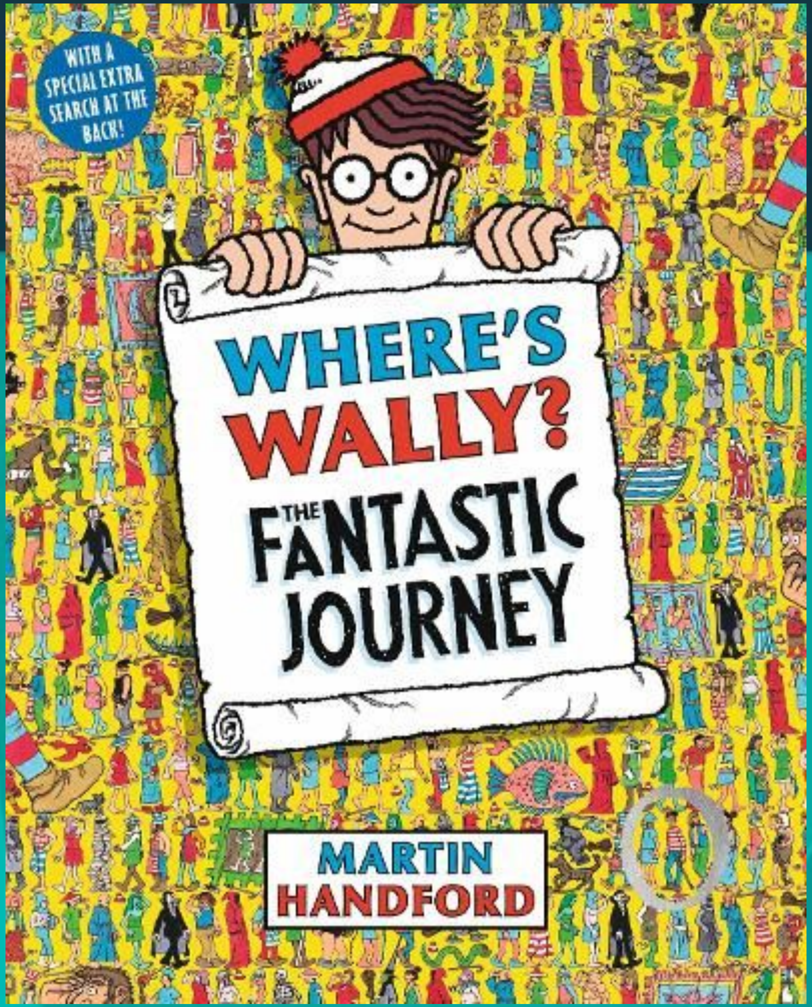
To Bayesian Optimisation and Beyond

Gaussian Processes as Decision Makers

Henry Moss

Bayesian Search

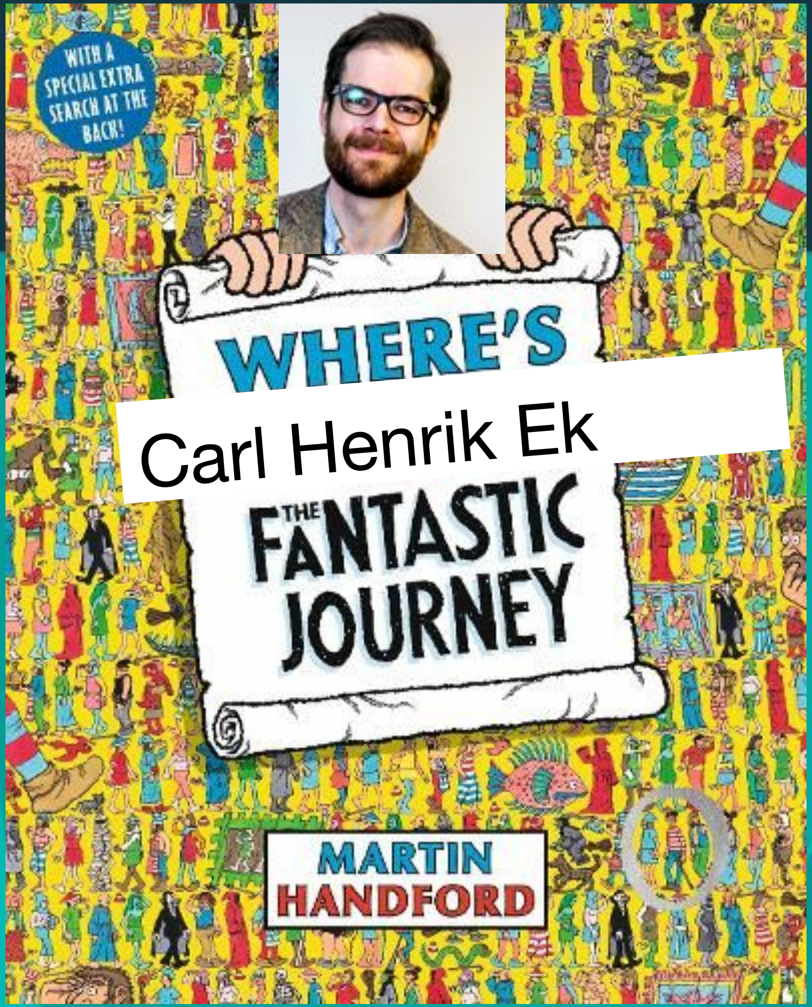
Bayesian Search



UNIVERSITY OF CAMBRIDGE

Lancaster University

Bayesian Search



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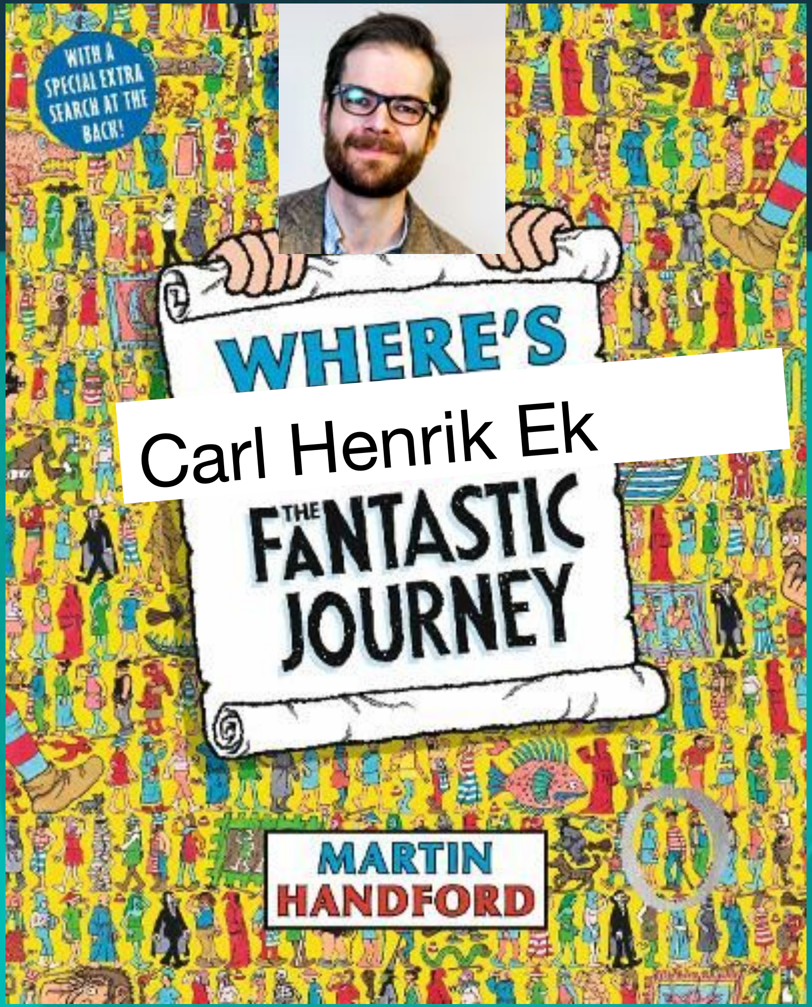
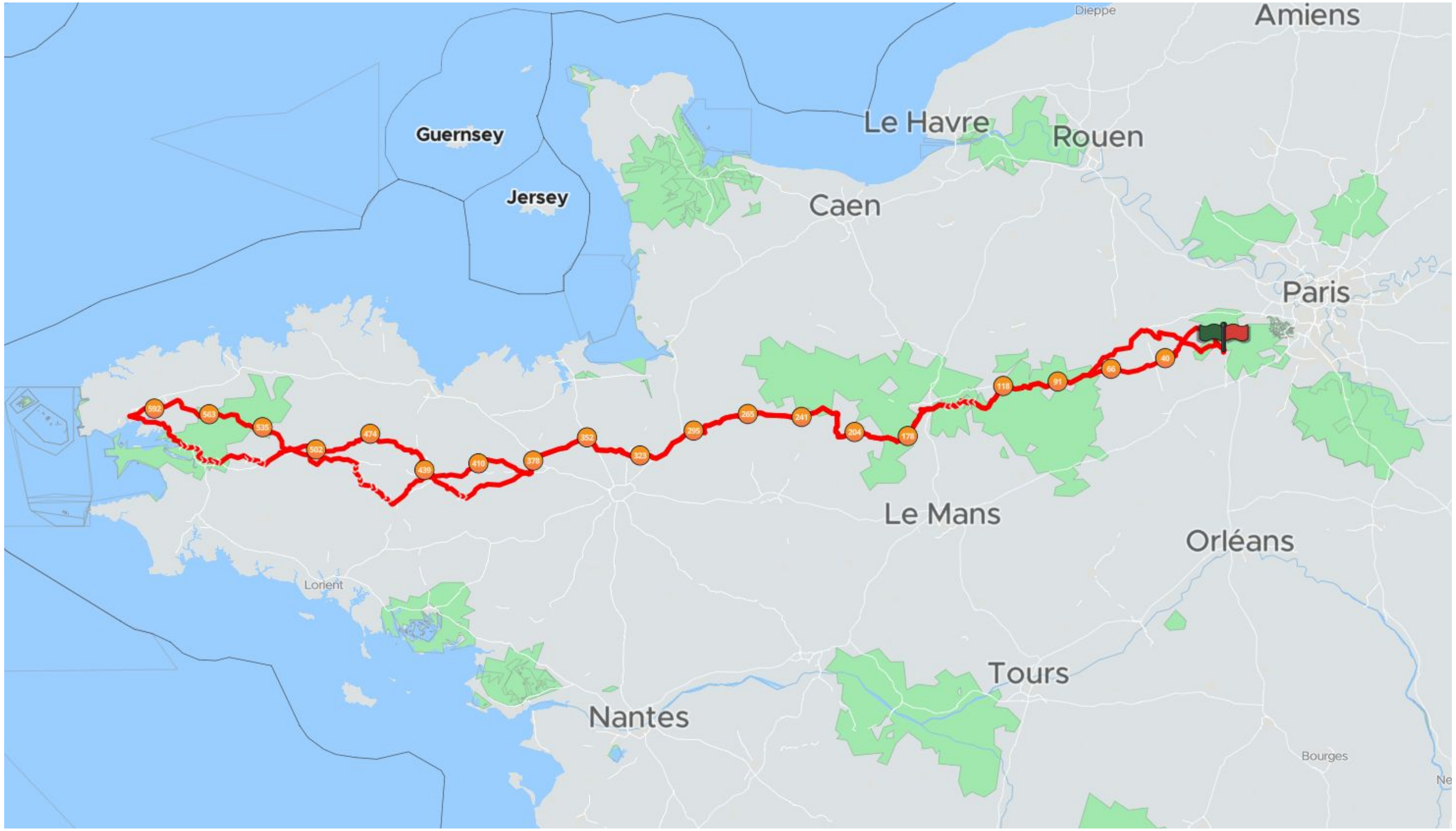
Bayesian Search



Where is Carl Henrik?



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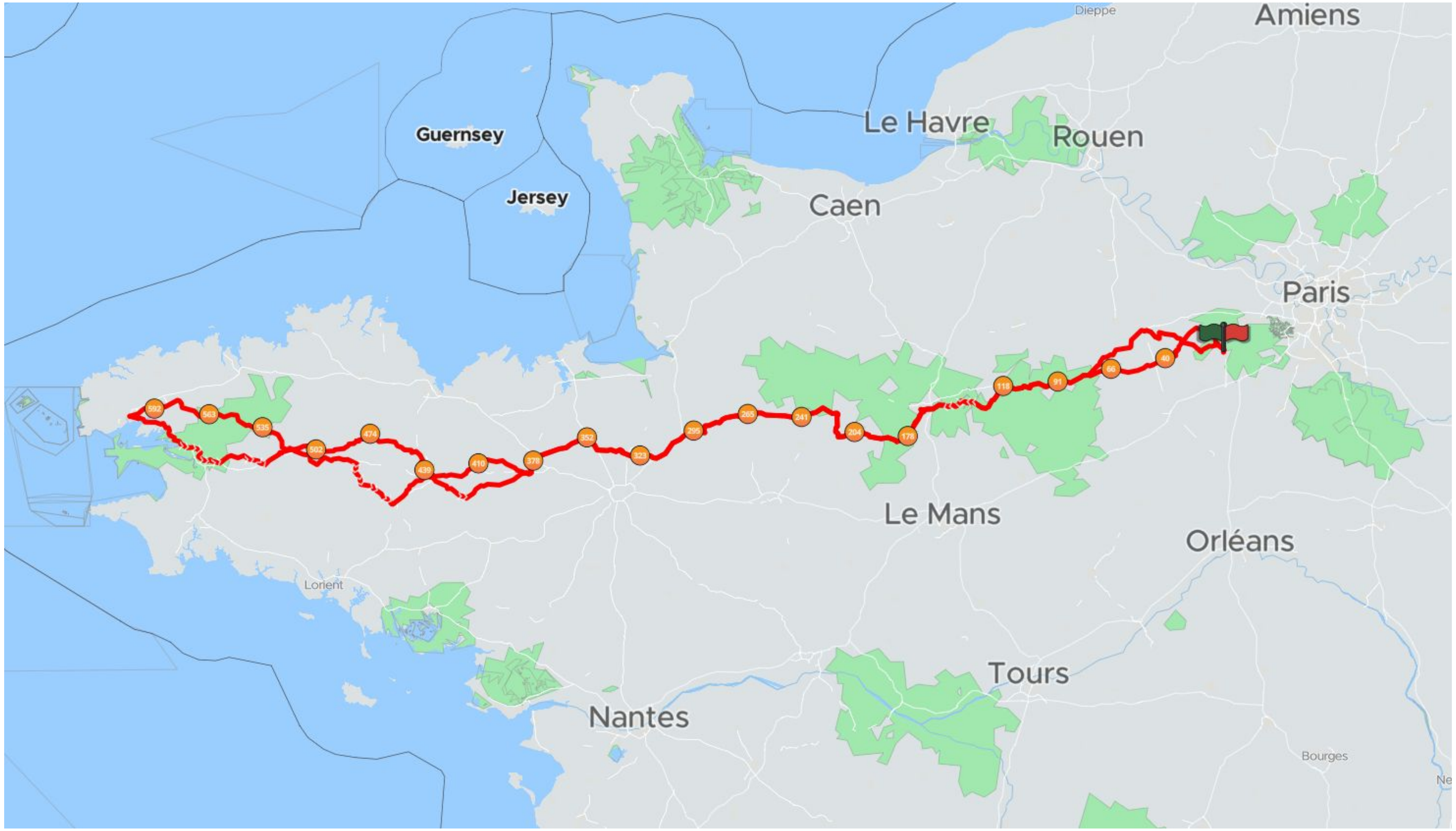

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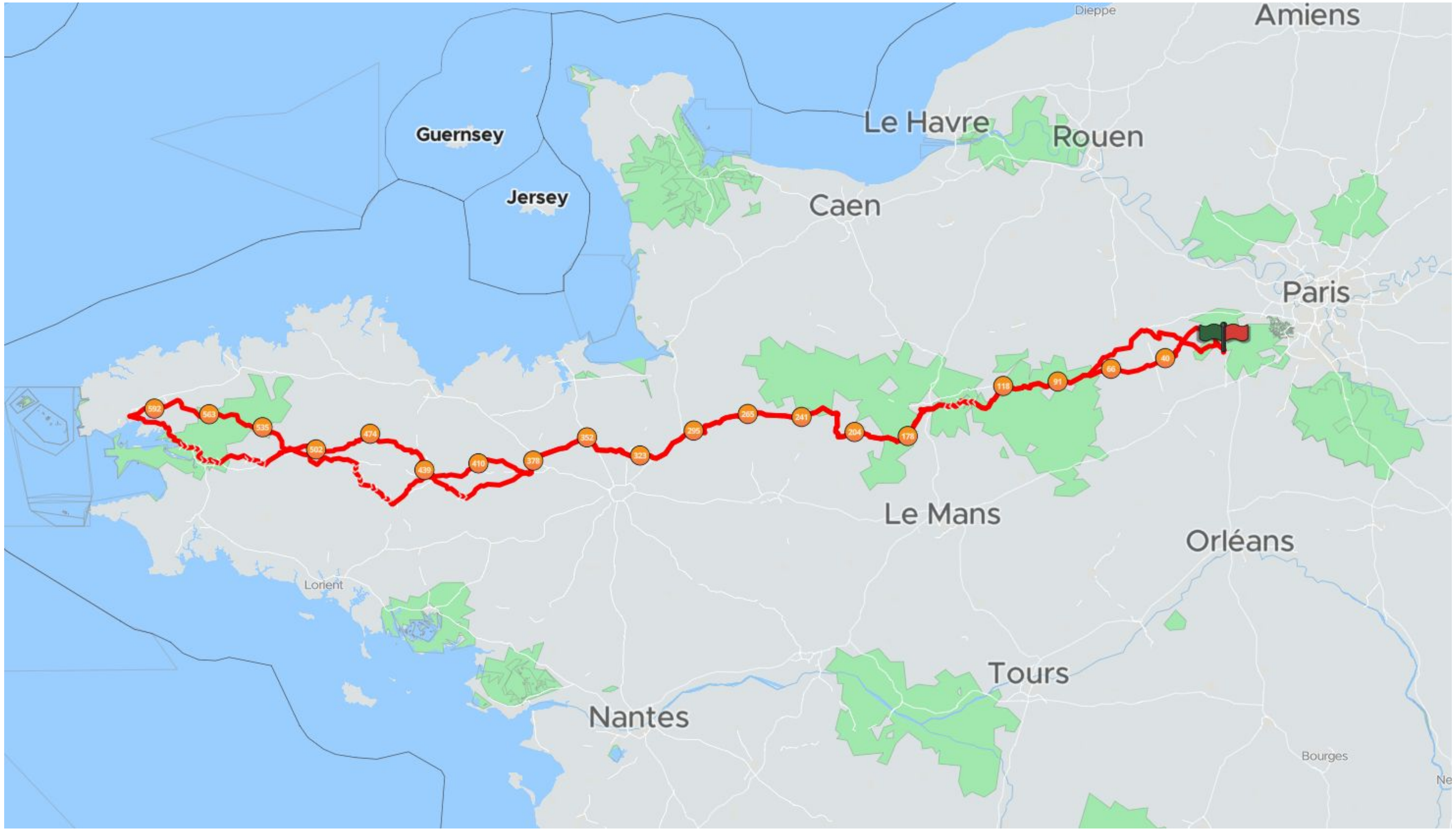

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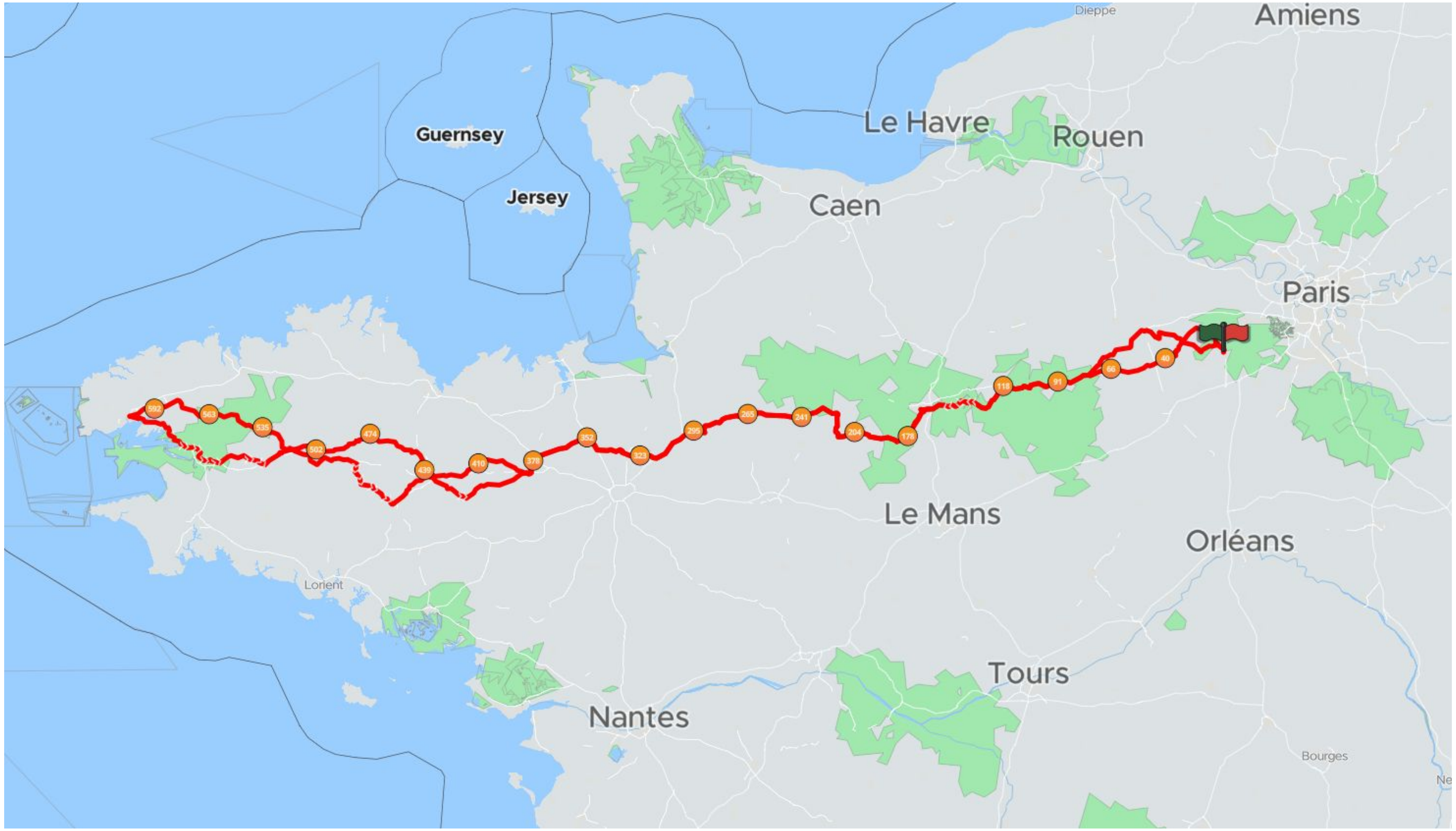
At 3:30 AM?



