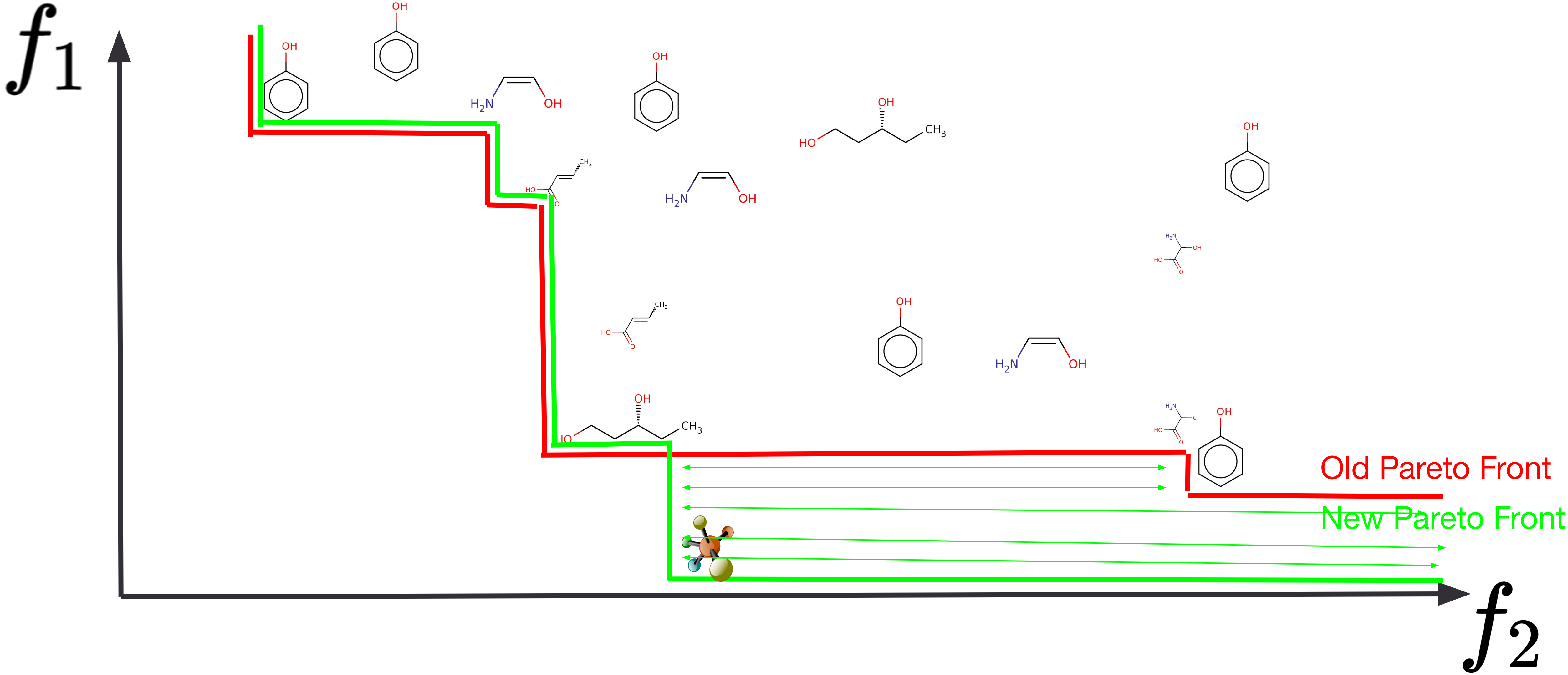
$U_{f_1,f_2}($$)$: what is the utility of evaluating  if it will return (f_1, f_2)

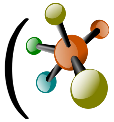
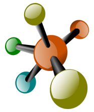


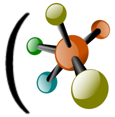
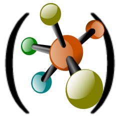
Multi-objective Optimisation

$U_{f_1,f_2}($  $)$: what is the utility of evaluating  if it will return (f_1, f_2)



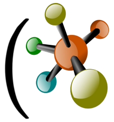
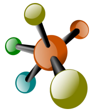
Multi-objective Optimisation

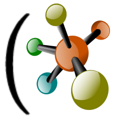
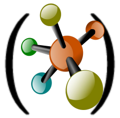
$U_{f_1,f_2}($  $)$: what is the utility of evaluating  if it will return (f_1, f_2)

- Use expected hyper-volume improvement $\alpha_{\mathrm{EHVI}}($  $) = \mathbb{E}_{f_1,f_2}(U_{f_1,f_2}($  $))$

$$f_1 \sim \mathcal{N}(\mu_1, \sigma_1^2)$$
$$f_2 \sim \mathcal{N}(\mu_2, \sigma_2^2)$$

Multi-objective Optimisation

$U_{f_1,f_2}\Big($  $\Big)$: what is the utility of evaluating  if it will return (f_1, f_2)

- Use expected hyper-volume improvement $\alpha_{\mathrm{EHVI}}\big($  $\big) = \mathbb{E}_{f_1,f_2}\big(U_{f_1,f_2}($  $)\big)$

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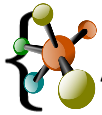
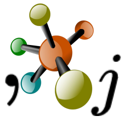
$\alpha_{\mathrm{EHVI}}\big(\{$  $_i,$  $_j\}\ \big) = ???$

A more sophisticated acquisition function?

Entropy Search

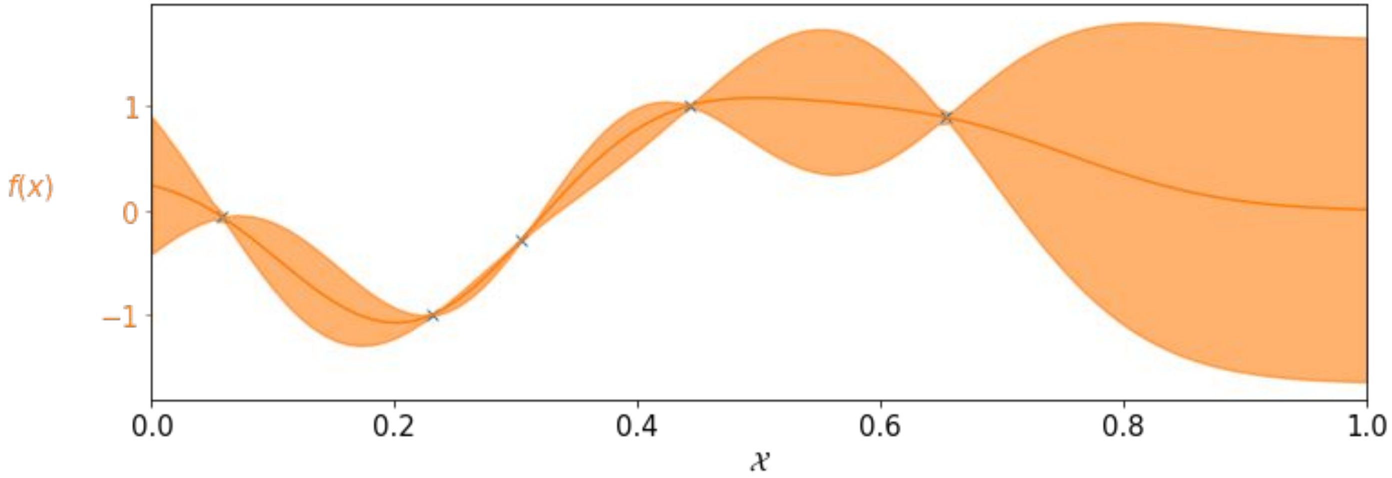
Quick Recap

$$\mathbf{x}^* = \arg\max_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x})$$