$$d = v \times t$$

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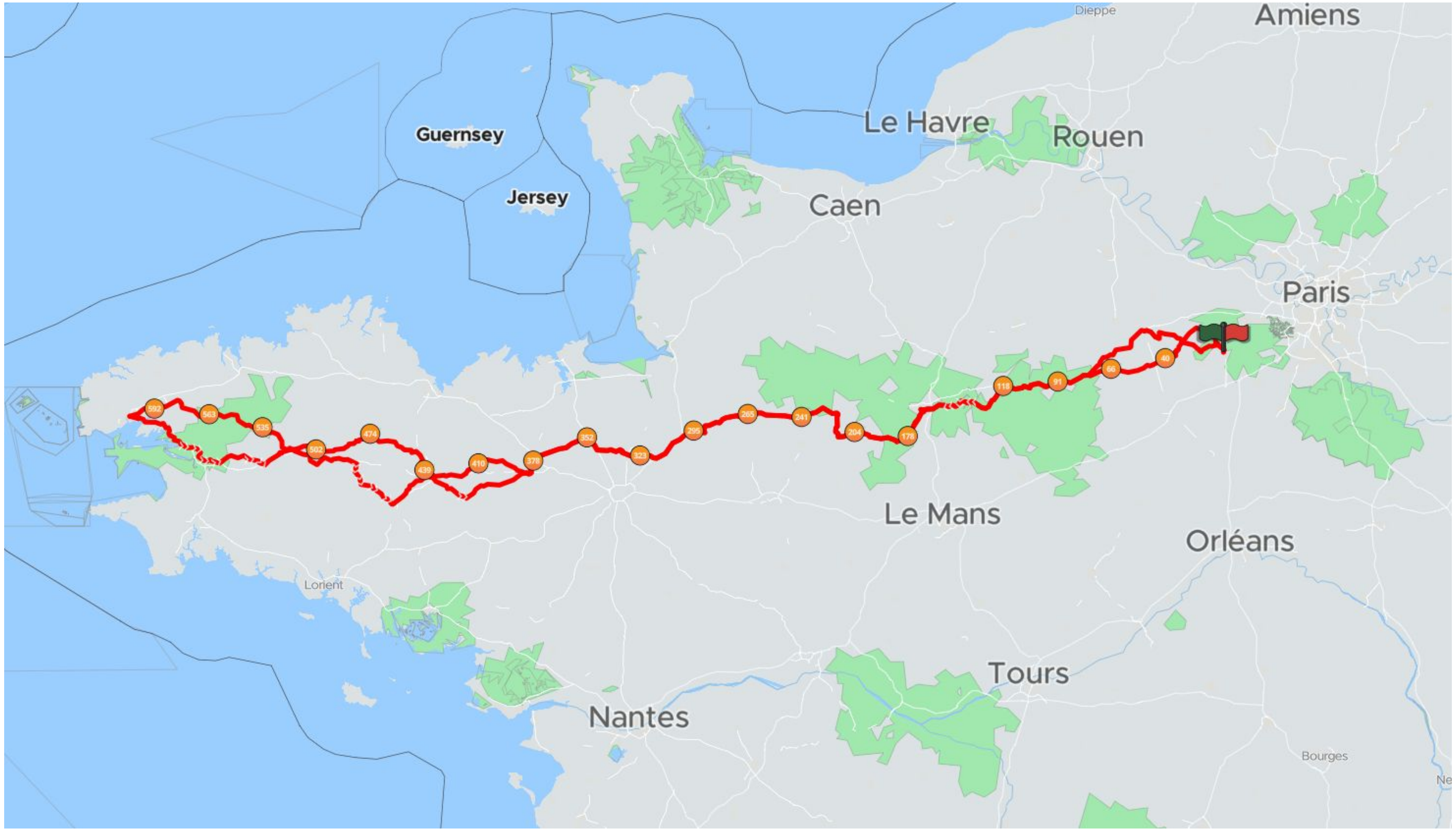

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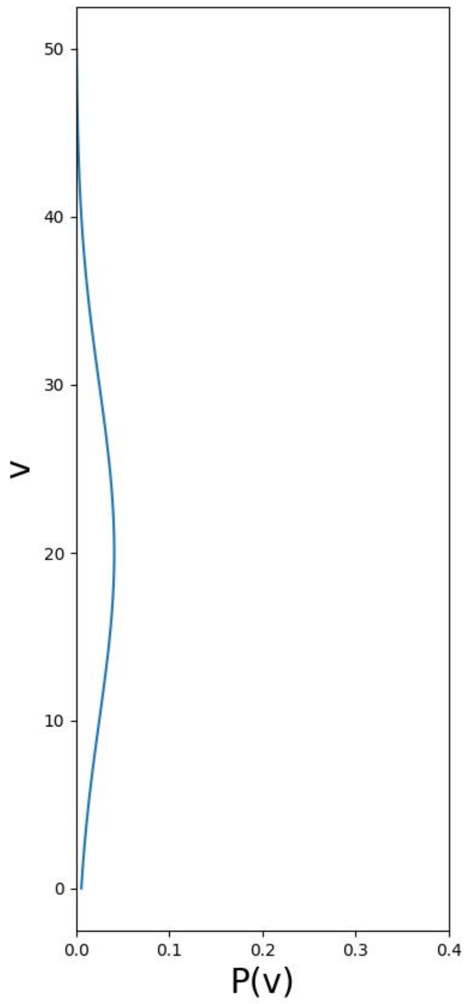

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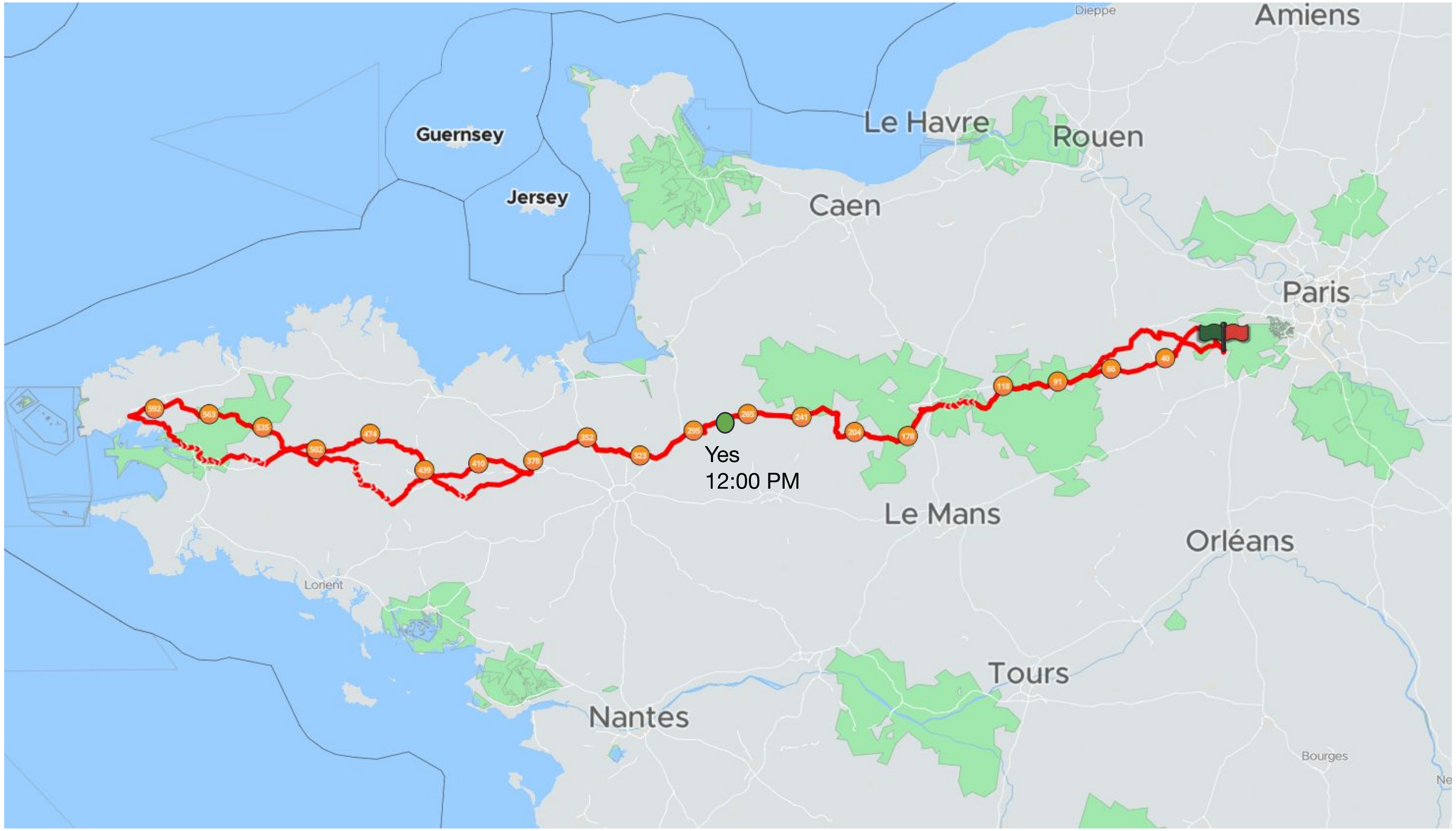

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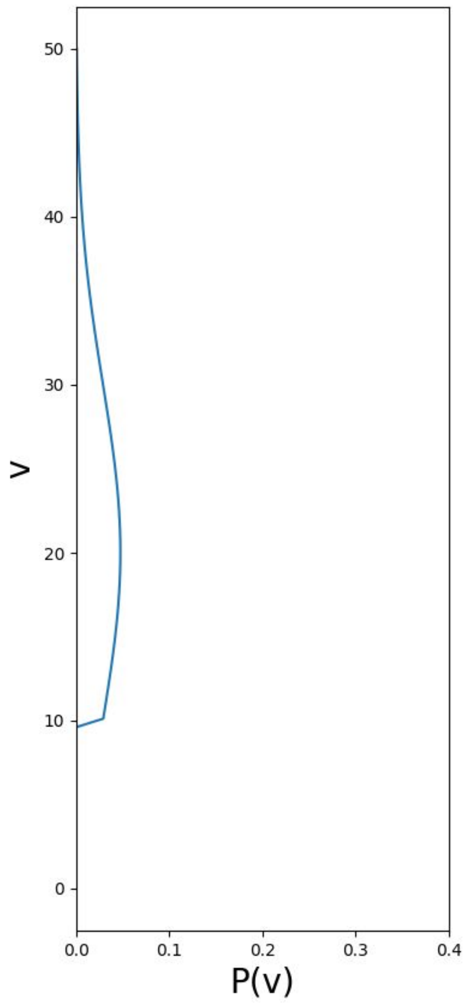

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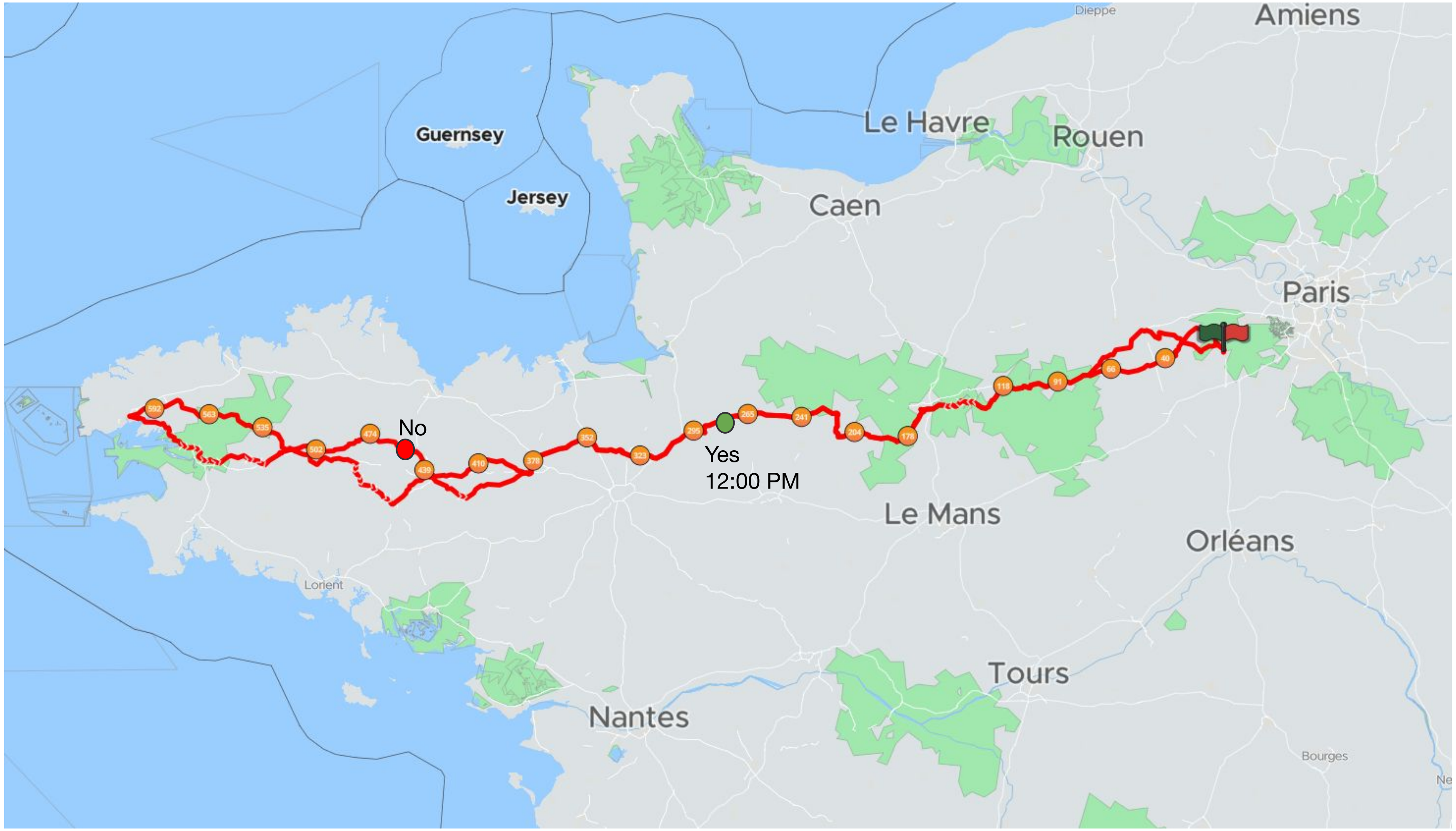

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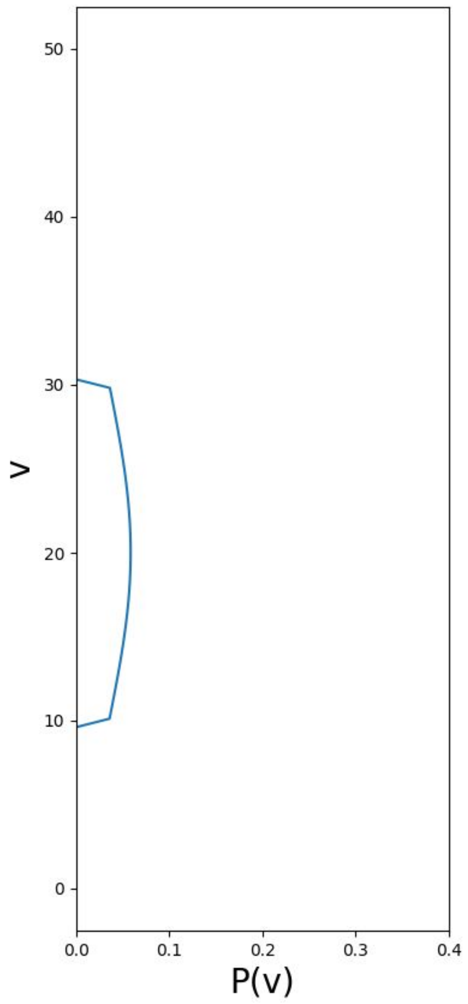

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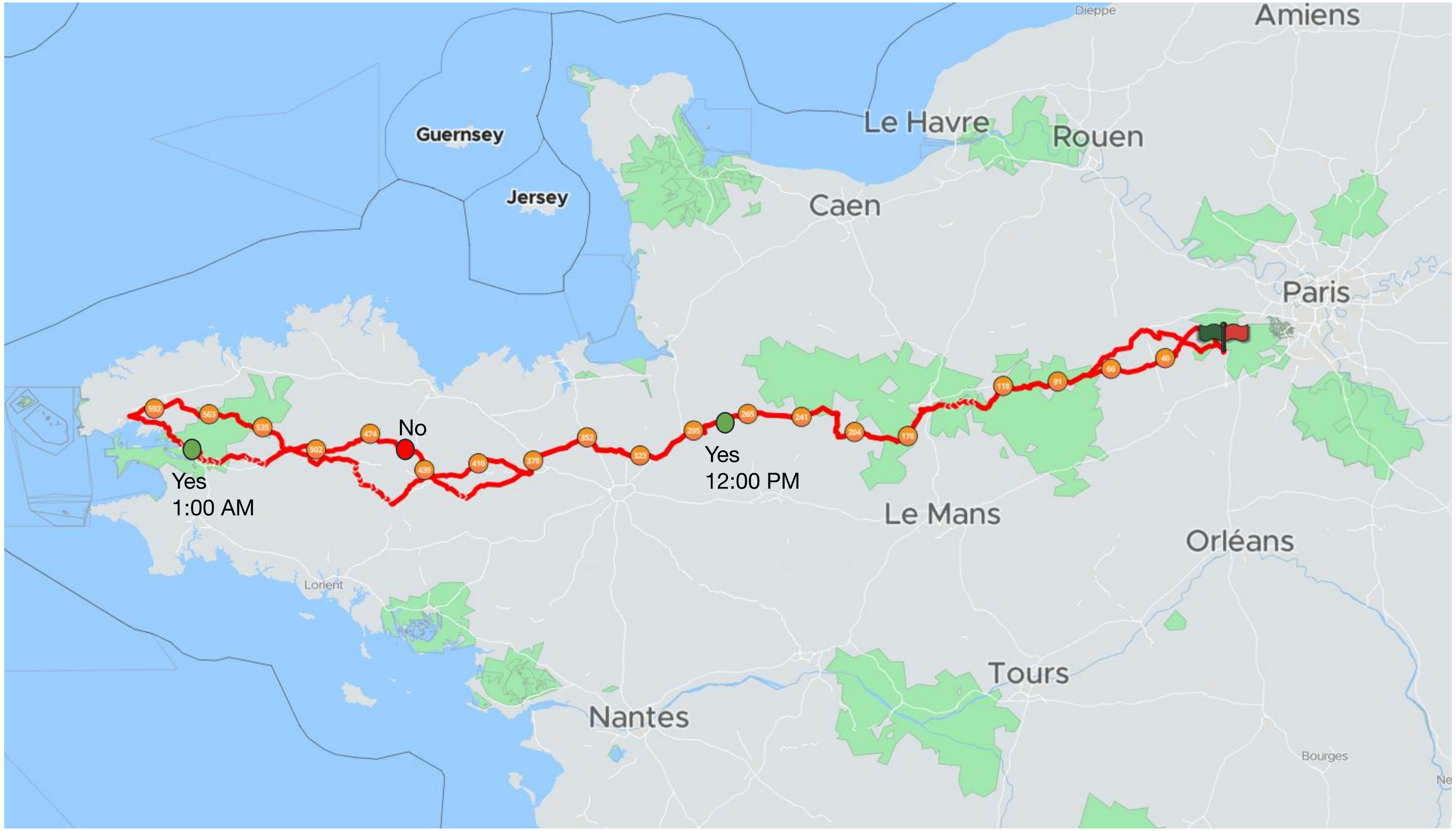

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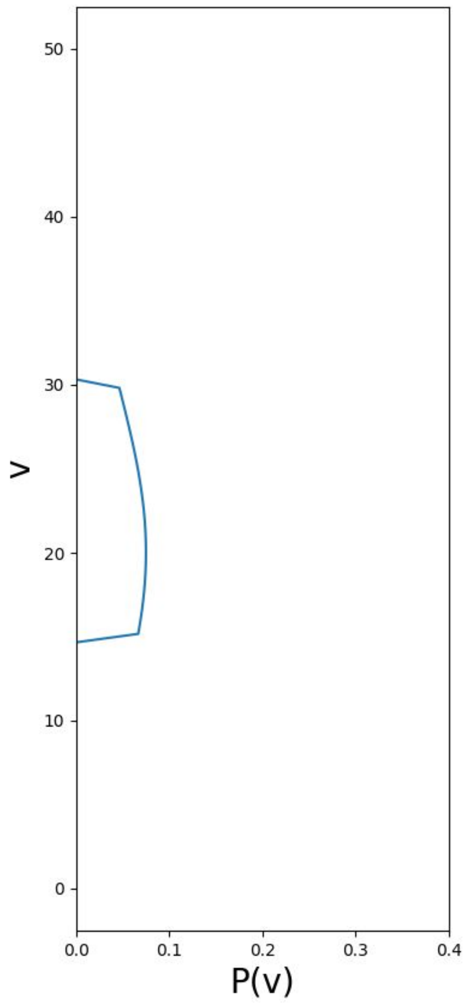

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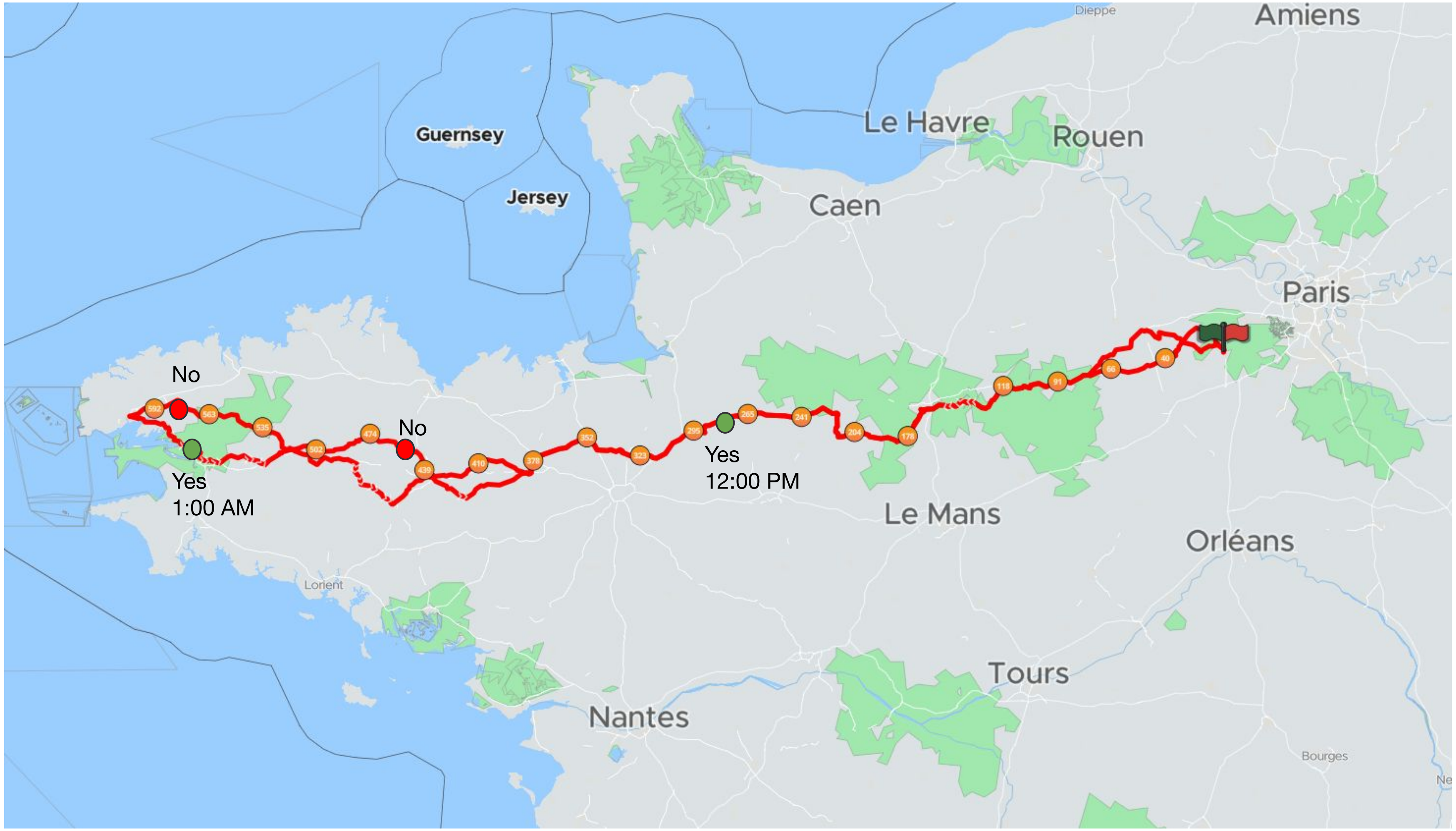

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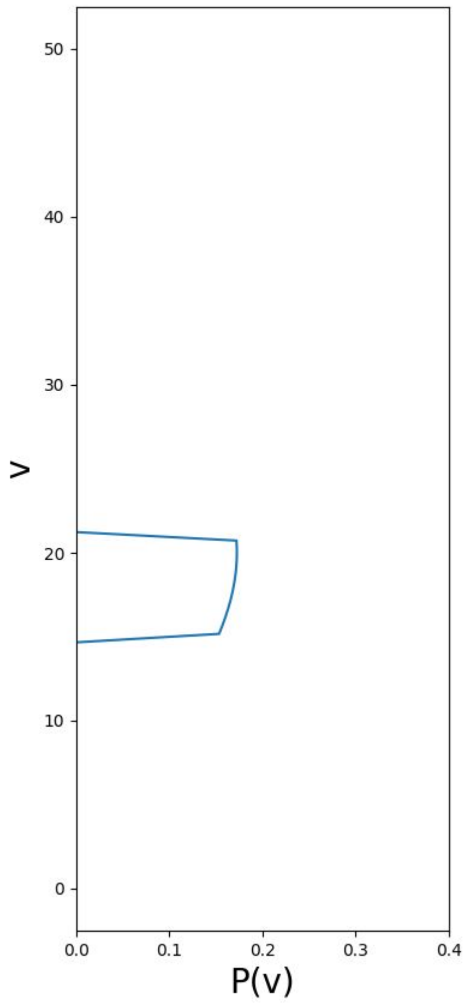

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But can we do better than **random**???

What is Active Learning?

Bayesian search for learning functions

Sequential data collection

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

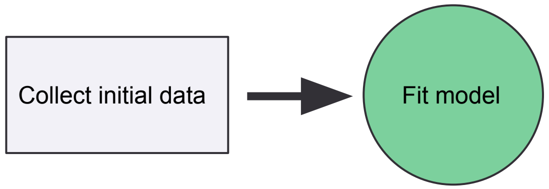
Sequential data collection

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

Collect initial data

Sequential data collection

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



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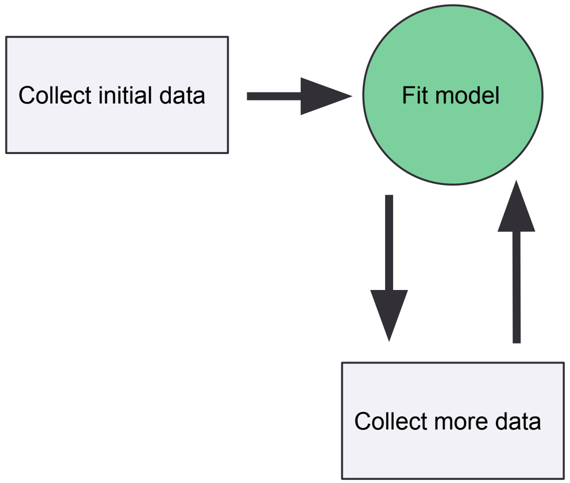
Let's make use of uncertainty estimates to make better models



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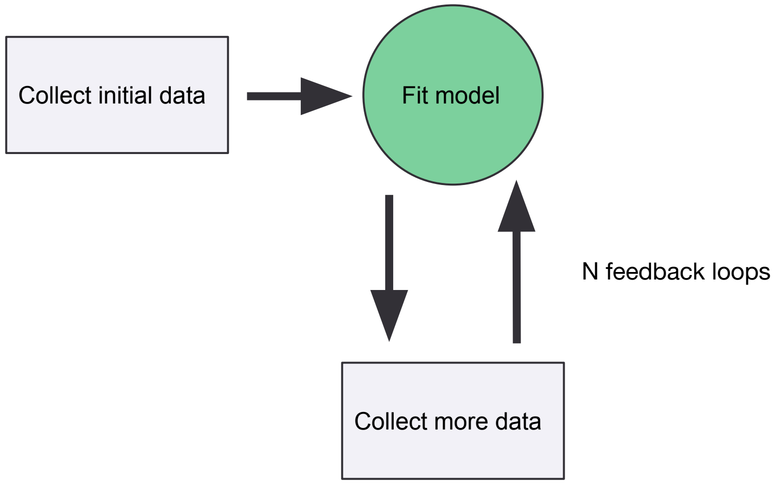

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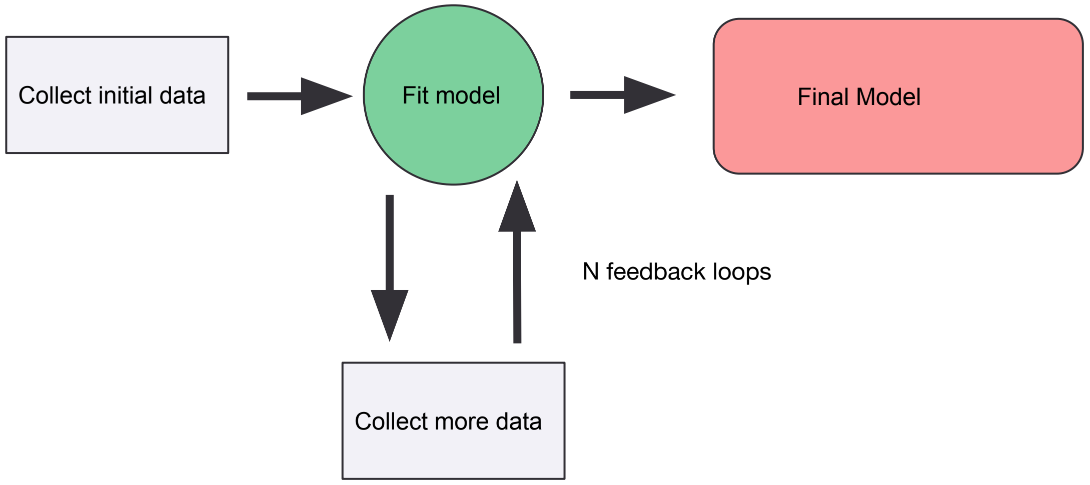

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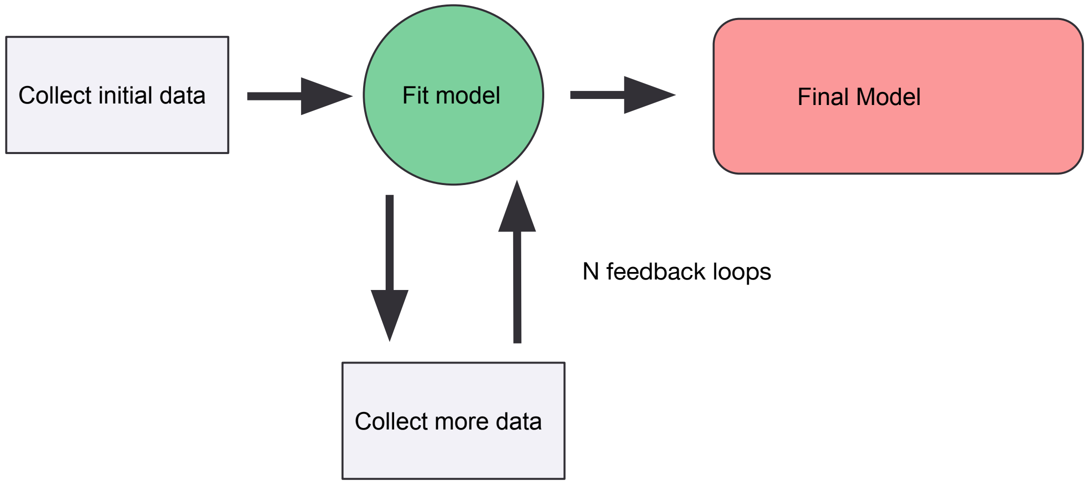

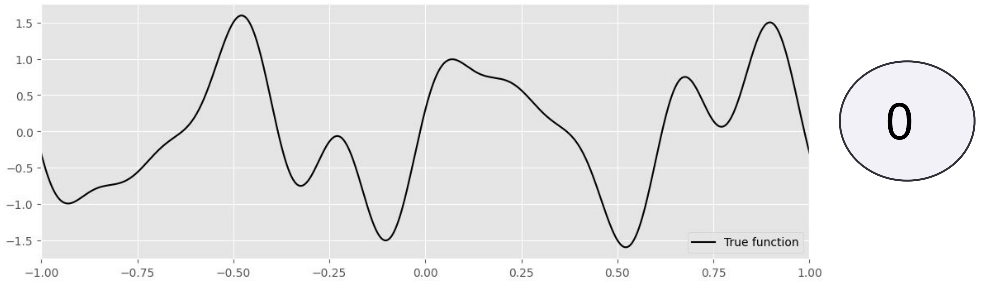

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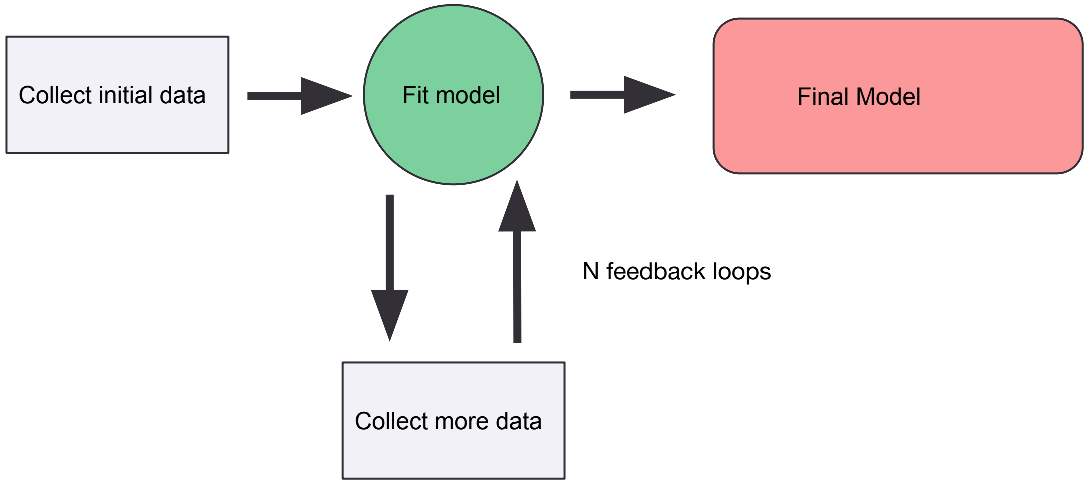

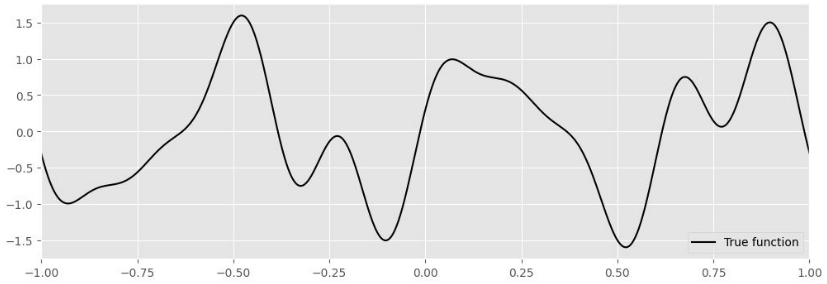

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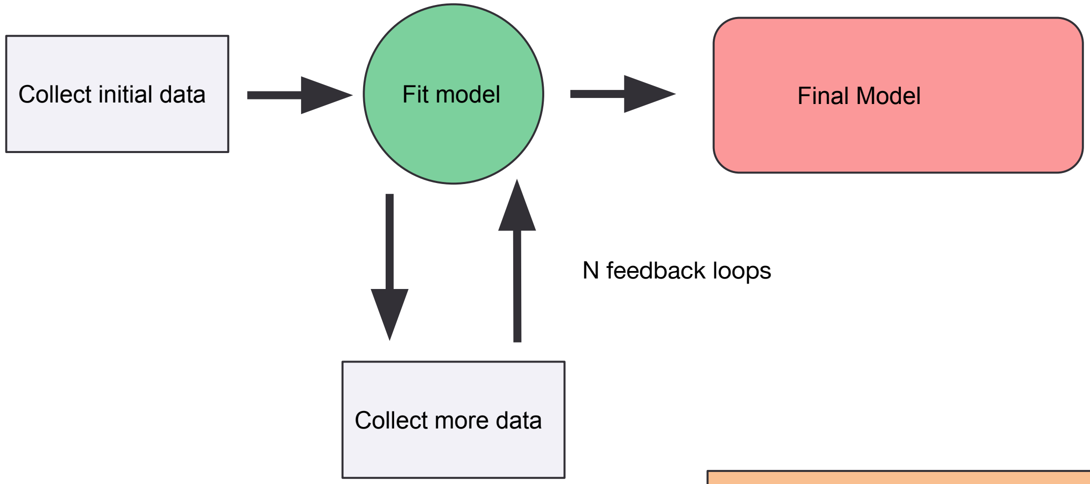

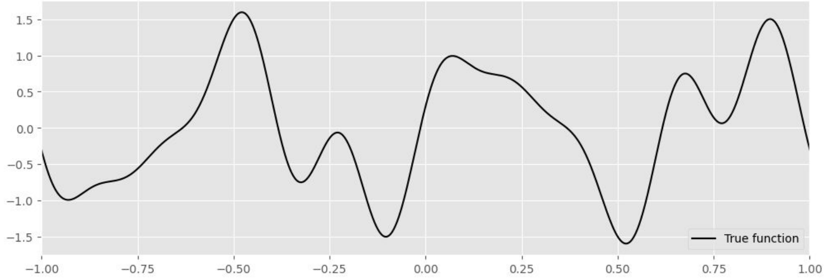

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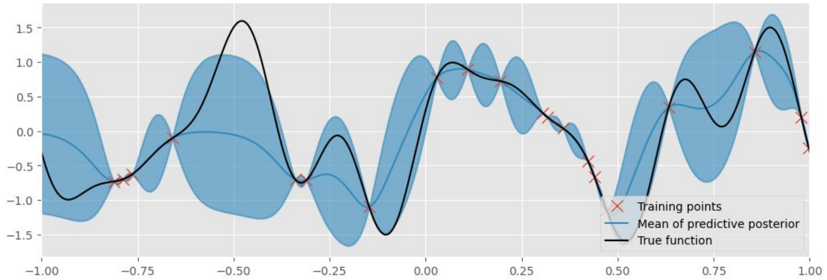

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These damn sausage plots!!!