Quick Recap

$$\mathbf{x}^* = \arg\max_{\mathbf{x}\in\mathcal{X}} f(\mathbf{x})$$

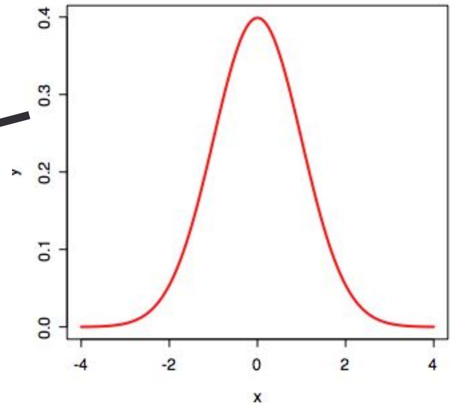
$$f(\mathbf{x})|D \sim \mathcal{GP}$$

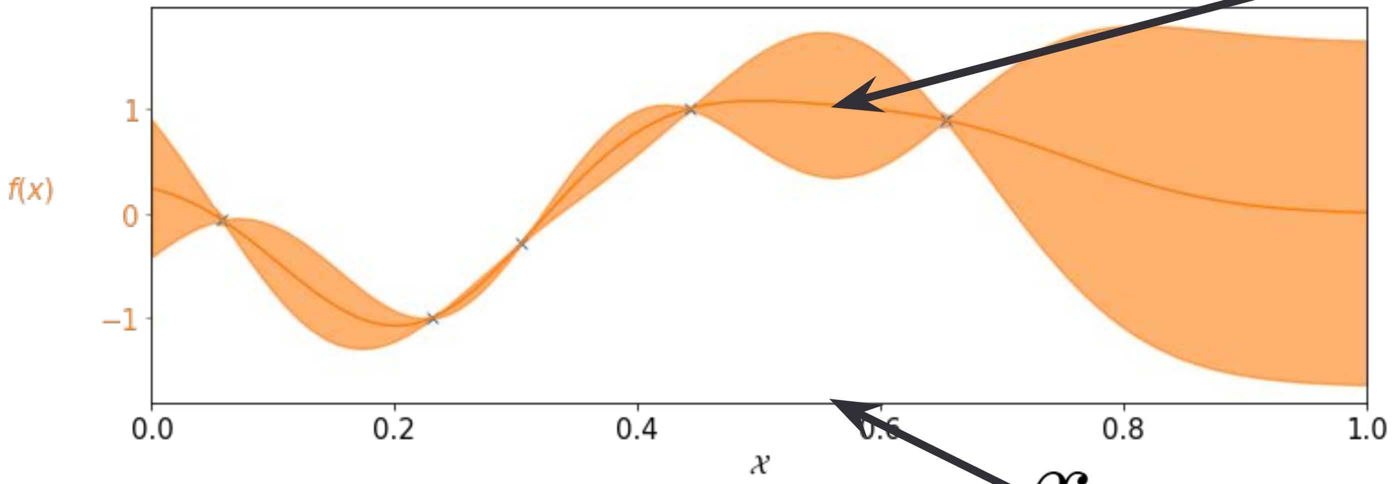


Quick Recap

$$\mathbf{x}^* = \arg\max_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x})$$

$$f(\mathbf{x}) | D \sim \mathcal{GP}$$



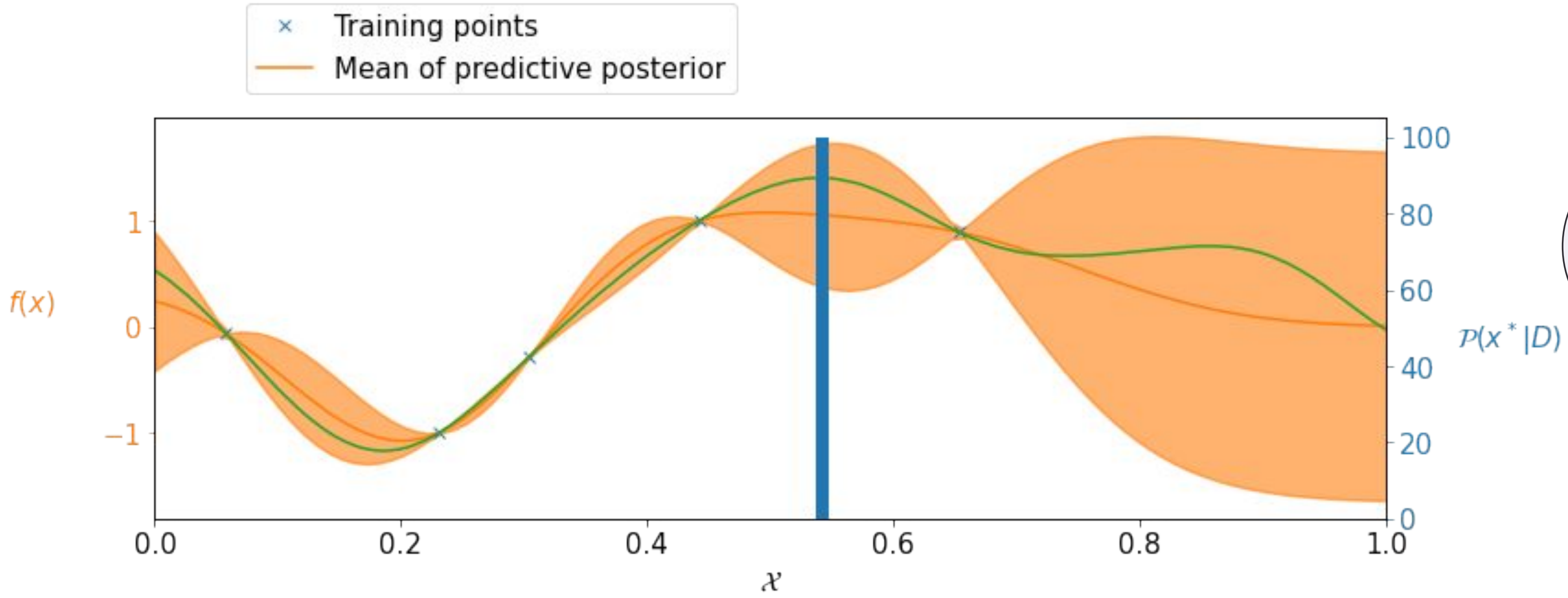


$$f(x) \sim N(\mu(x), \sigma^2(x))$$

x

What is our best guess for $\mathbf{x}^*$?

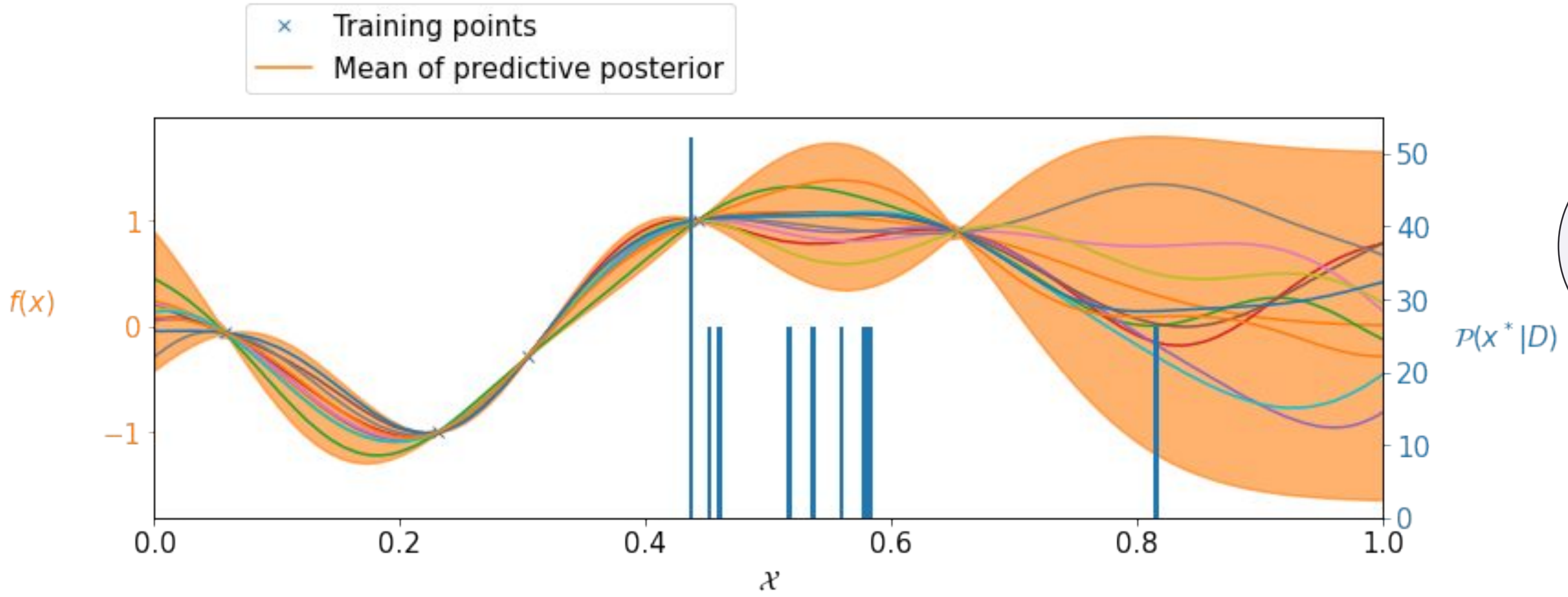
$P(\mathbf{x}^*|D)$ based on one sample



1 sample

What is our best guess for $\mathbf{x}^*$?

$P(\mathbf{x}^*|D)$ based on 10 samples



10 samples

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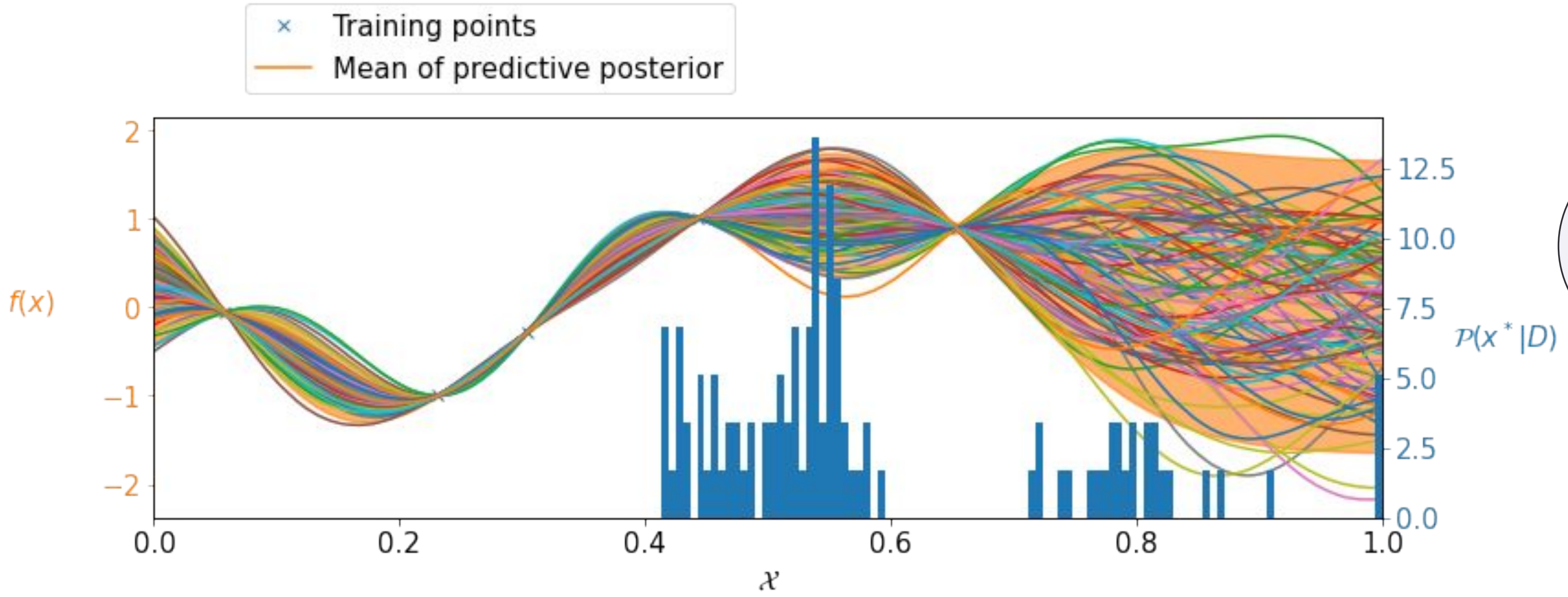
What is our best guess for $\mathbf{x}^*$?