Sequential data collection

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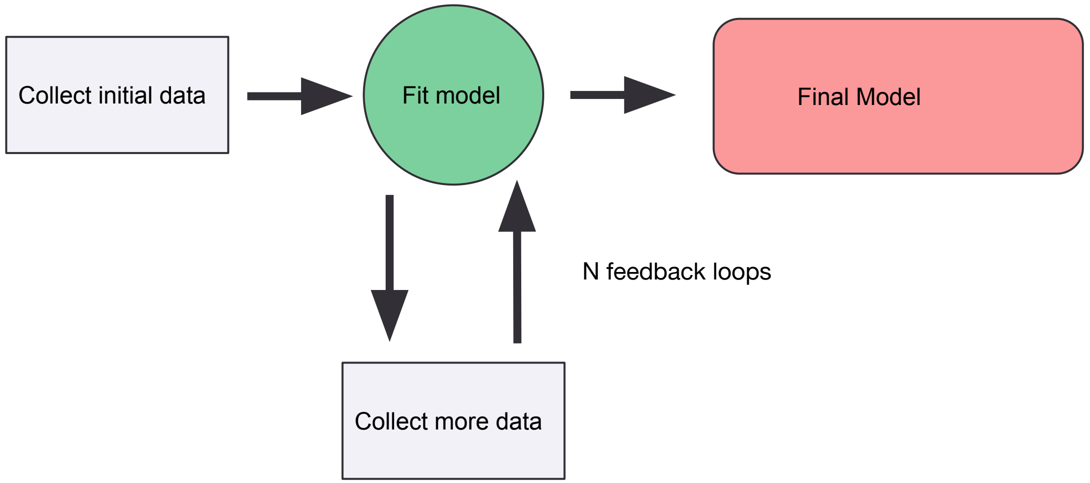

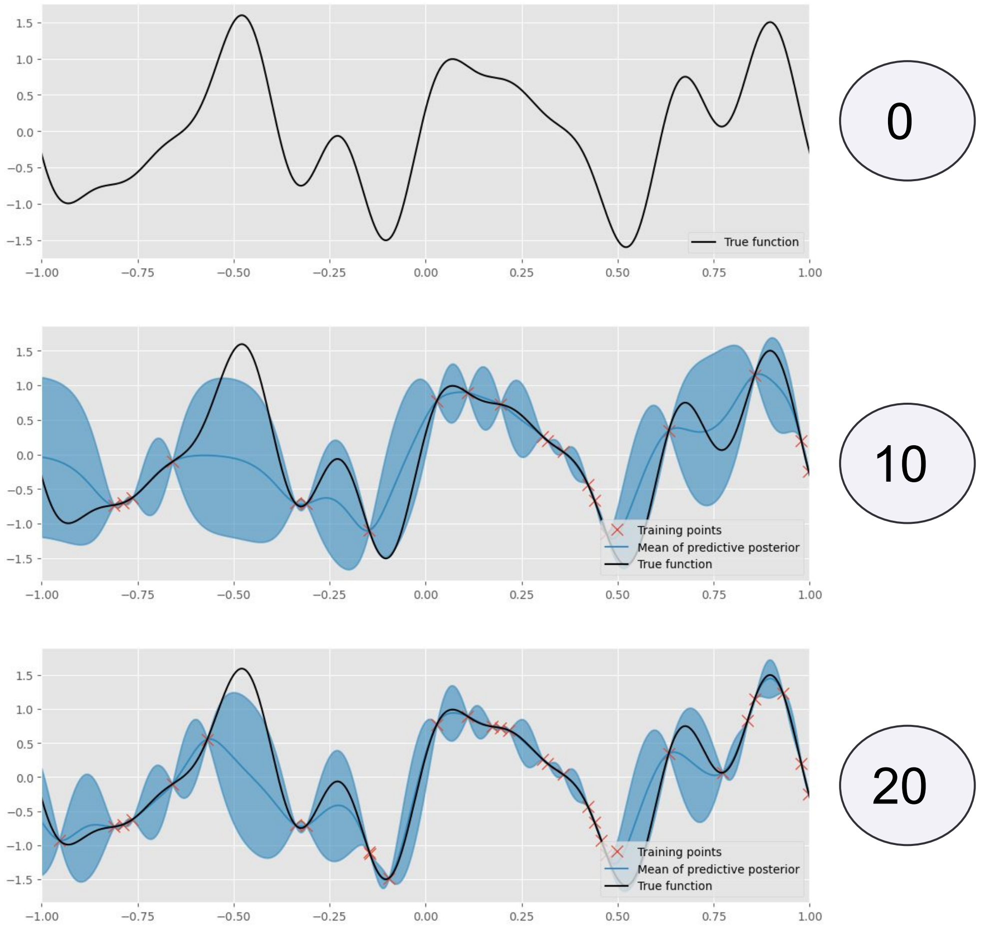

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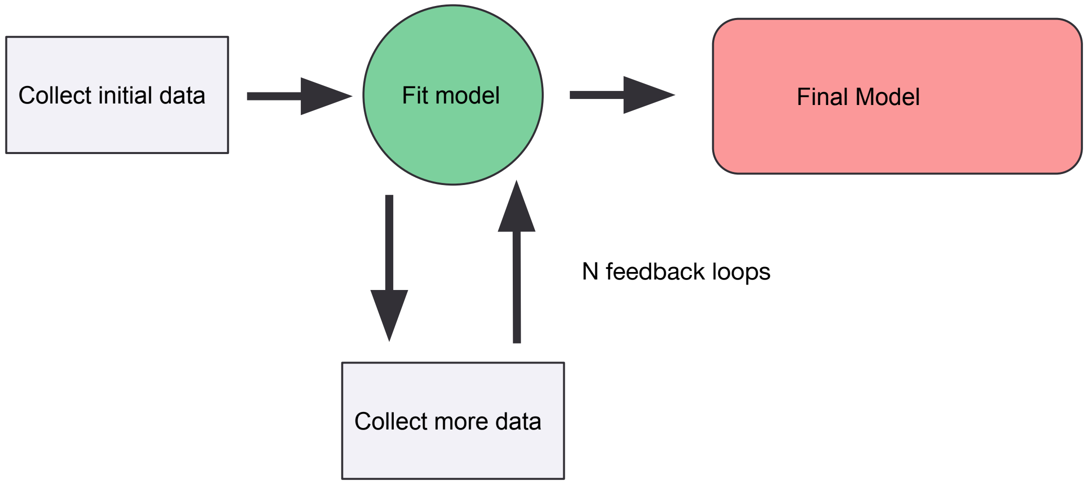

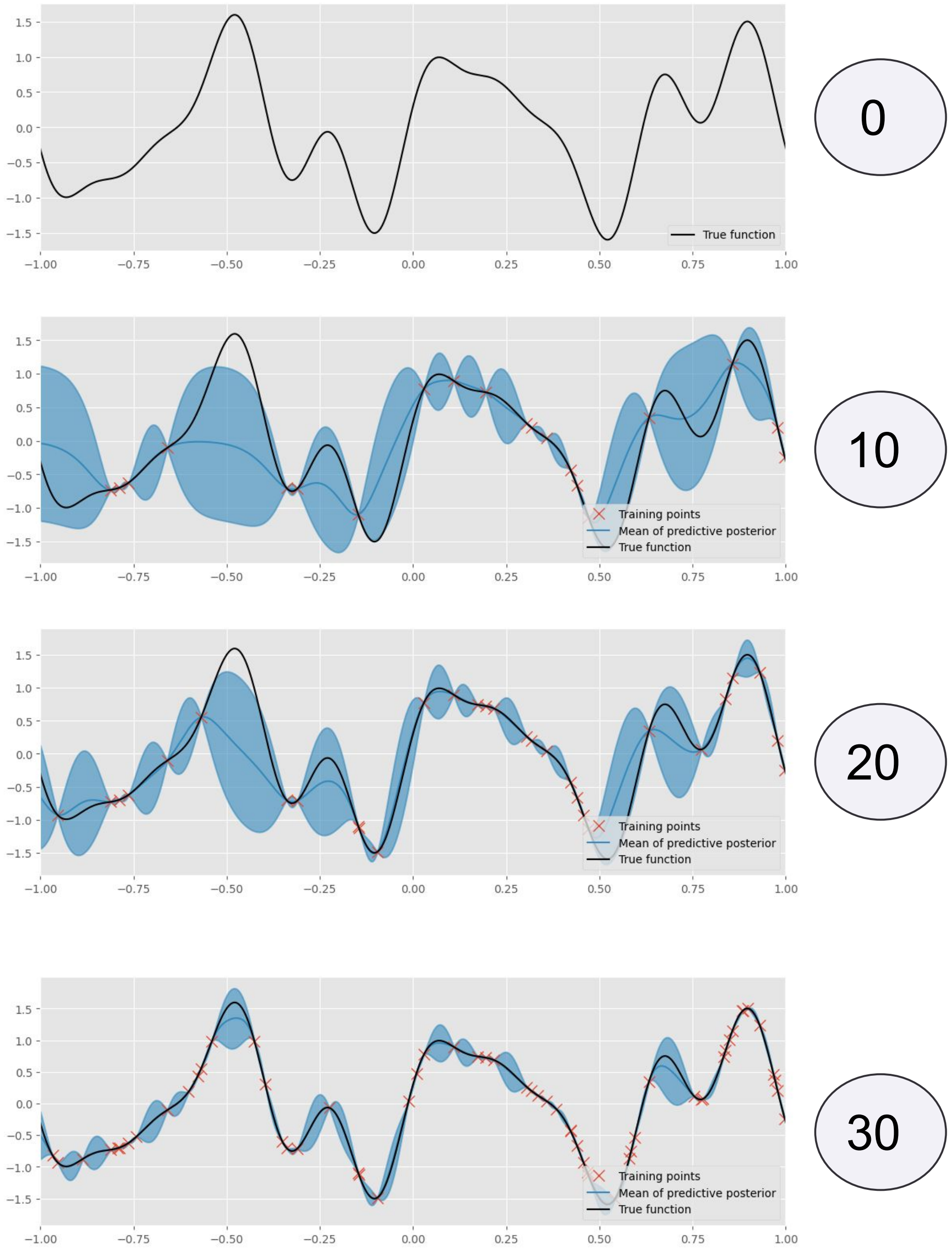

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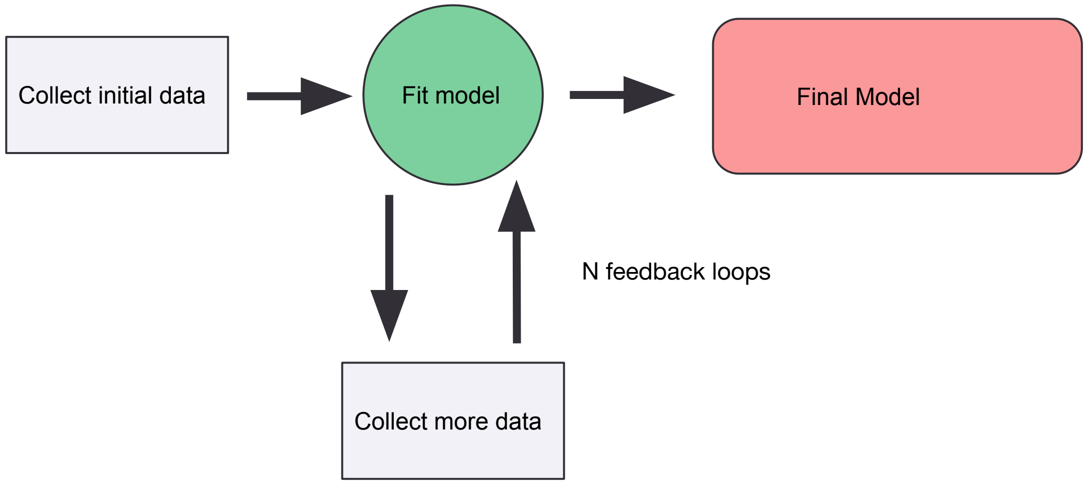

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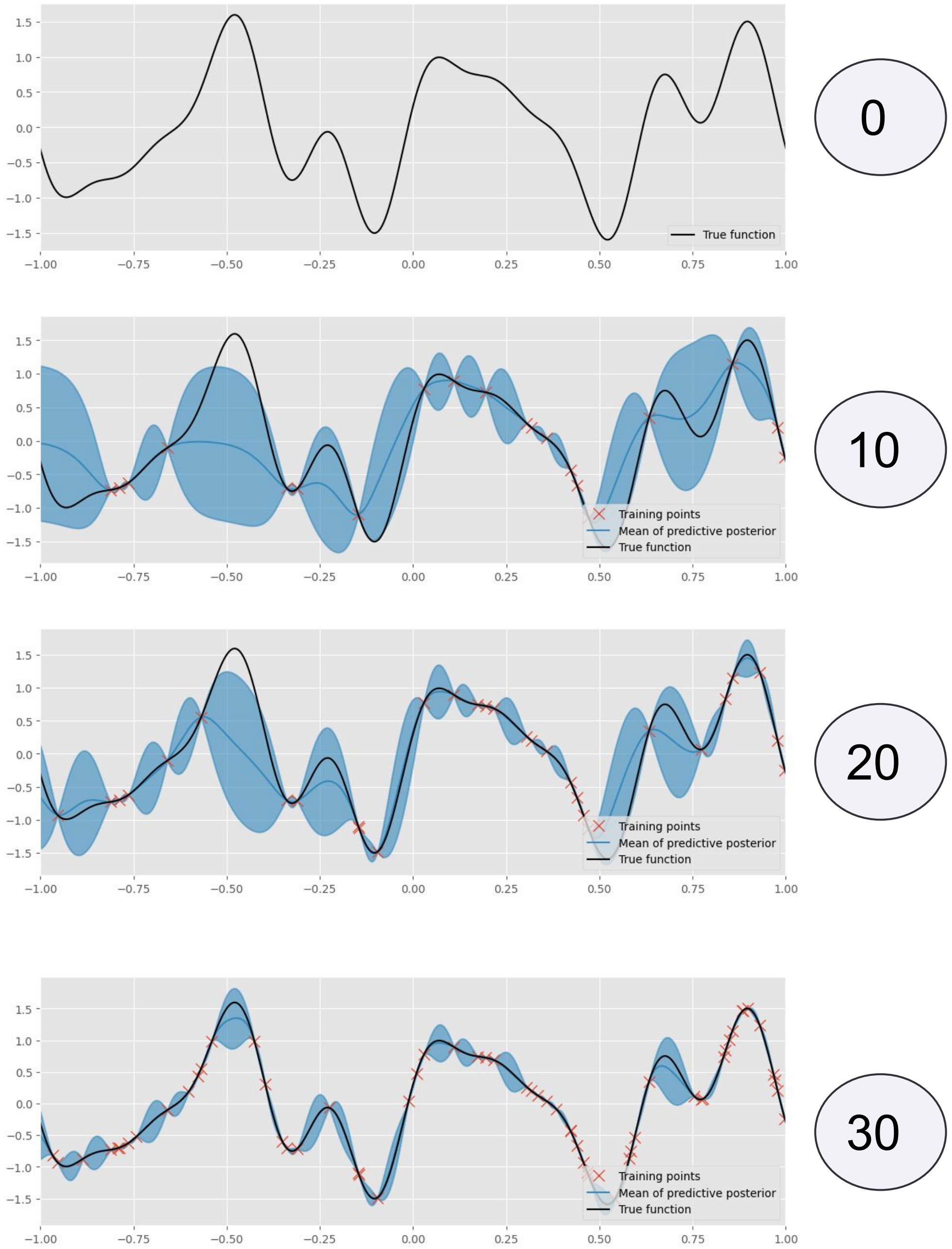

Active learning

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

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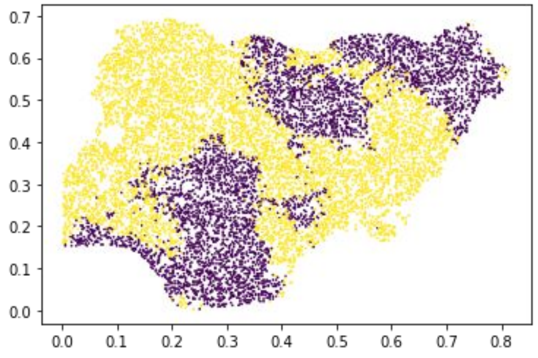

Malaria incidence in Nigeria

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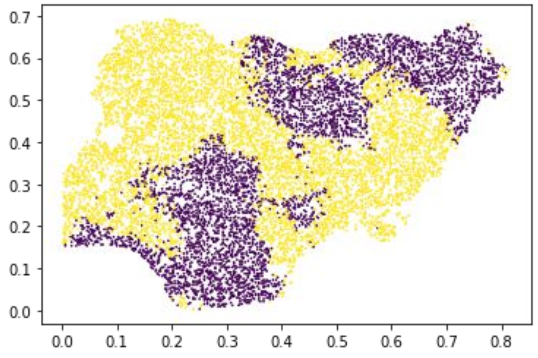

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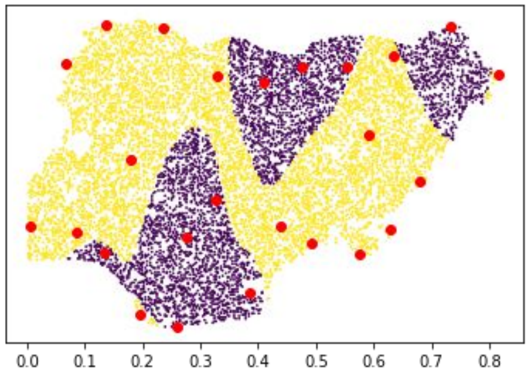

Model on Random data

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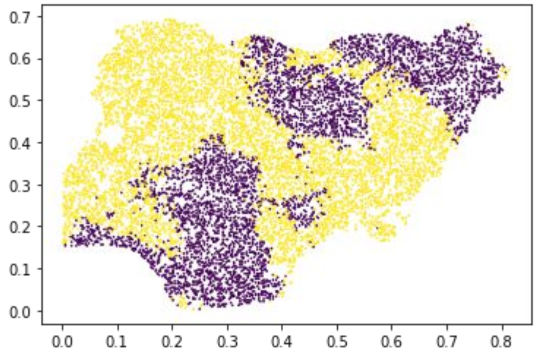

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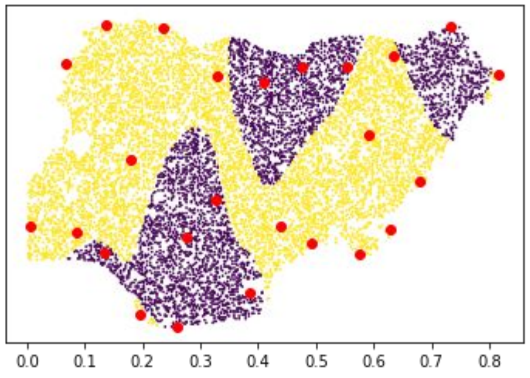

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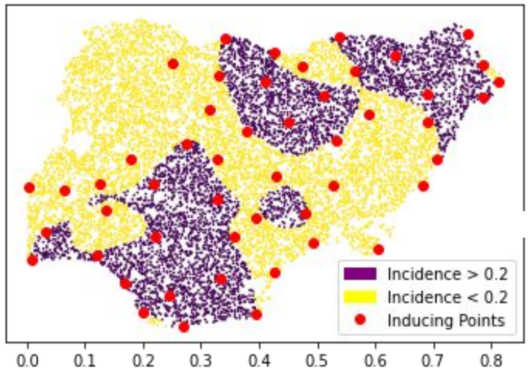

Model from data chosen by Active learning

So, Bayesian Optimisation?

i.e. Active learning for optimisation

A molecular design pipeline

Efficiently explore molecule space

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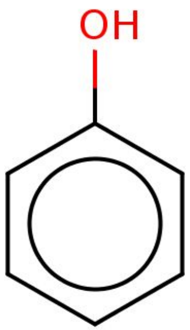
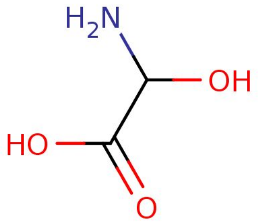
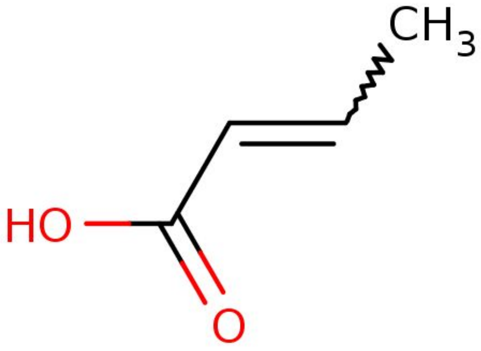
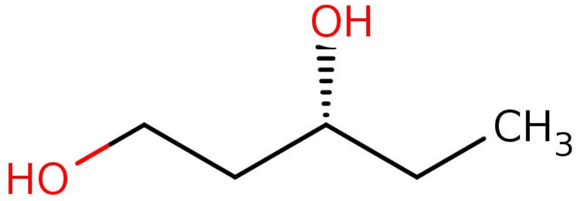
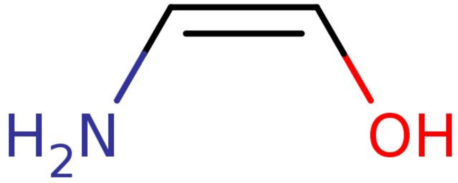
- **Large** library of candidates











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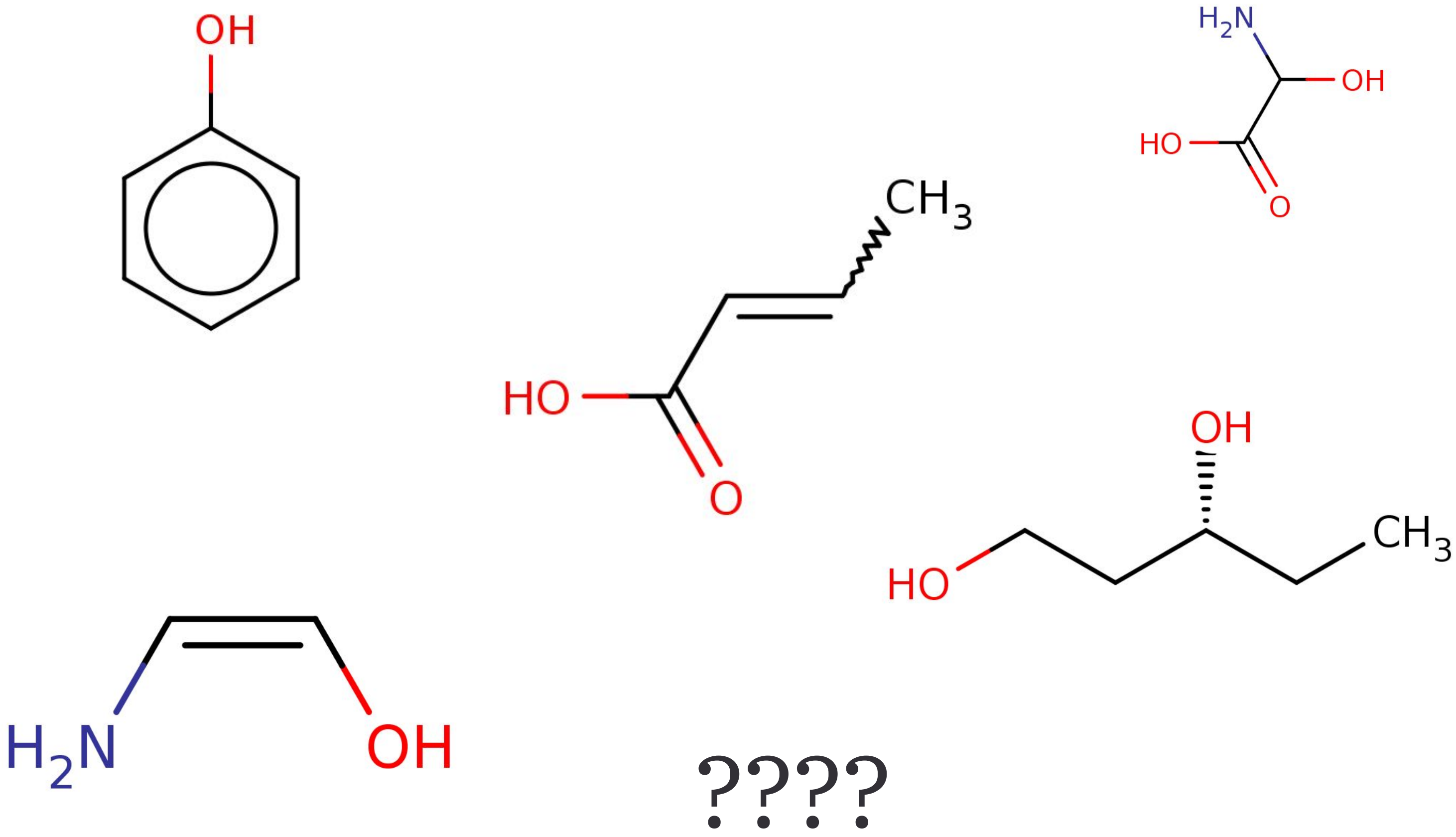
A molecular design pipeline