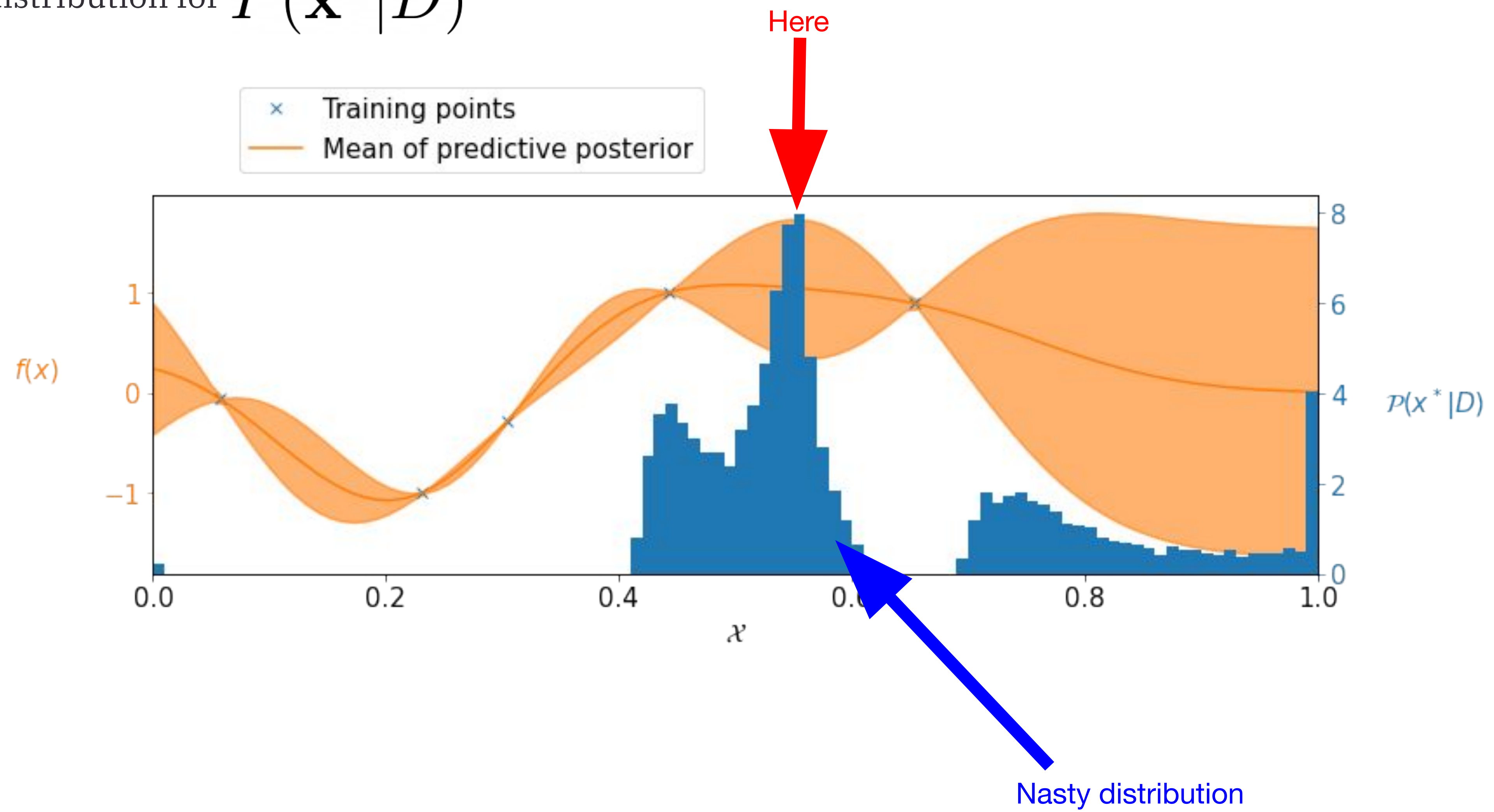
$P(\mathbf{x}^*|D)$ based on 100 samples



100 samples

What is our best guess for $\mathbf{x}^*$?

Empirical distribution for $P(\mathbf{x}^*|D)$



Where shall we evaluate next ?

We want to learn about $\mathbf{x}^*$

- Expected Improvement (EI) maximises $\alpha_{EI}(\mathbf{x}) = E[\max(f(\mathbf{x}) - f^*, 0)]$

Where shall we evaluate next ?

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Only needs $f(\mathbf{x})|D$

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Where shall we evaluate next ?

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Only needs $f(\mathbf{x})|D$

Does not use full knowledge of $P(\mathbf{x}^*|D)$

Entropy search seeks to reduce our uncertainty in $P(\mathbf{x}^*|D)$

How to measure uncertainty?

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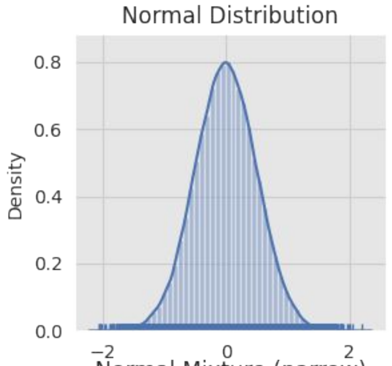
$X \sim \mathcal{N}(\mu, \sigma^2)$	σ^2	$\log(\sigma\sqrt{2\pi e})$
$X \sim U(a, b)$	$\frac{(b-a)^2}{12}$	$\log(b-a)$

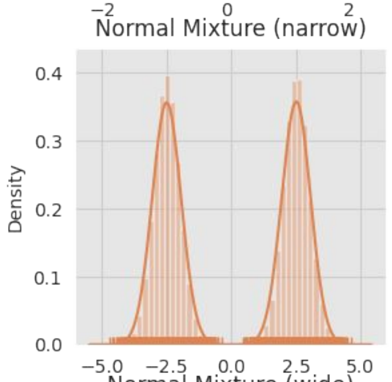
How to measure uncertainty?

Should we use entropy?

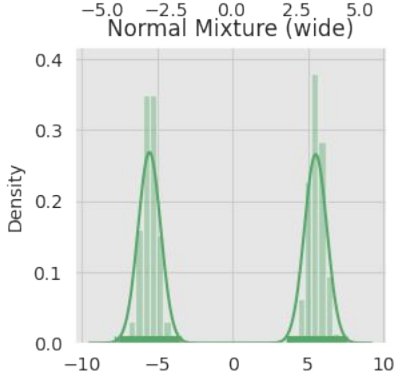
$$H(X) = E\left[-\log(p(X))\right]$$



H(X) = 0.7



H(X) = 1.4



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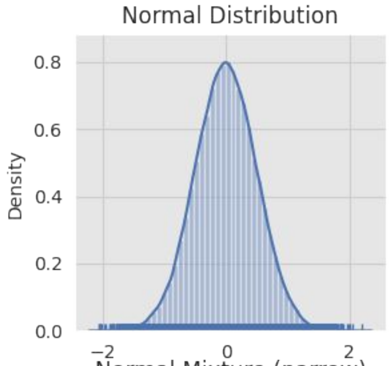
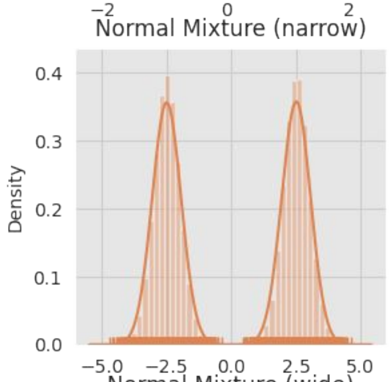
How to measure uncertainty?

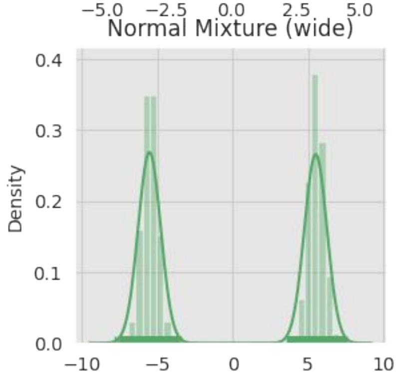
Should we use variance (i.e. dispersion)?