Efficiently explore molecule space

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



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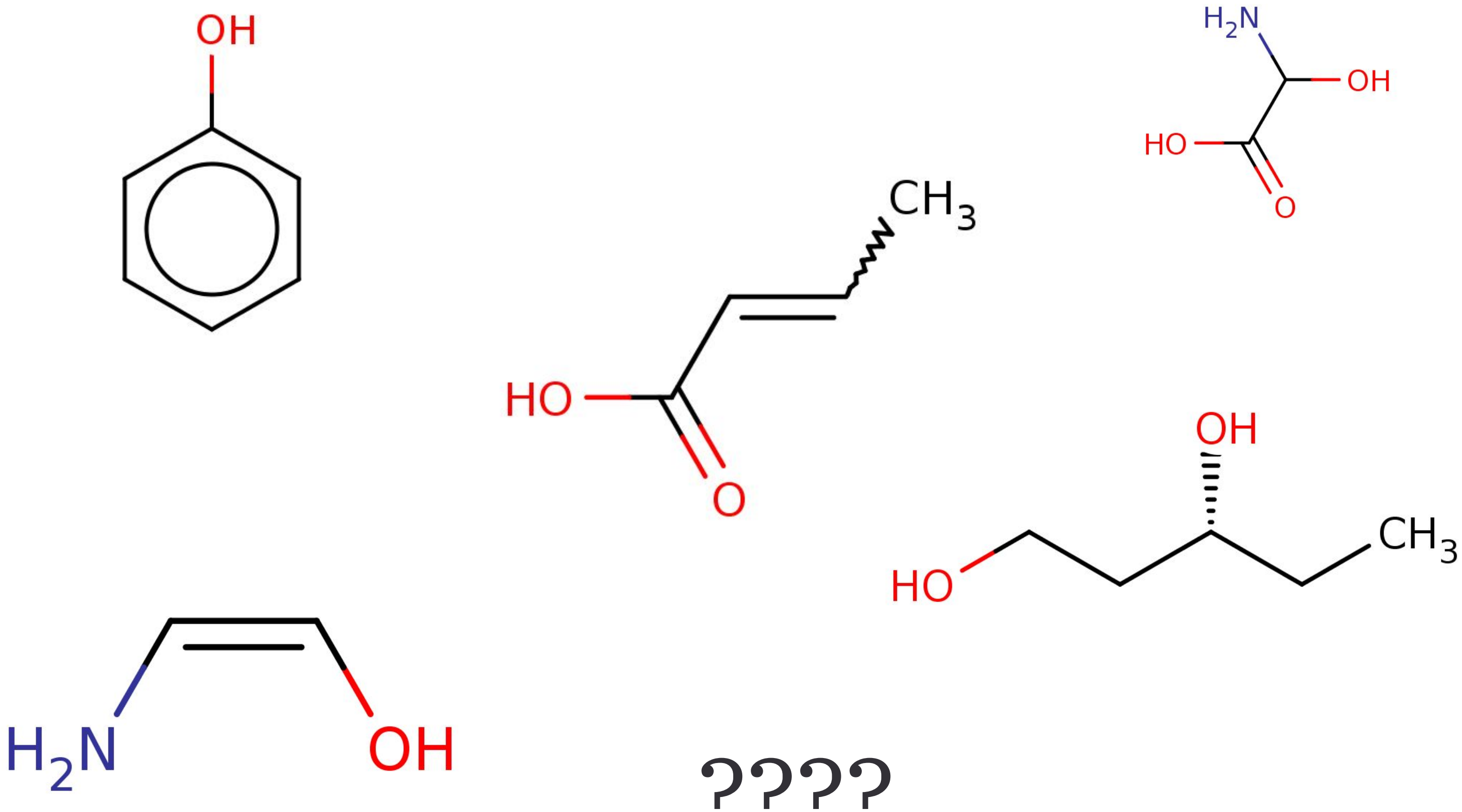

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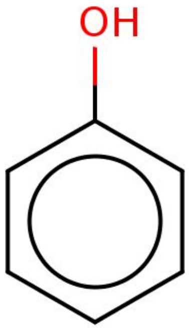

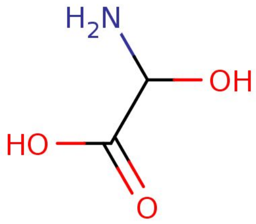

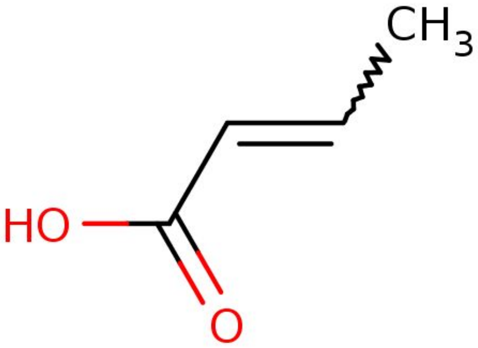

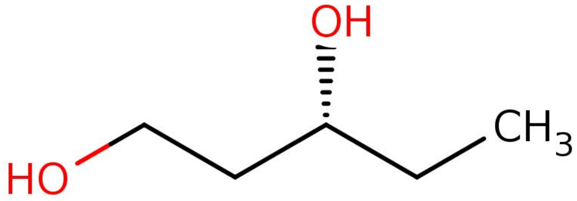

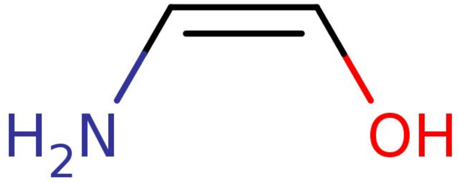

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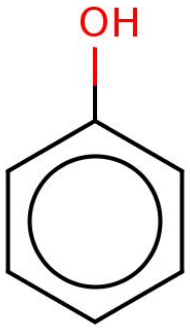

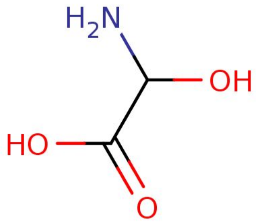

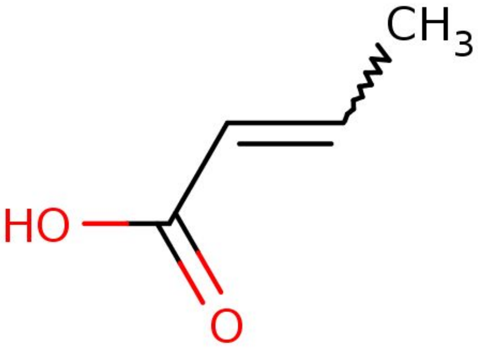

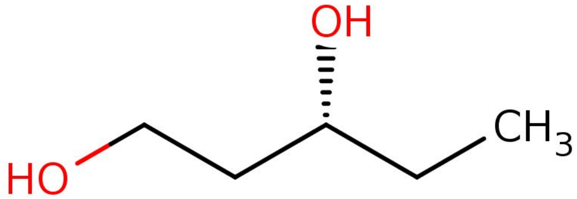

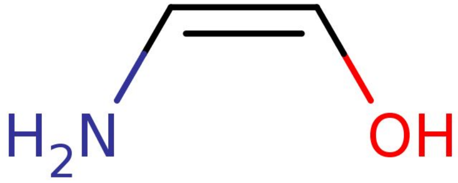

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- **Large** library of candidates
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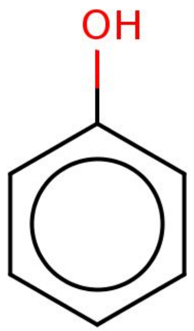
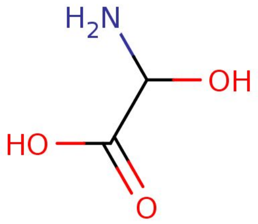
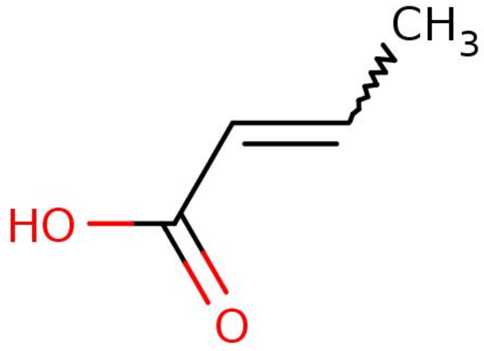
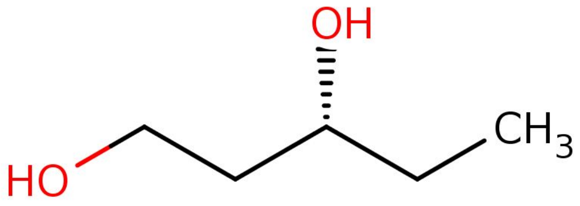
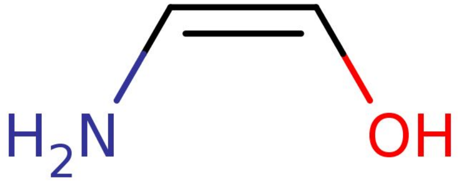
- Want molecules with high **affinity**
    - Also easy to make











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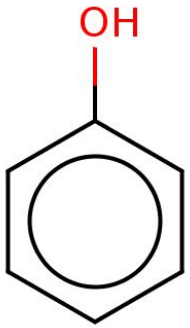
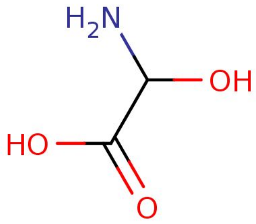
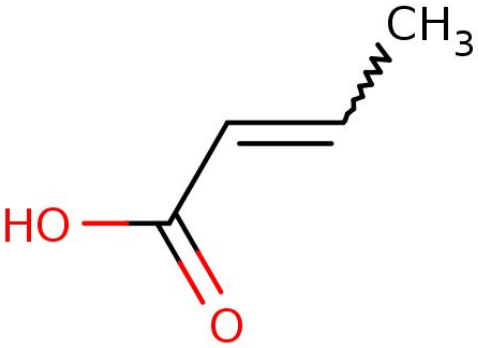
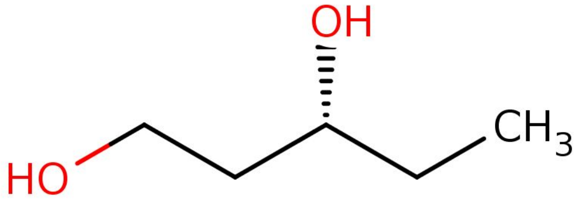
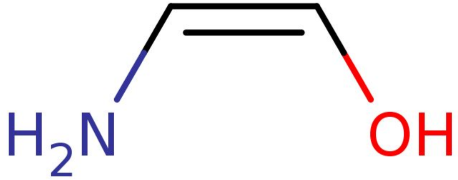
    - Also easy to make
    - Don’t stick to themselves











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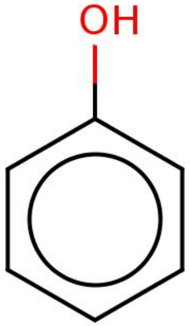
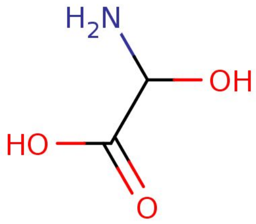
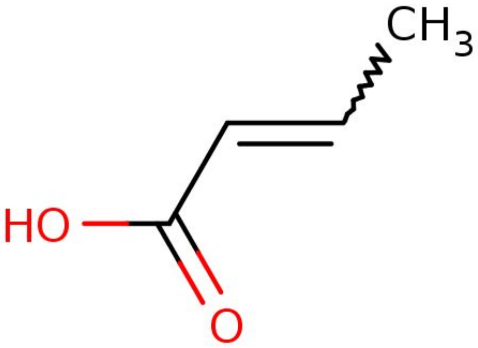
A molecular design pipeline

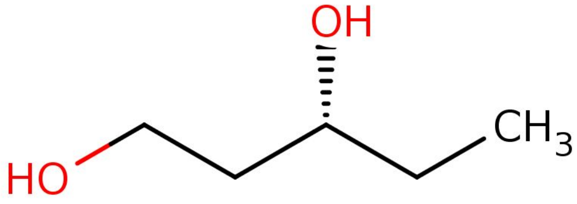
Efficiently explore molecule space

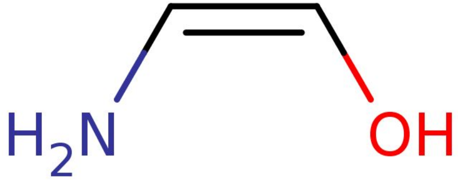
- **Large** library of candidates
- **Expensive** experiments (<10)
- High degree of **parallelism**
- Want molecules with high **affinity**
  - Also easy to make
  - Don’t stick to themselves
  - Stable











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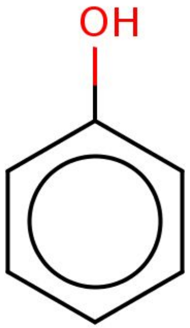

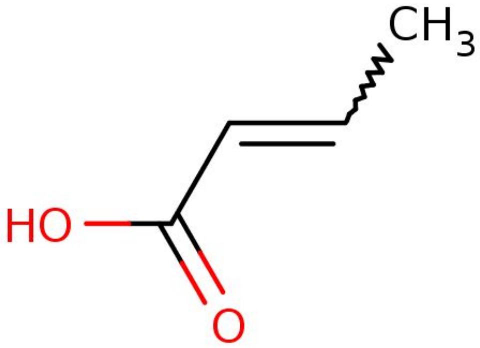

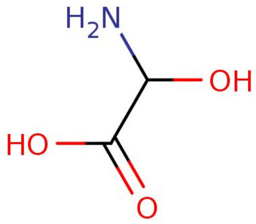

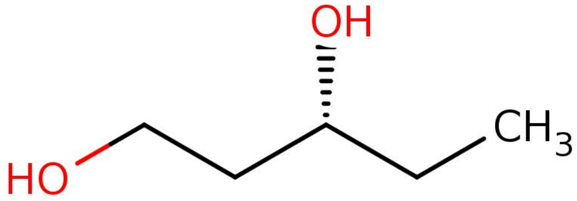

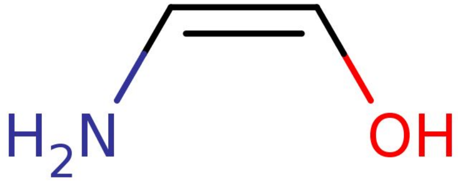

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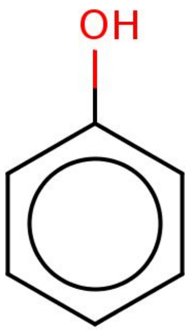

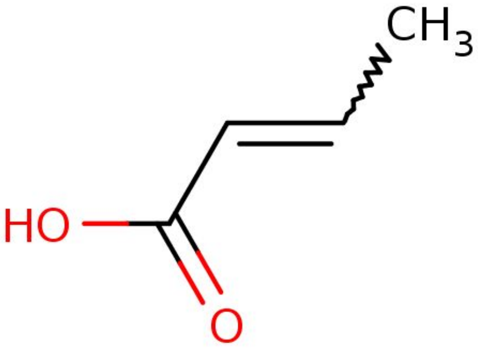

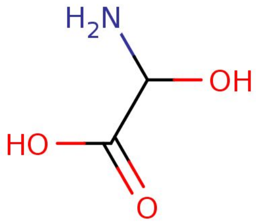

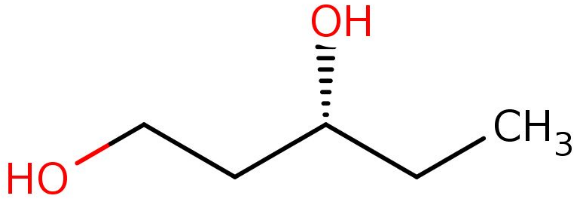

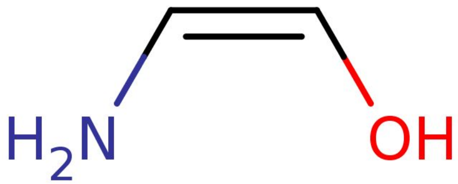

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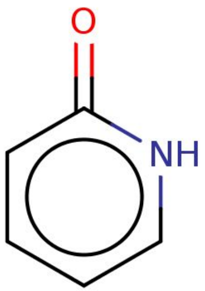
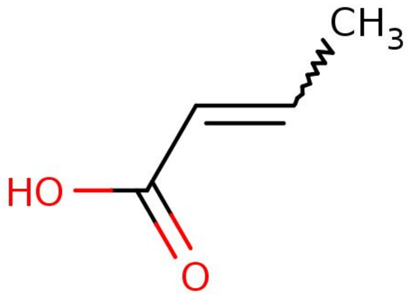
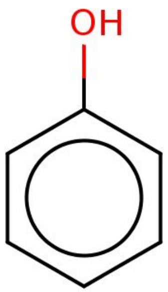
Any ideas?

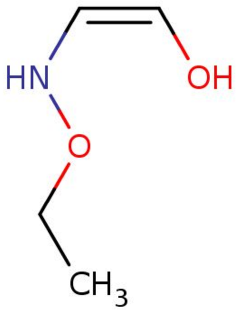
A Simpler Example

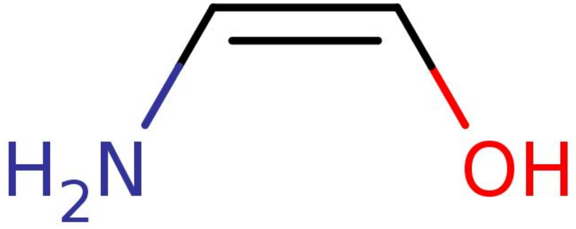
Can evaluate **at most** 4

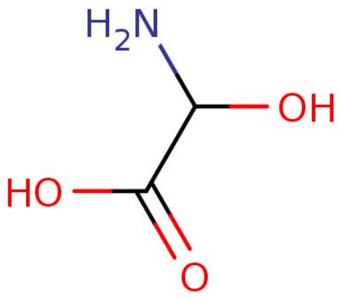






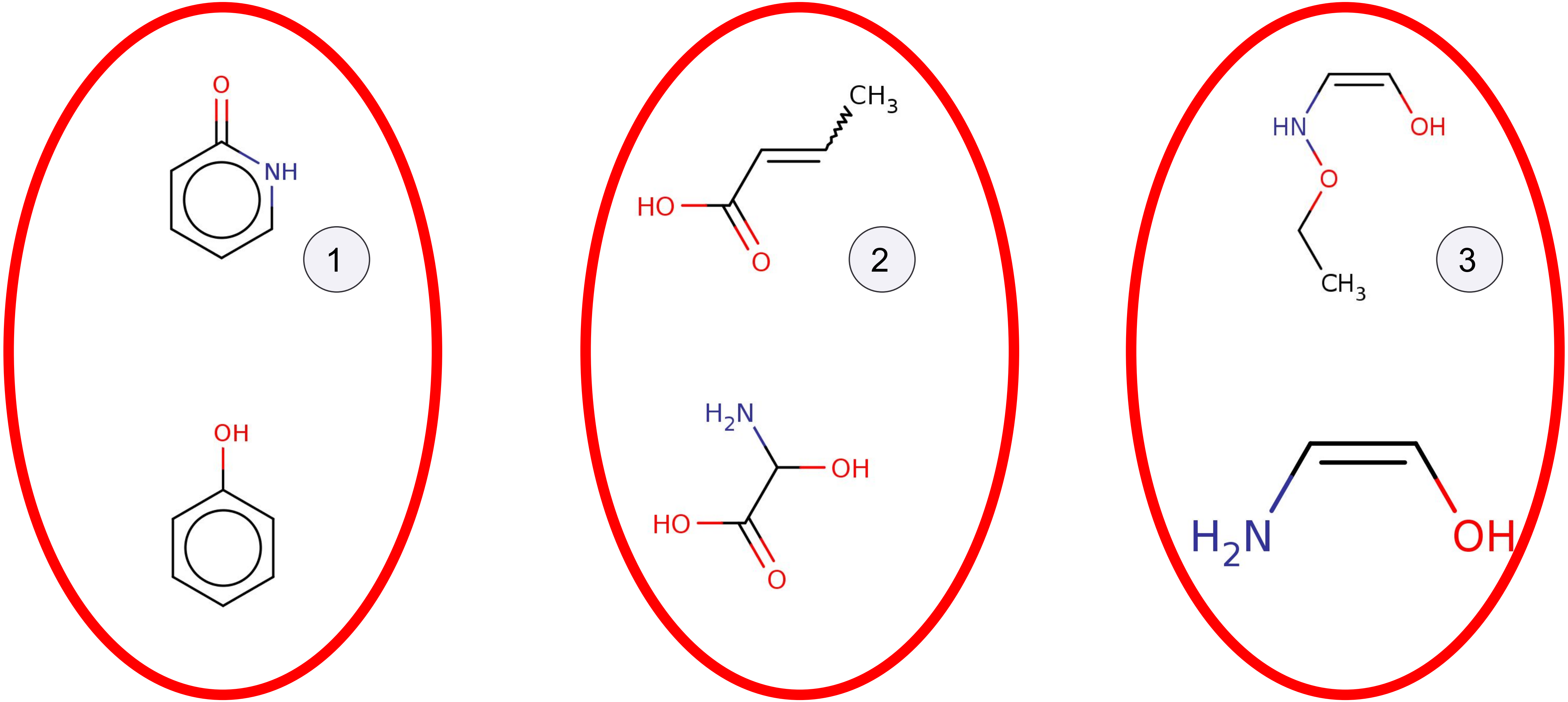






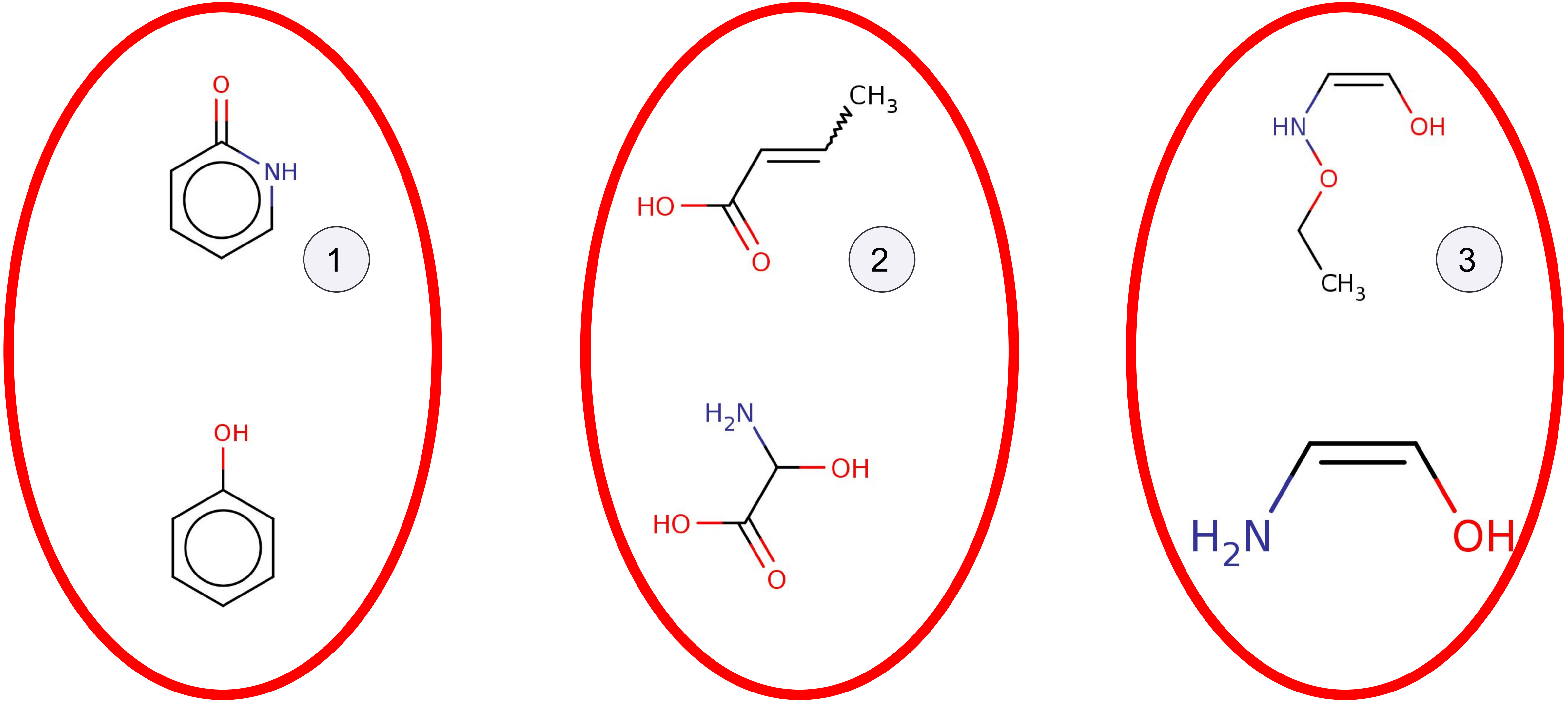
A Simpler Example (grouped)

Can evaluate **at most** 4



A Simpler Example (grouped)

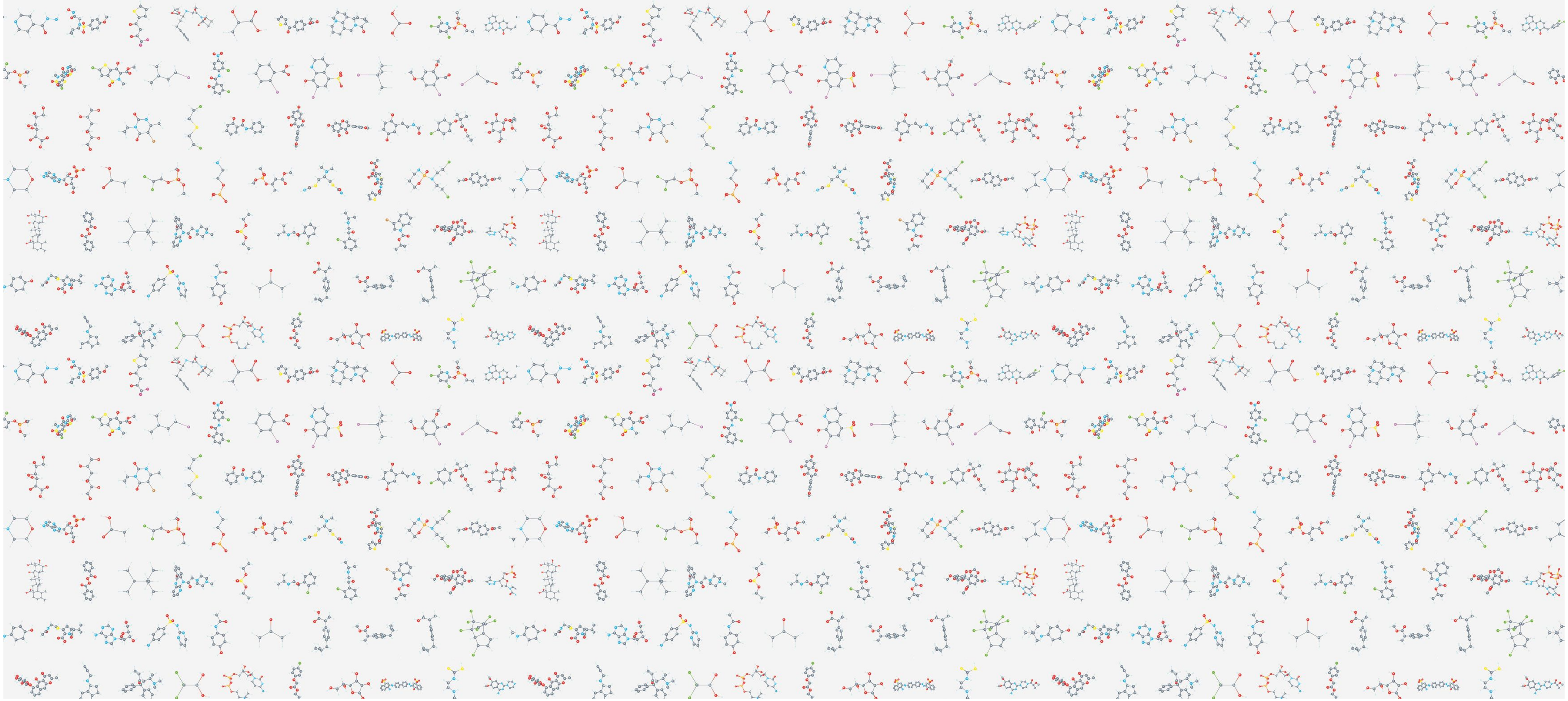
Can evaluate **at most** 4



Explore v.s. **exploit**?

What about at scale?

eek



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

What about at scale?

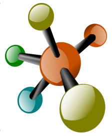
eek

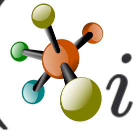
Use a GP!

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

An Aside: GPs for Molecules

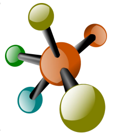
Structured Input Spaces

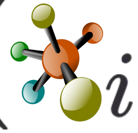
$y_i = f($$_i) + \epsilon_i$

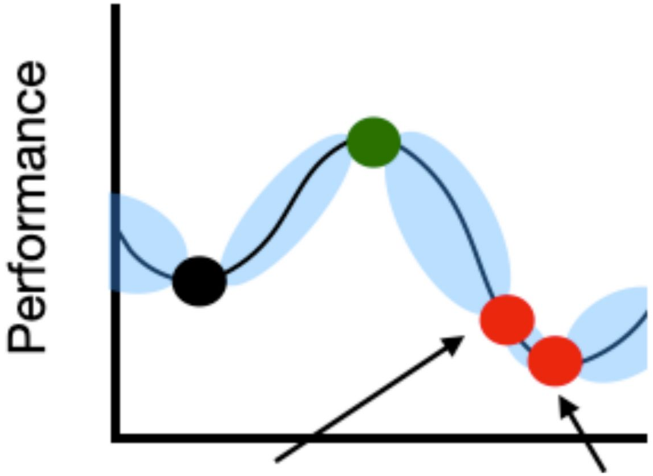
$D_N = \{($$_i, y_i)\}_i^N$

An Aside: GPs for Molecules

Structured Input Spaces

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

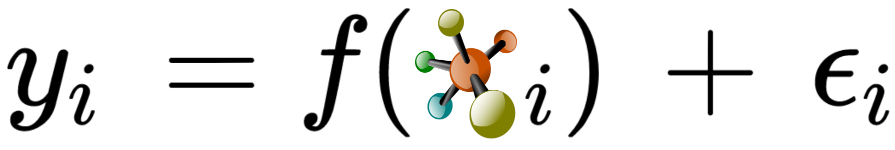
$D_N = \{($$_i, y_i)\}_i^N$

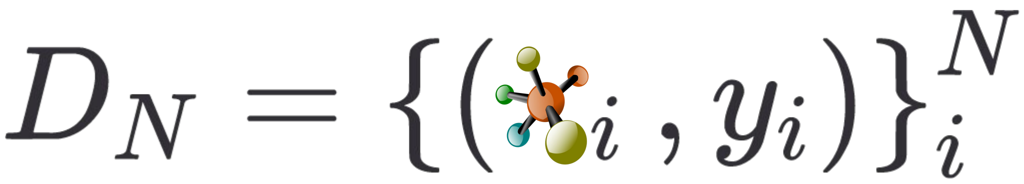


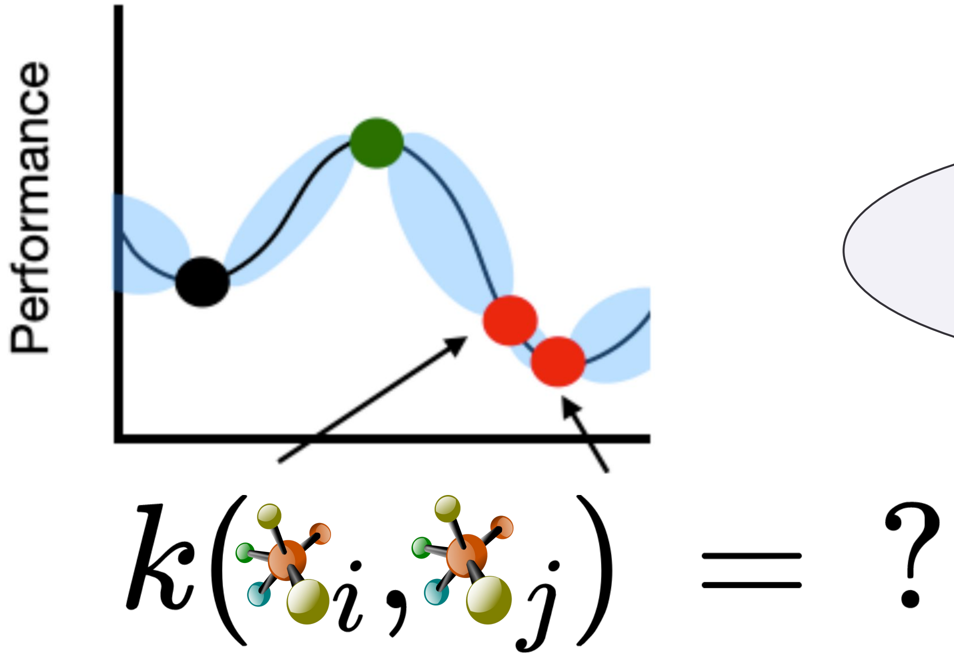
What do we require to define a GP?

An Aside: GPs for Molecules

Structured Input Spaces



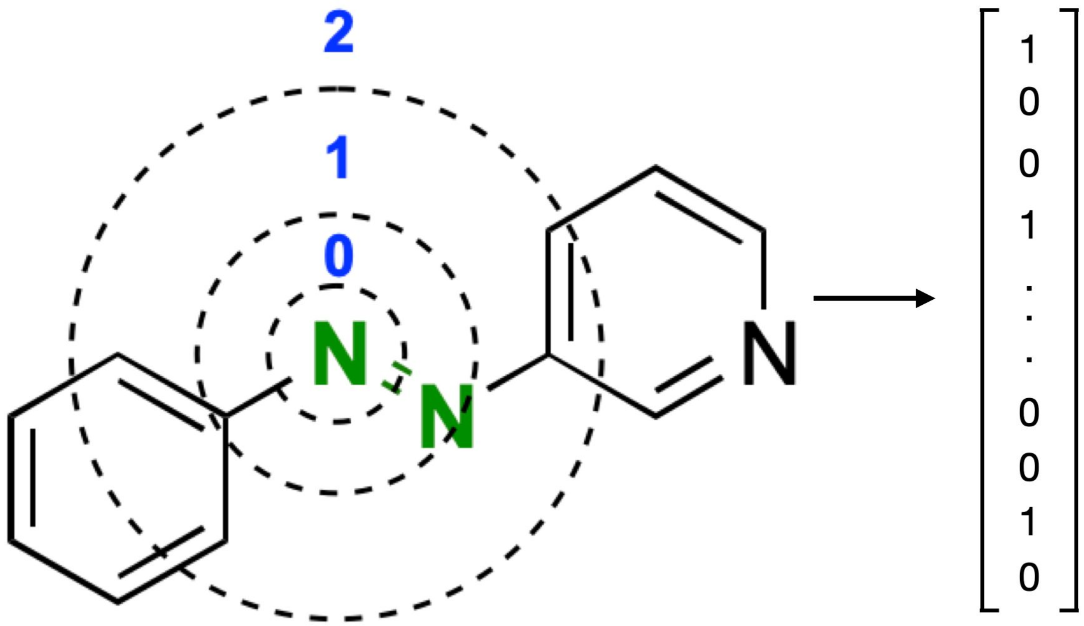




What do we require to define a GP?

An Aside: GPs for Molecules

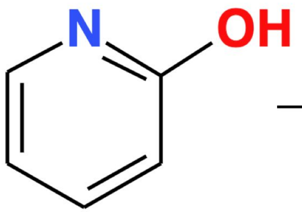
Fingerprint Kernels



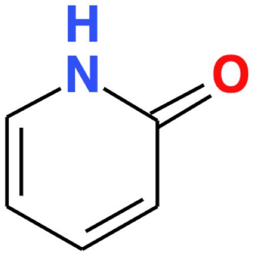
An Aside: GPs for Molecules

String kernels between SMILES strings

$$k(\cdot_i, \cdot_j) = k(str(\cdot_i),\ str(\cdot_j))$$



$\longrightarrow$ $Oc1ncccc1$



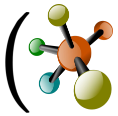
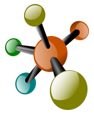
$\longrightarrow$ $O = c1[nH]cccc1$

Automatically choosing next molecules

Using GP posteriors and utility functions

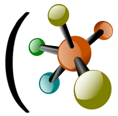
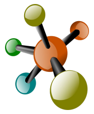
Automatically choosing next molecules

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

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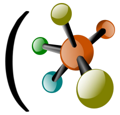
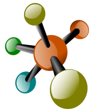
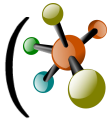
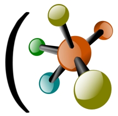
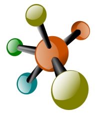
- $U_f($  $)$: what is the utility of evaluating  (if it will return f)

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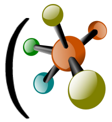
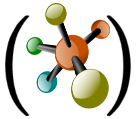
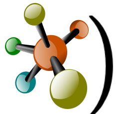
  - Has there been an improvement? $U_f($  $) = \mathbb{1}_{(f > f^\star)}$
  - How big was the improvement? $U_f($  $) = \max(f - f^\star, 0)$

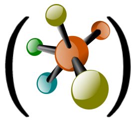
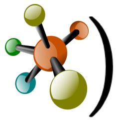
Automatically choosing next molecules

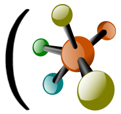
Using GP posteriors and utility functions

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

Automatically choosing next molecules

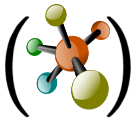
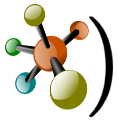
Using GP posteriors and utility functions

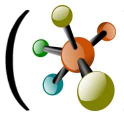
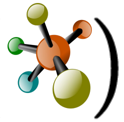
- $\alpha($$) = \mathbb{E}_f[U_f($$)]$: what utility is predicted by my model of f

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

Automatically choosing next molecules

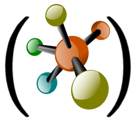
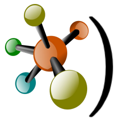
Using GP posteriors and utility functions

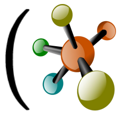
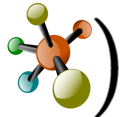
- $\alpha($  $) = \mathbb{E}_f[U_f($  $)]$: what utility is predicted by my model of f

  - 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

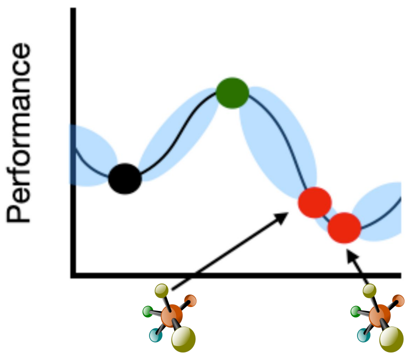
- $\alpha($  $) = \mathbb{E}_f[U_f($  $)]$: what utility is predicted by my model of f

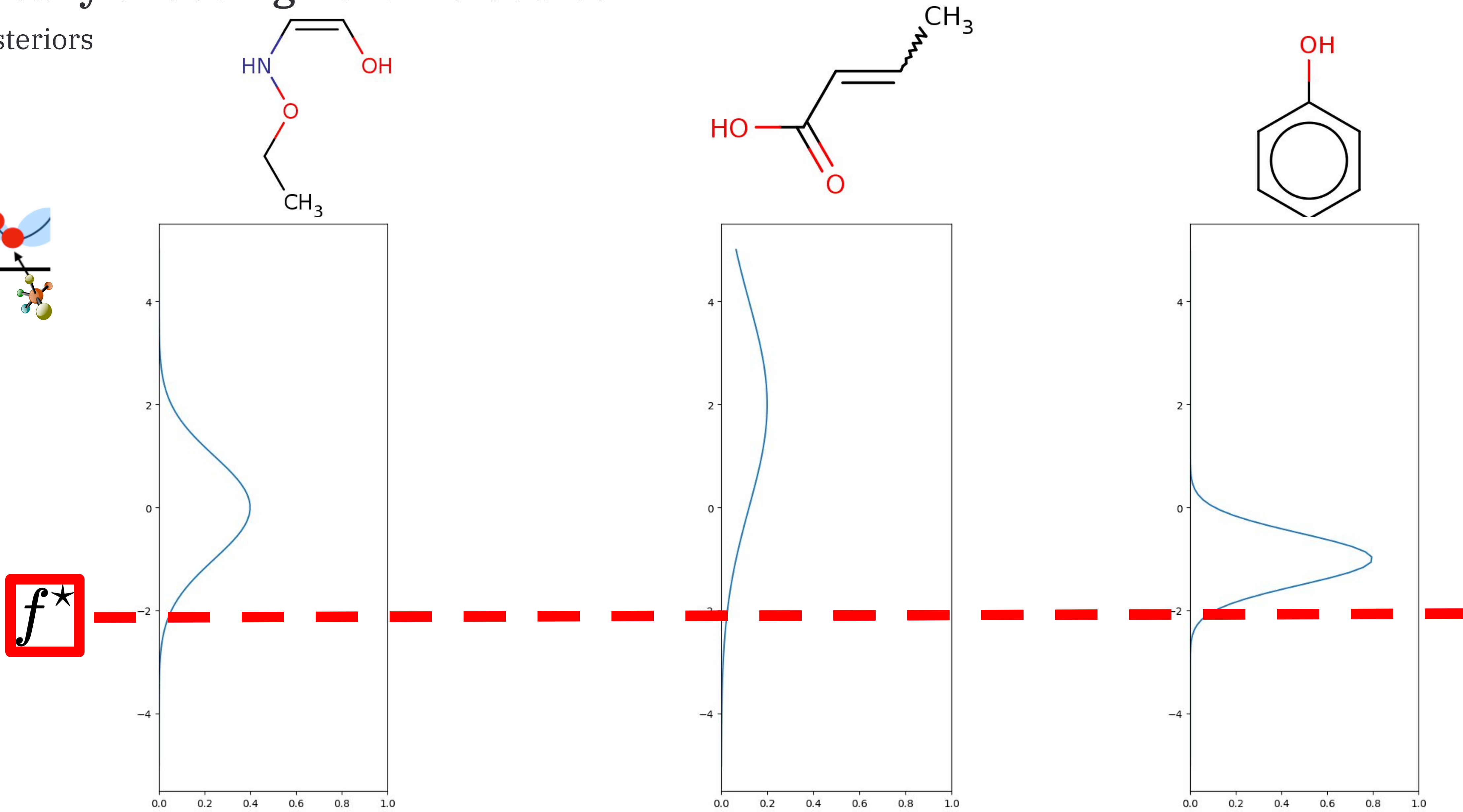
    - What the probability of improvement? $\alpha_{\mathrm{PI}}($  $) = \mathbb{E}_f\left[\mathbb{1}_{(f > f^\star)}\right]$
    - How much improvement do we expect? $\alpha_{\mathrm{EI}}($  $) = \mathbb{E}_f[\max(f - f^\star, 0)]$