Var(X) = 0.5



Var(X) = 6.5



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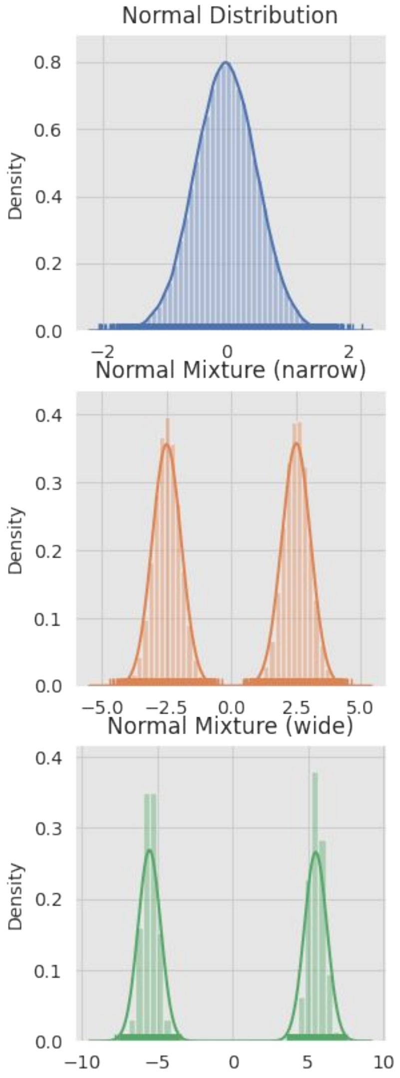

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Perhaps not good for multi-modal distributions ?

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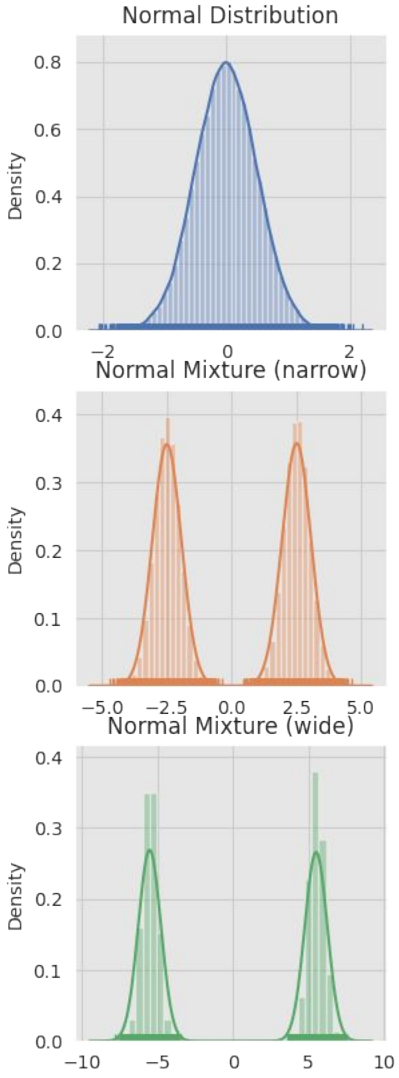

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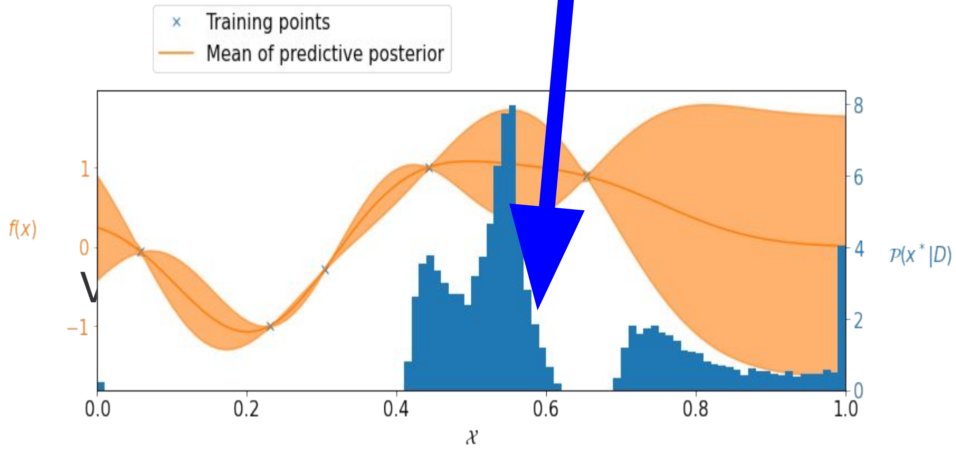

Entropy Search

Reduce global uncertainty in $P(\mathbf{x}^* | D)$

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- Make evaluation that provides the largest expected reduction in entropy

$$\alpha_{ES}(\mathbf{x}) = H(\mathbf{x}^*|D) - E_y[H(\mathbf{x}^*|D \cup \{y, \mathbf{x}\})]$$

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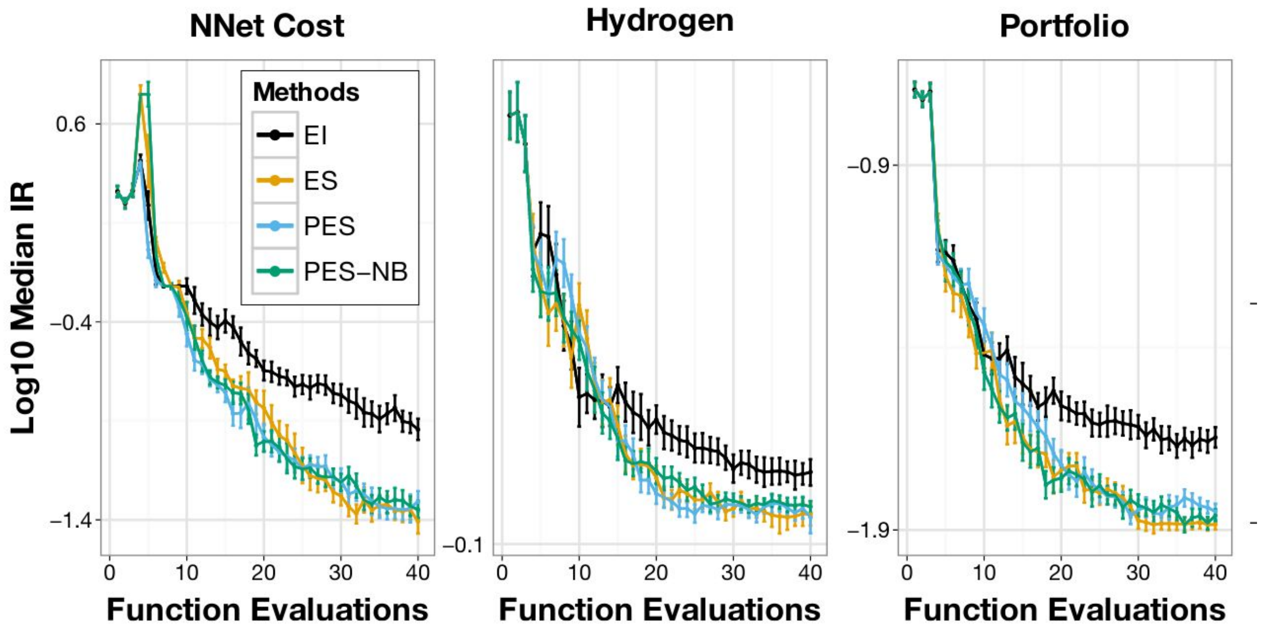
Fiendishly difficult to calculate!