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

Automatically choosing next molecules

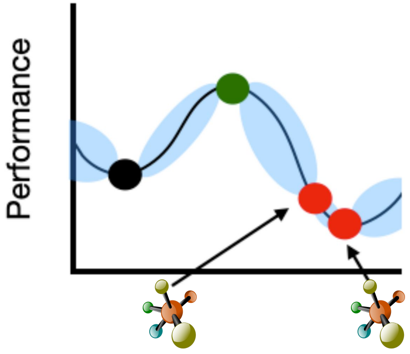
Using GP posteriors

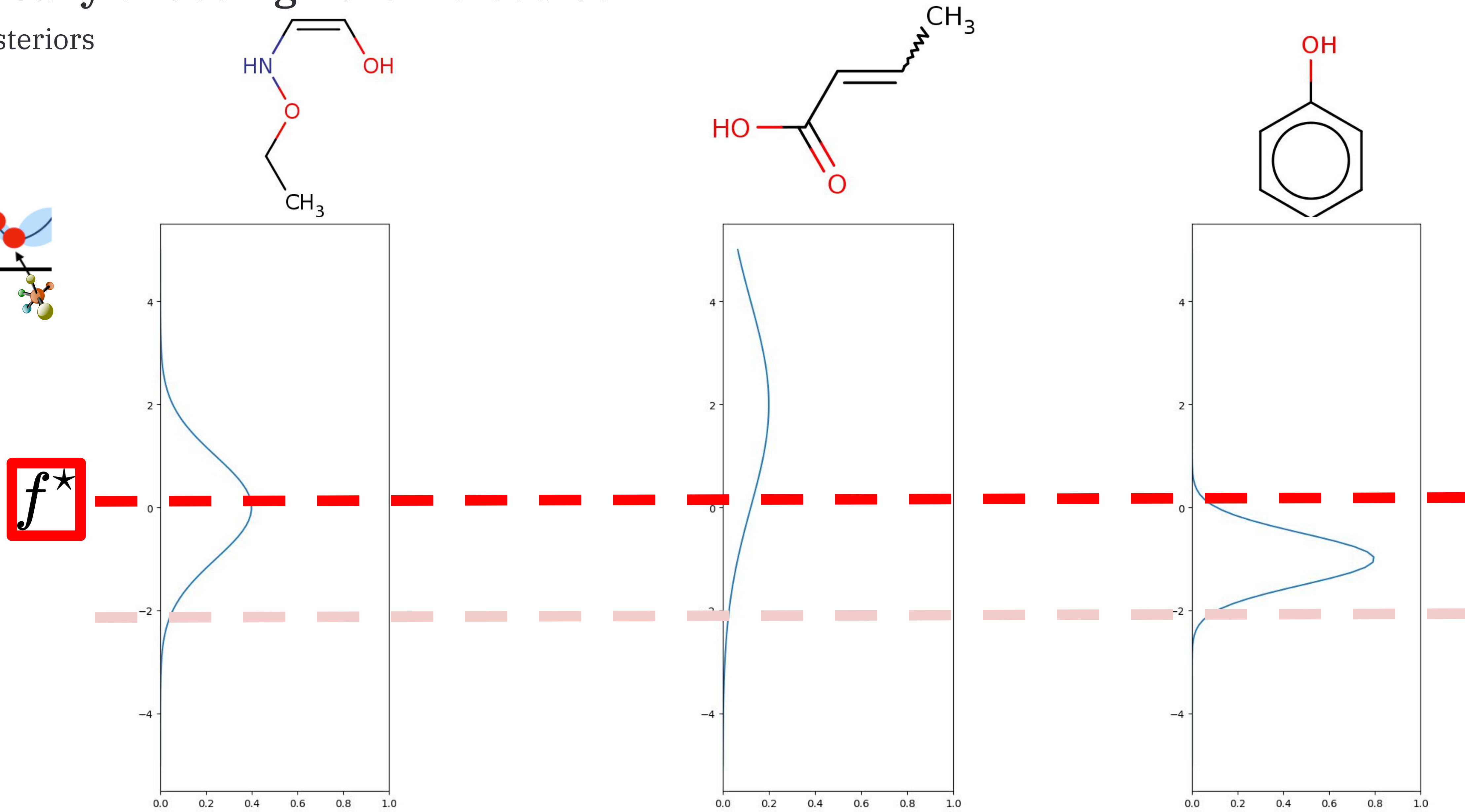




Automatically choosing next molecules

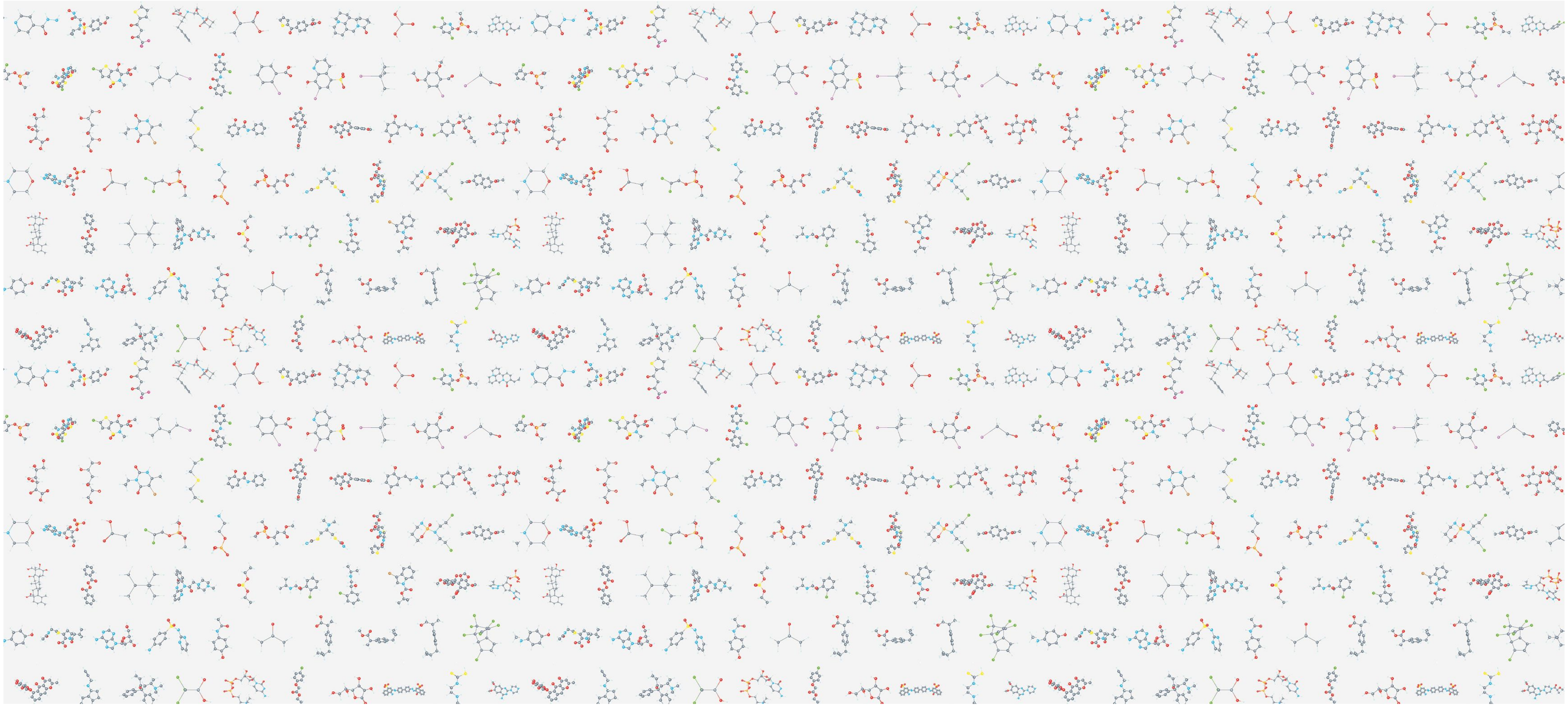
Using GP posteriors





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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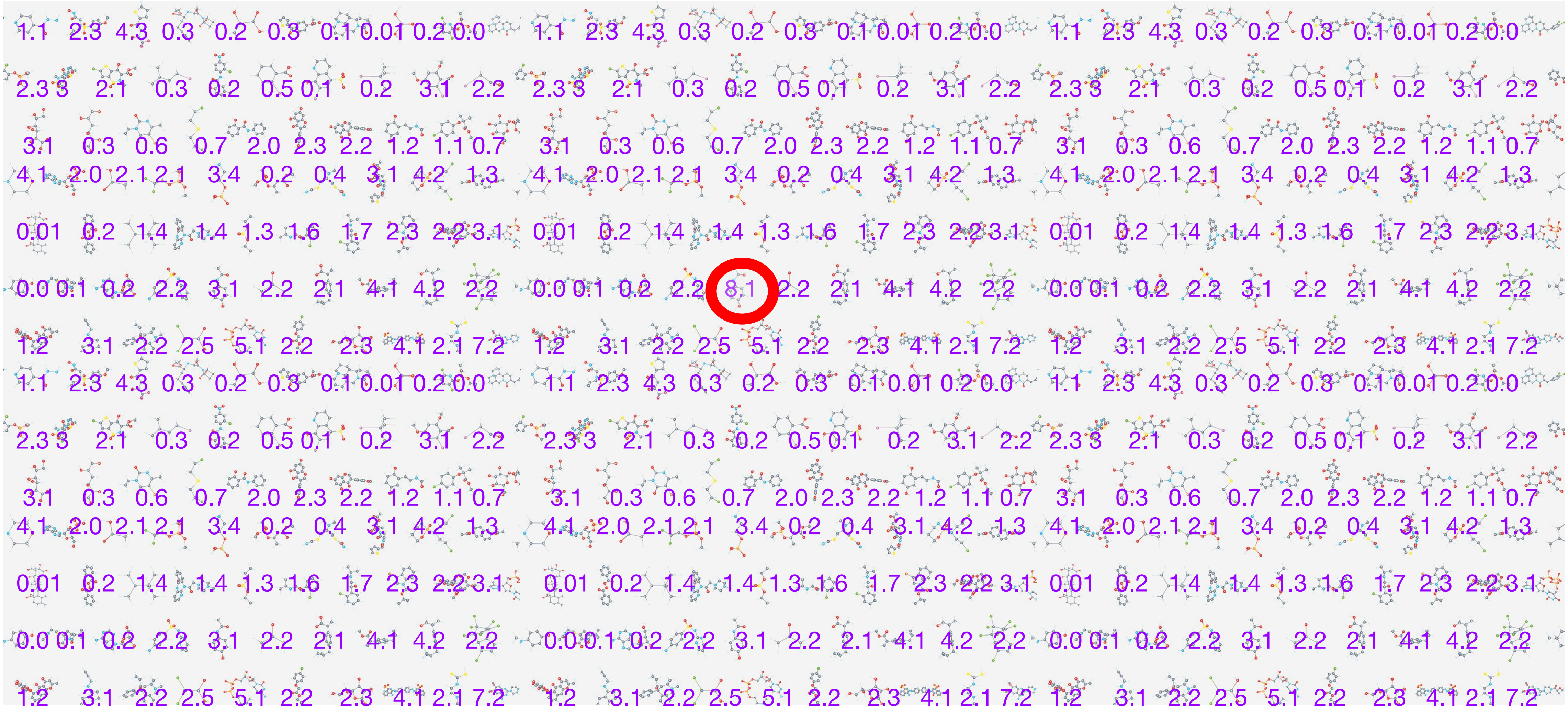

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Automatically choosing next molecules

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

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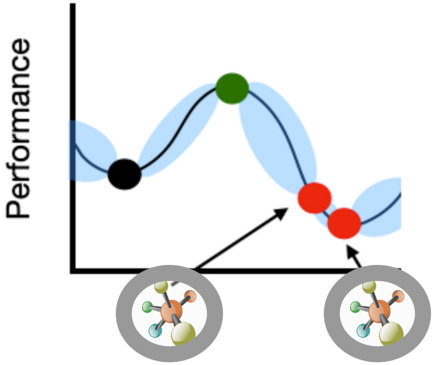
2. Fit GP model to measurements



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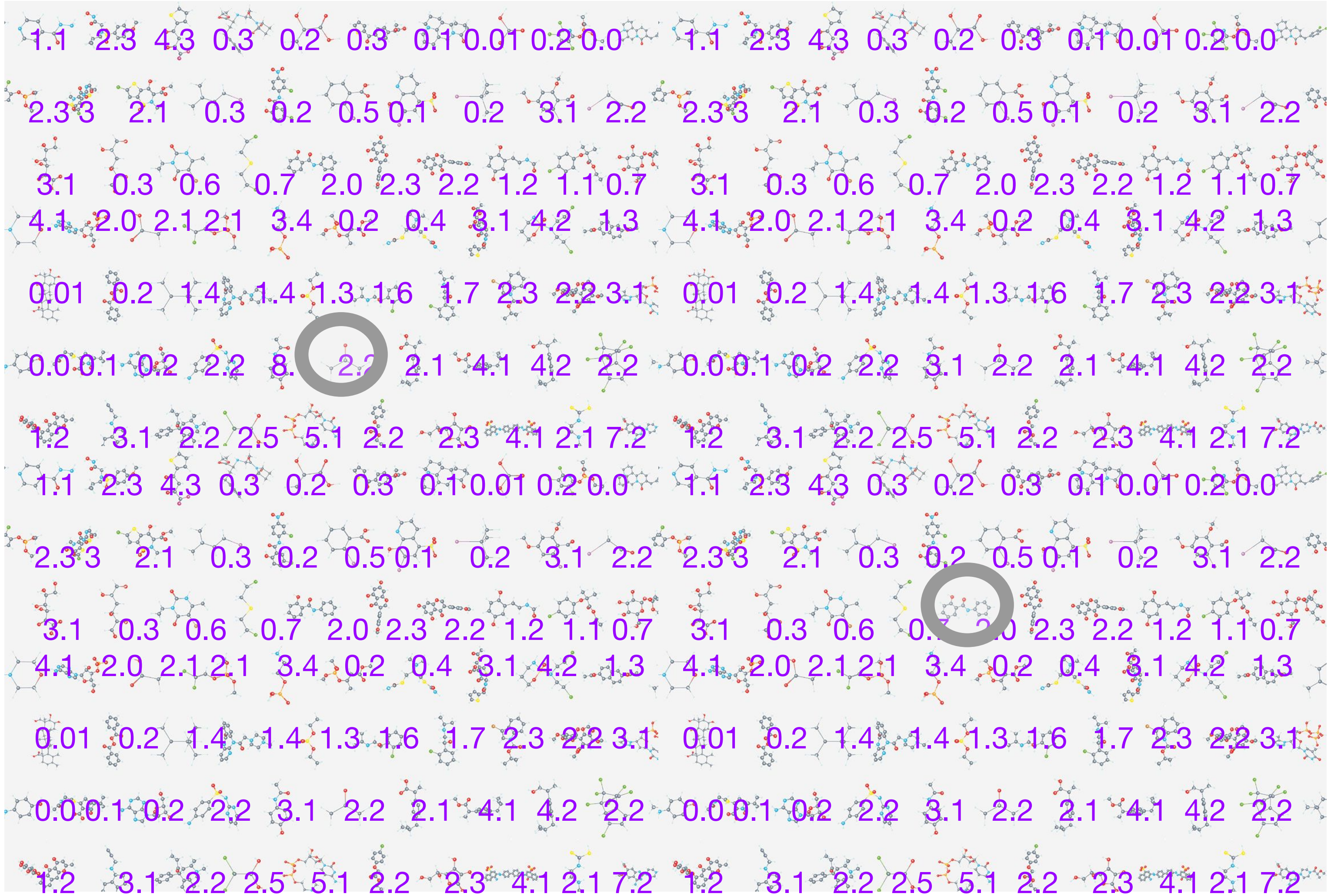

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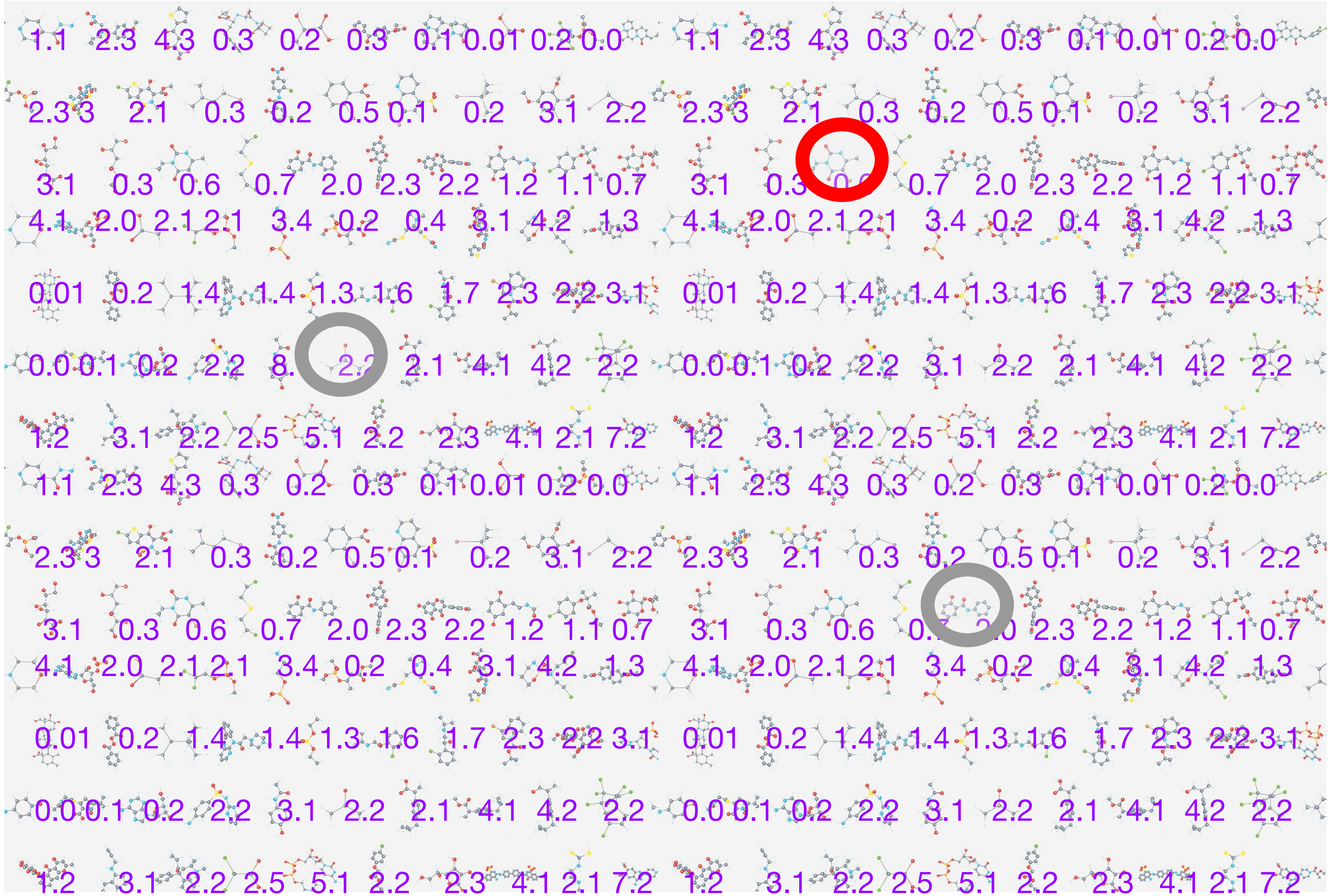