- **What is** $H(\mathbf{x}^*|D)$ **?**
- **What is** $H(\mathbf{x}^*|D, \{y, \mathbf{x}\})$**???**

It can be worth calculating these horrible quantities

They can provide highly efficient optimization



For details see

- Entropy Search is $O(n^2e^{2d} + e^{3d})$(Henning and Schuler, 2012)
- Predictive Entropy Search is $O(n^2e^{2d} + n^3e^d)$ (Hernandez-Lobato et al. 2014)

There is a better way!

Min-value Entropy Search

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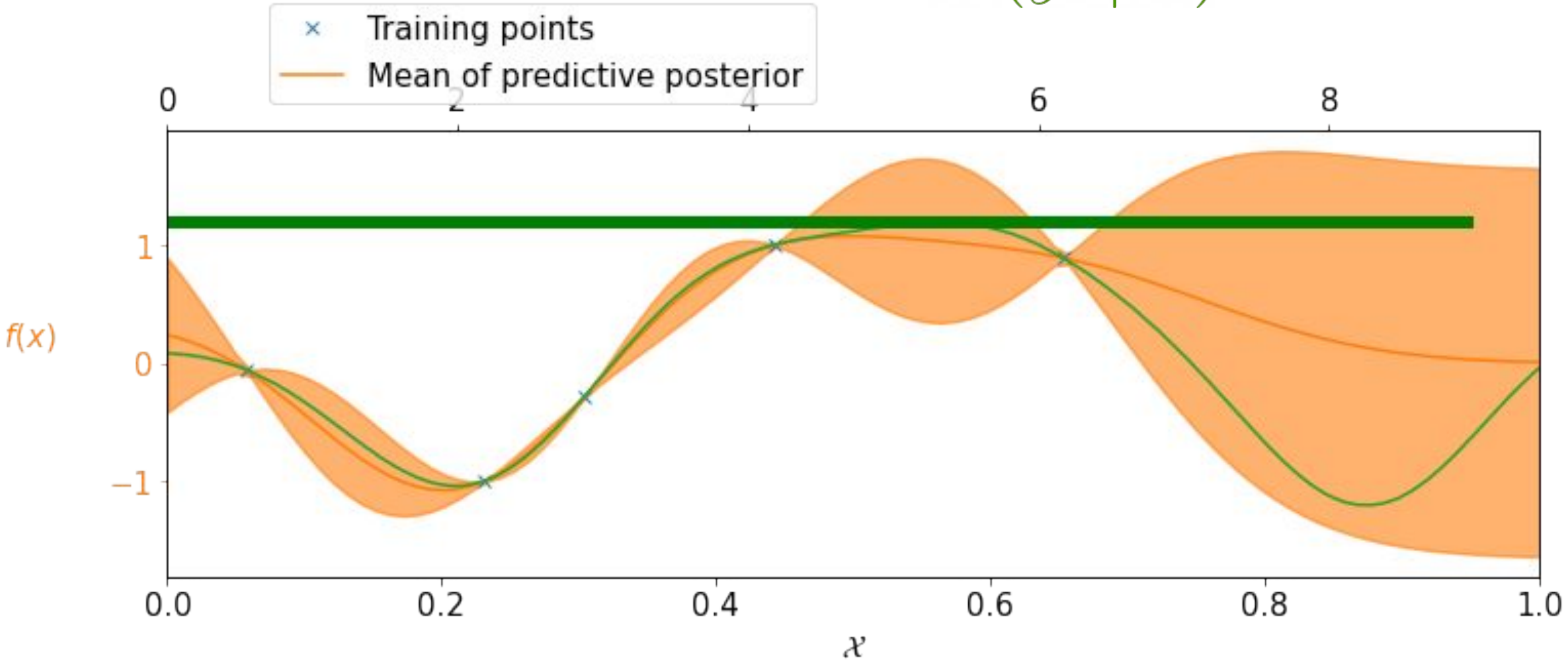

1 sample

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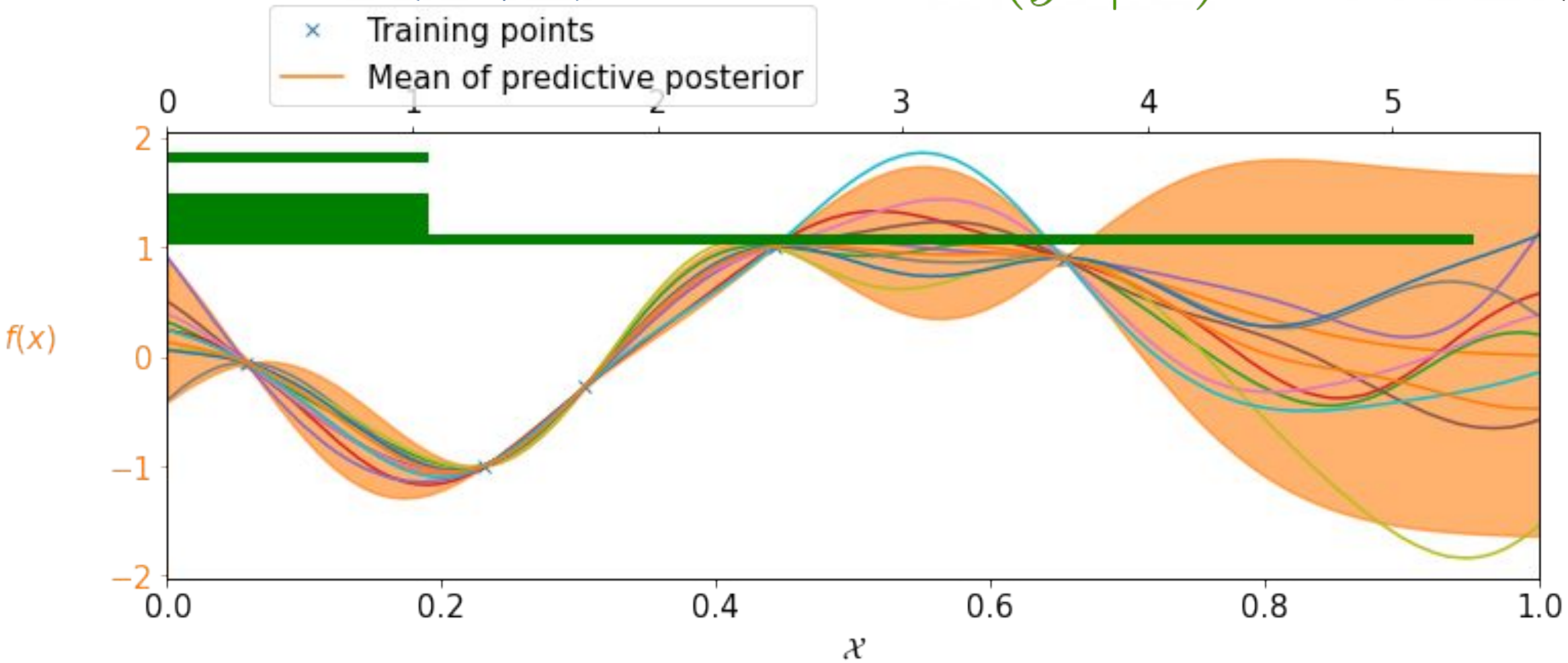

10 samples

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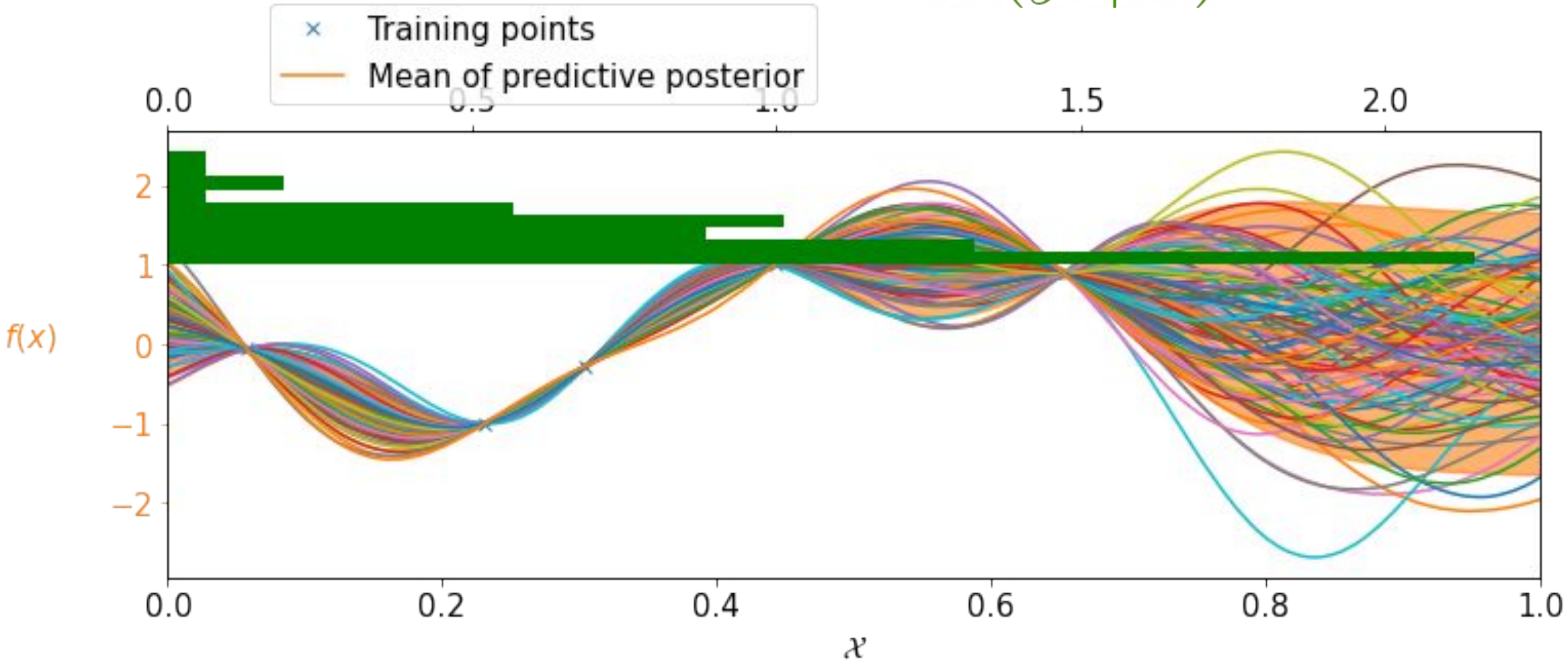

100 samples

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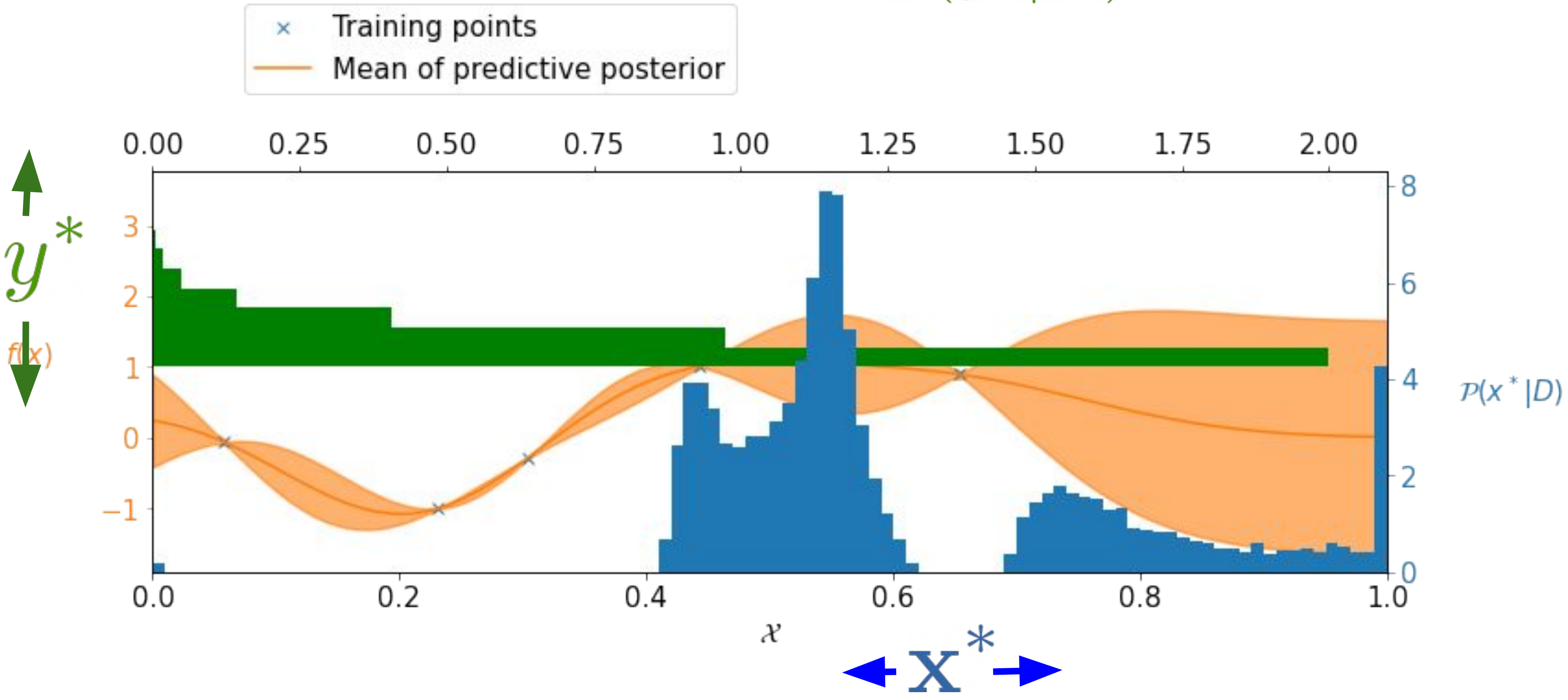

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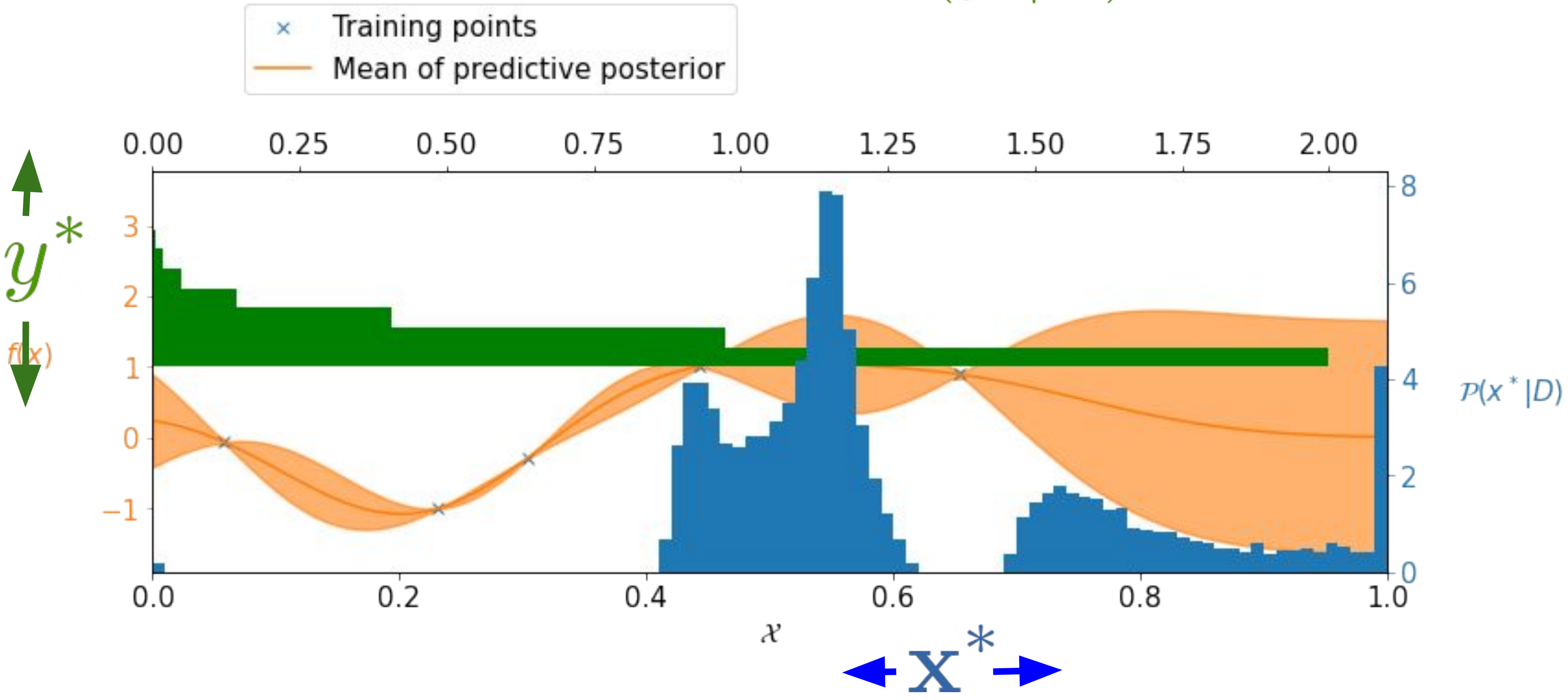

$$\alpha_{MES}(\mathbf{x}) = H(y|D) - E_{y^*|D}[y|D \cup y^*]$$

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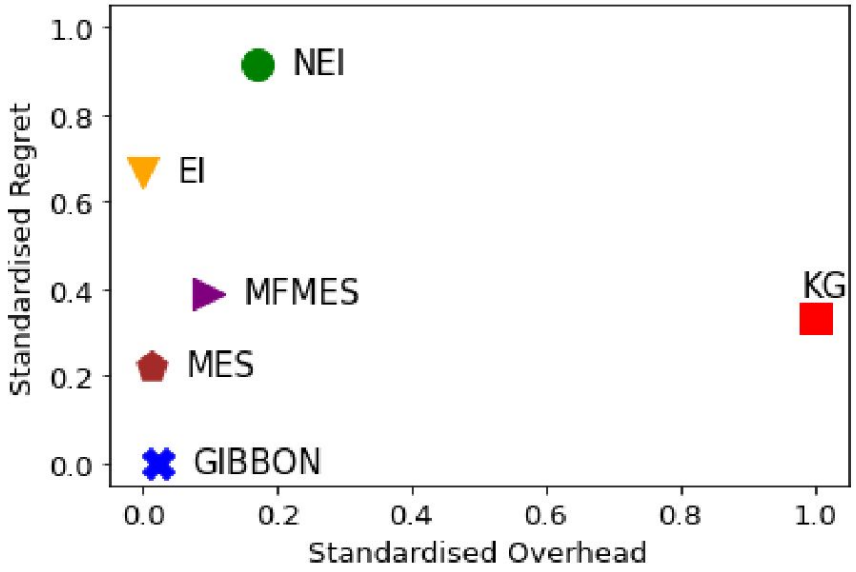
Current uncertainty

Expected uncertainty after the evaluation

Crucially $\mathbf{y}^* \in R$, whereas $\mathbf{x}^* \in R^d$

MES in practice

Highly effective optimization at low cost!



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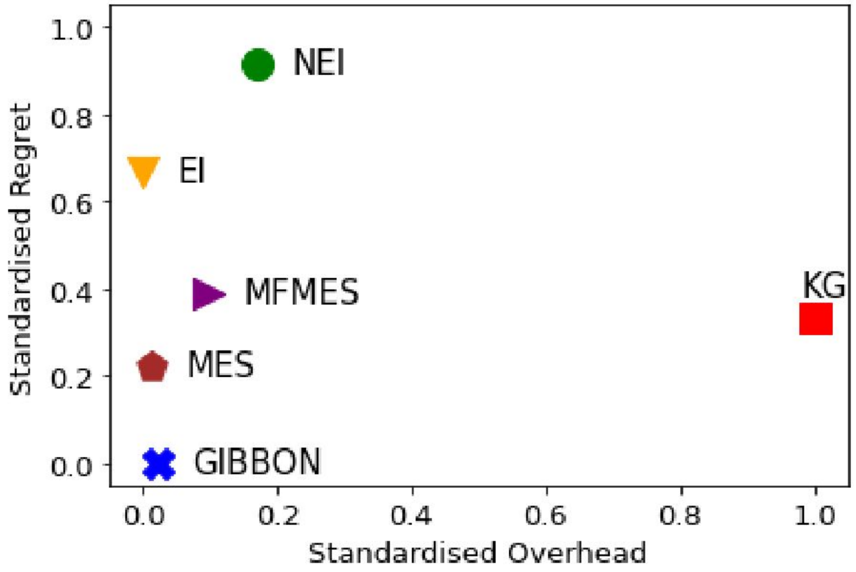

- Max-Value Entropy Search is $O(n^2 e^d)$ for noiseless optimisation (Wang and Jegelka, 2017).
- MUMBO is $O(n^2 e^d)$ for noisy optimisation (Moss et al., 2020)
- GIBBON is $O((n^2 + B^2)e^d + B^3)$ for batches of size B (Moss et al. 2021)

Thanks for listening

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