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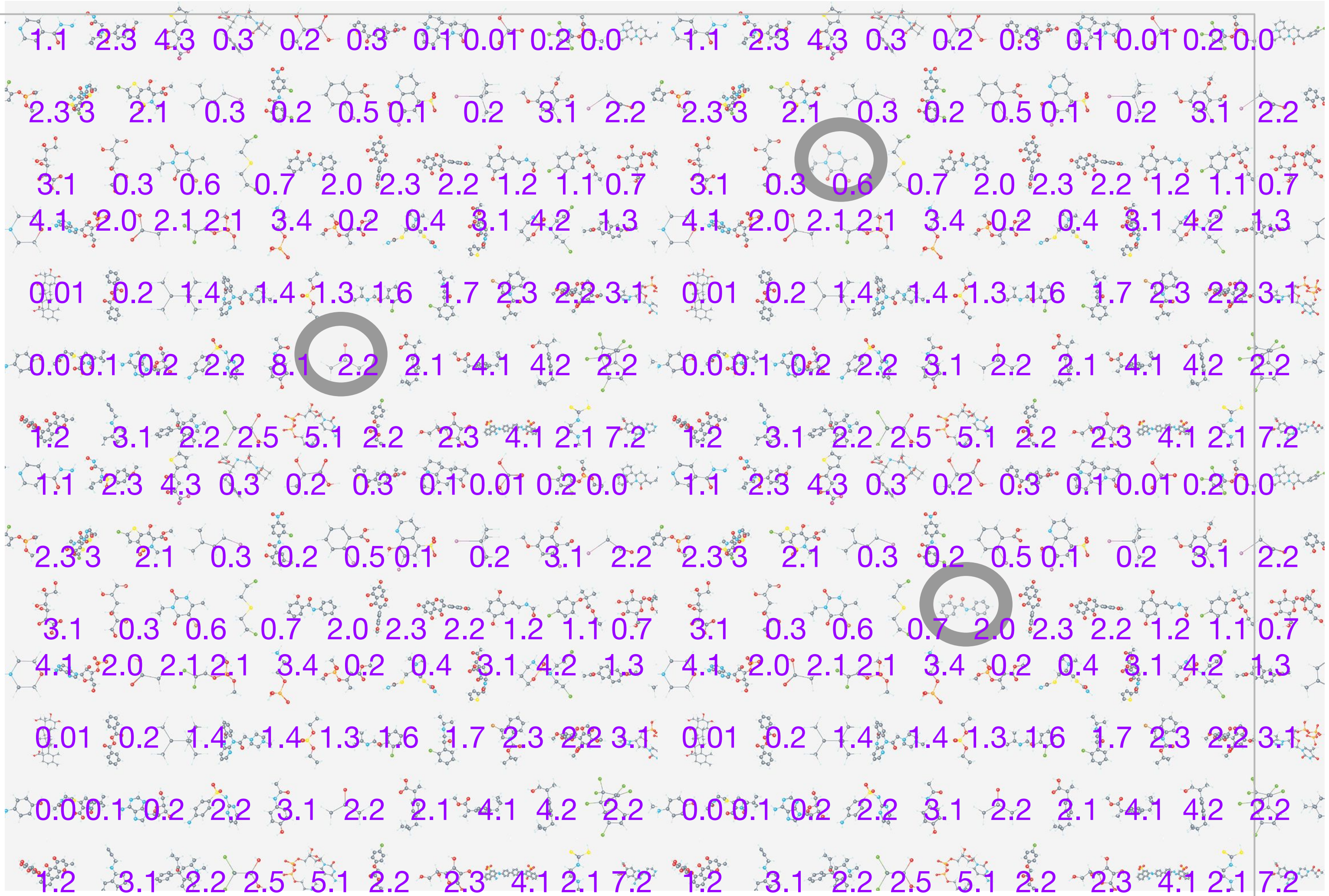

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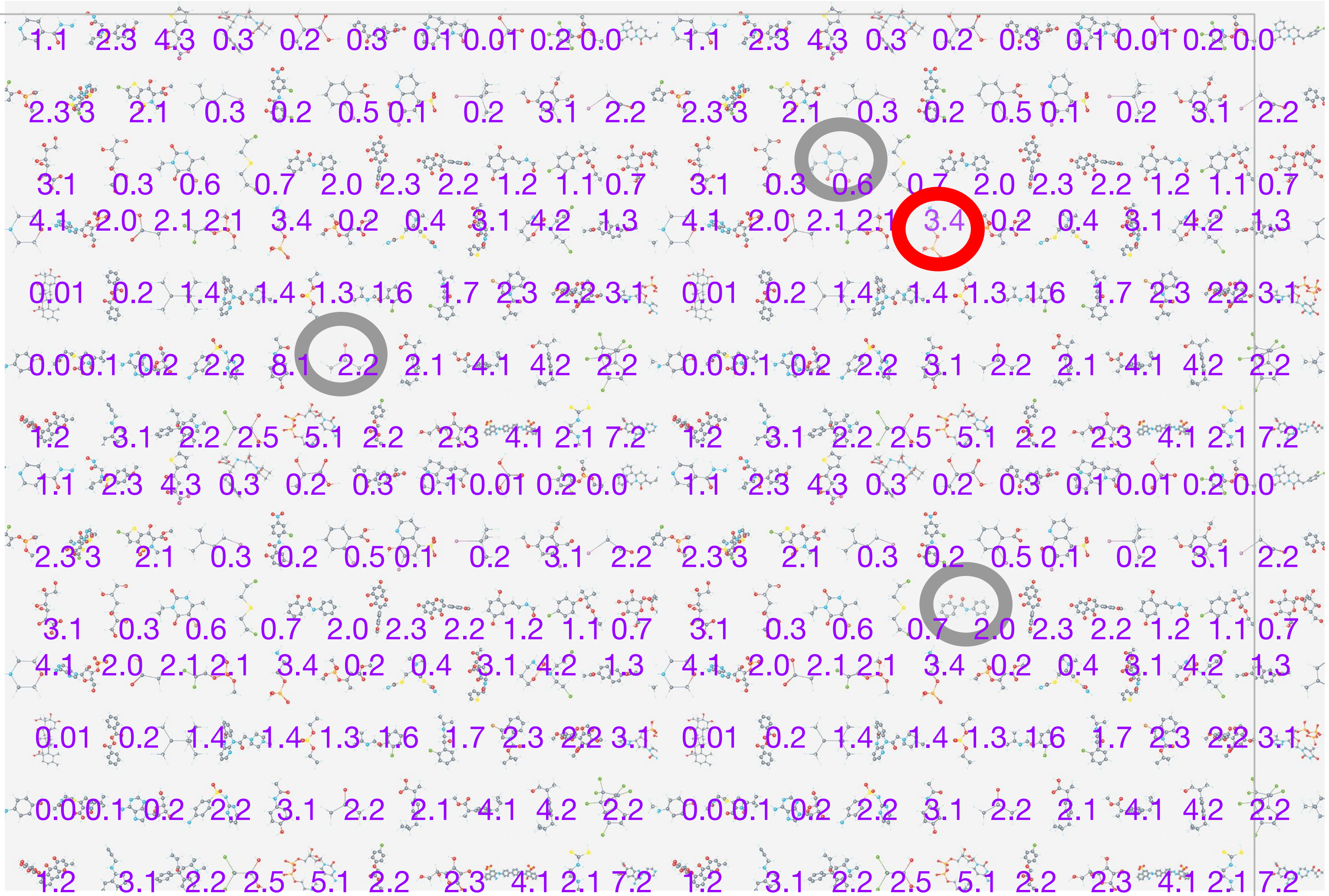

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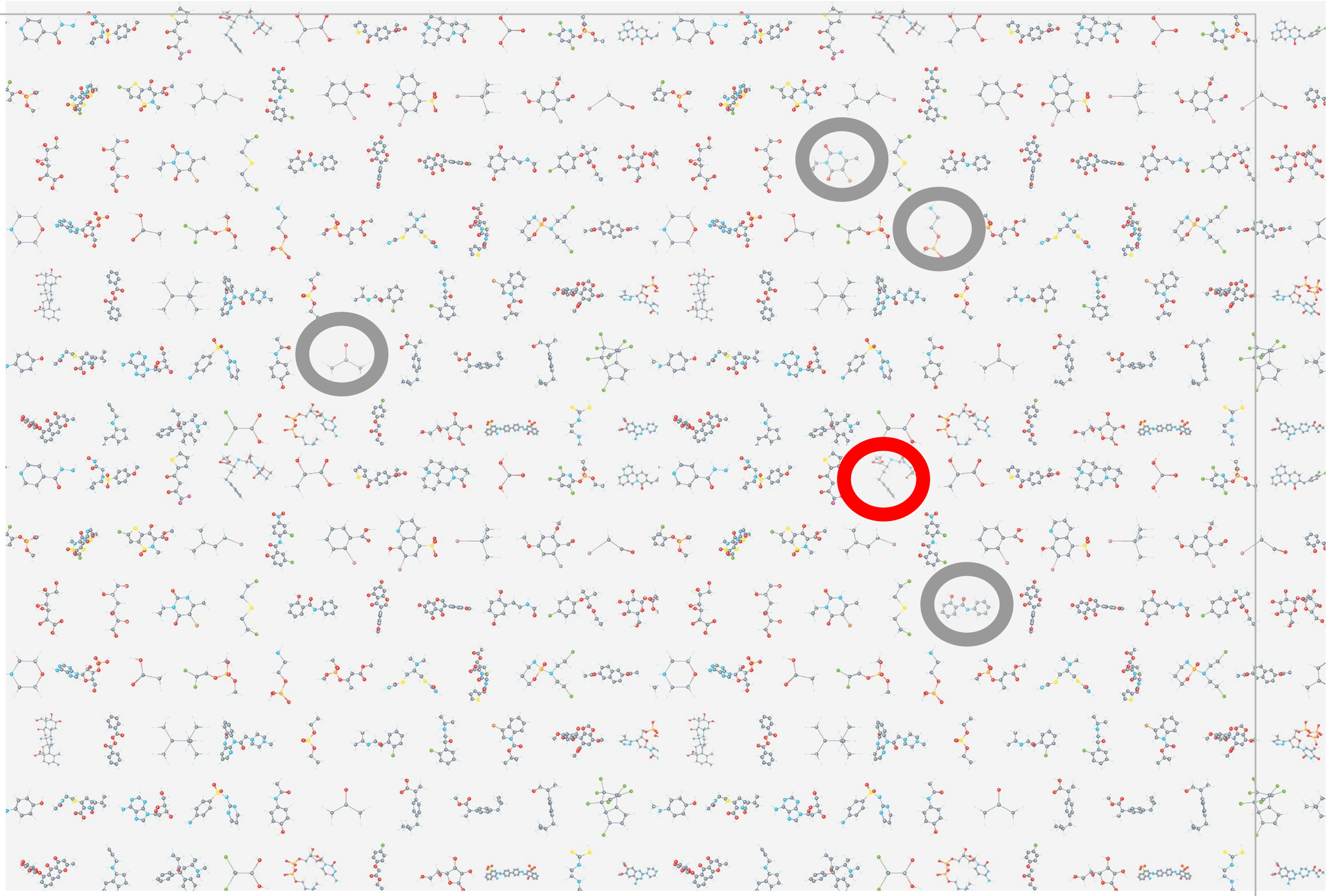

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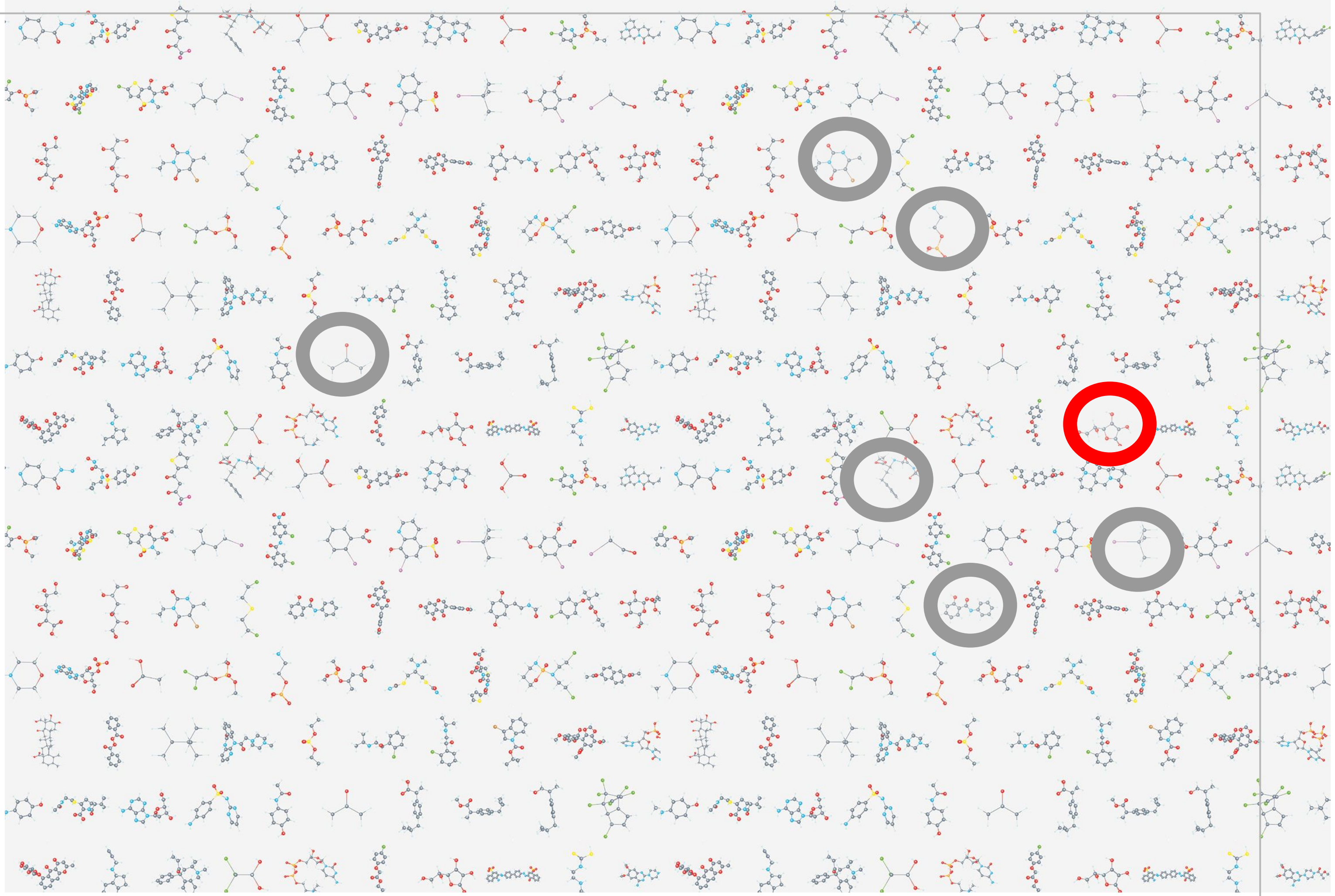

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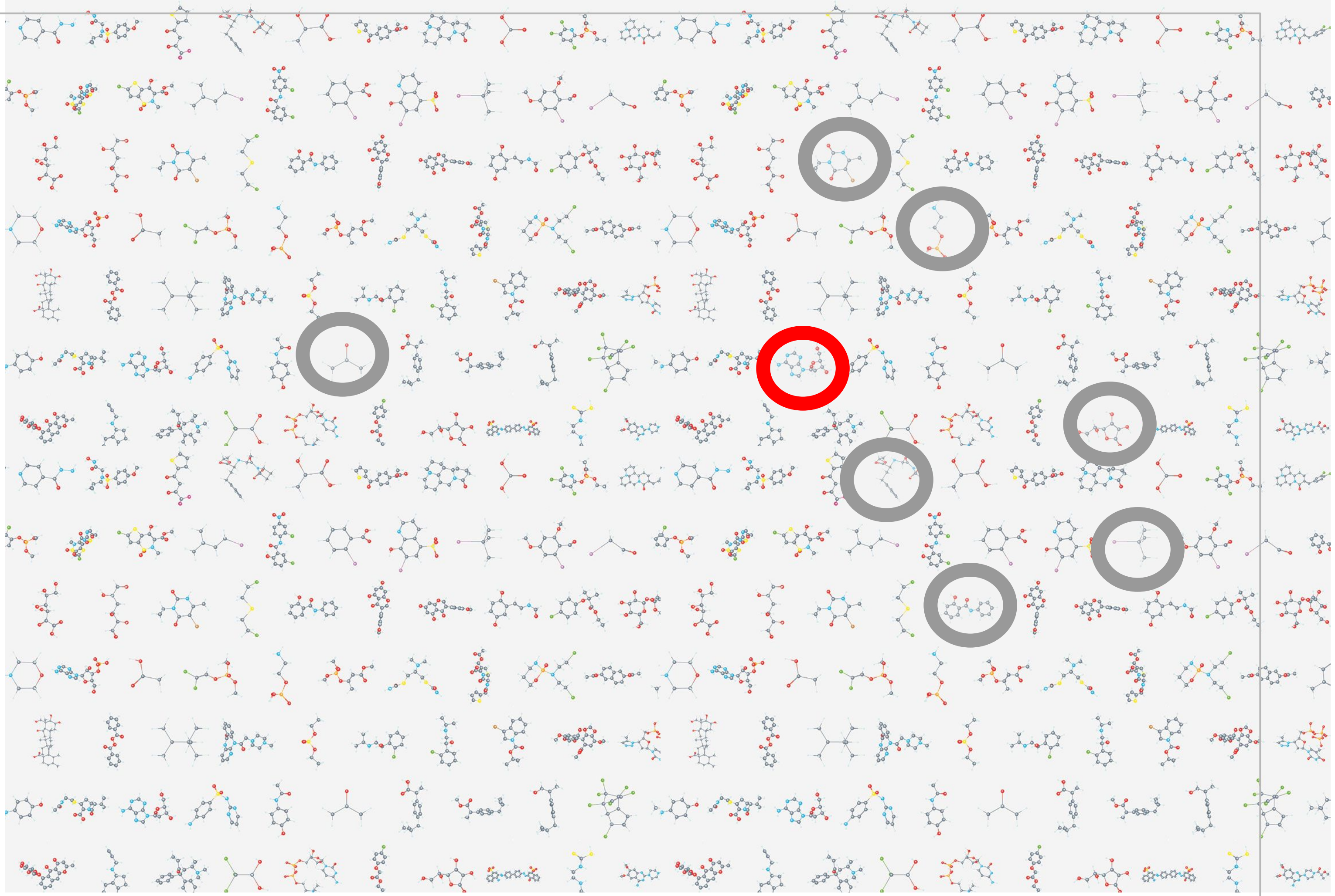

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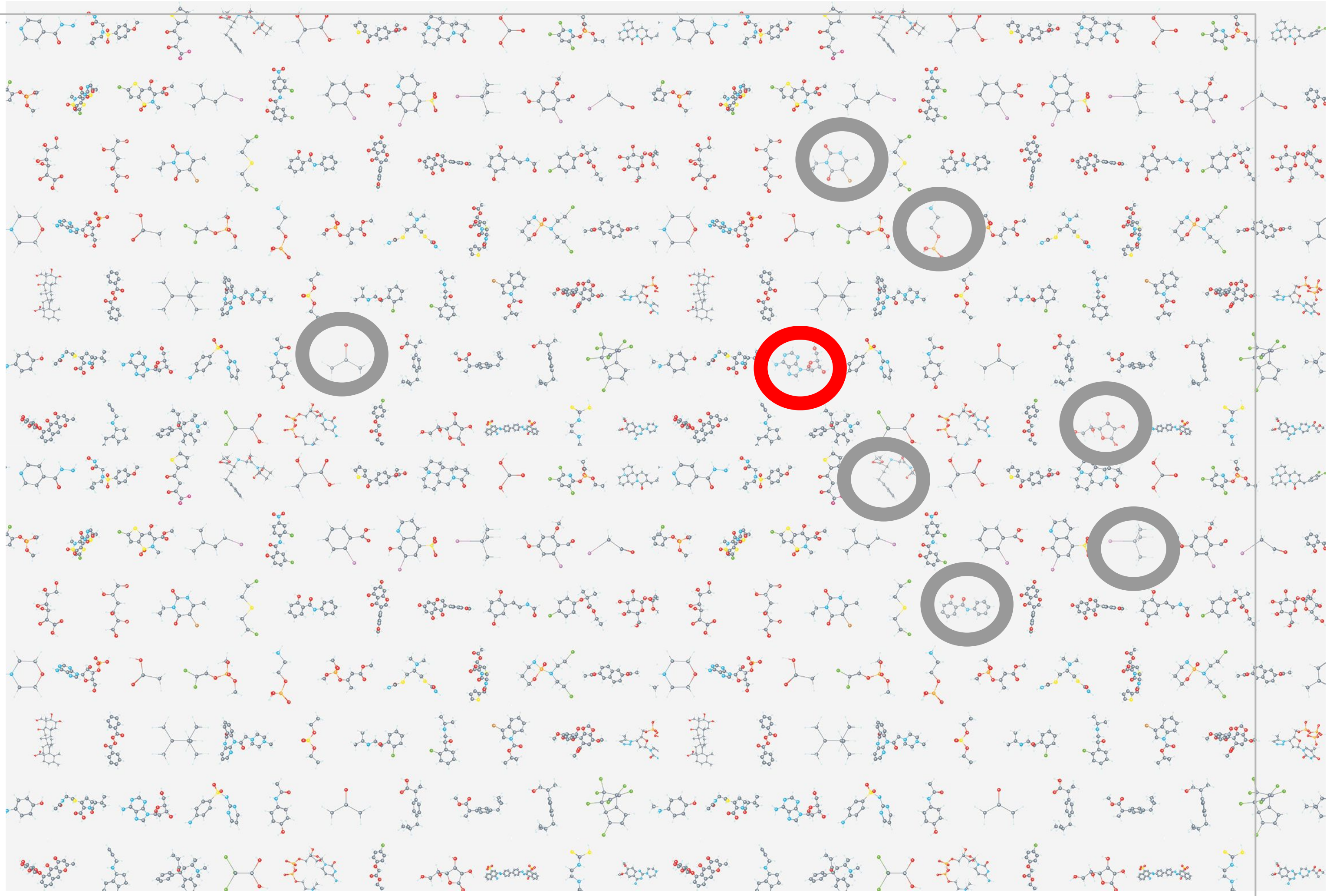
And so on ………



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

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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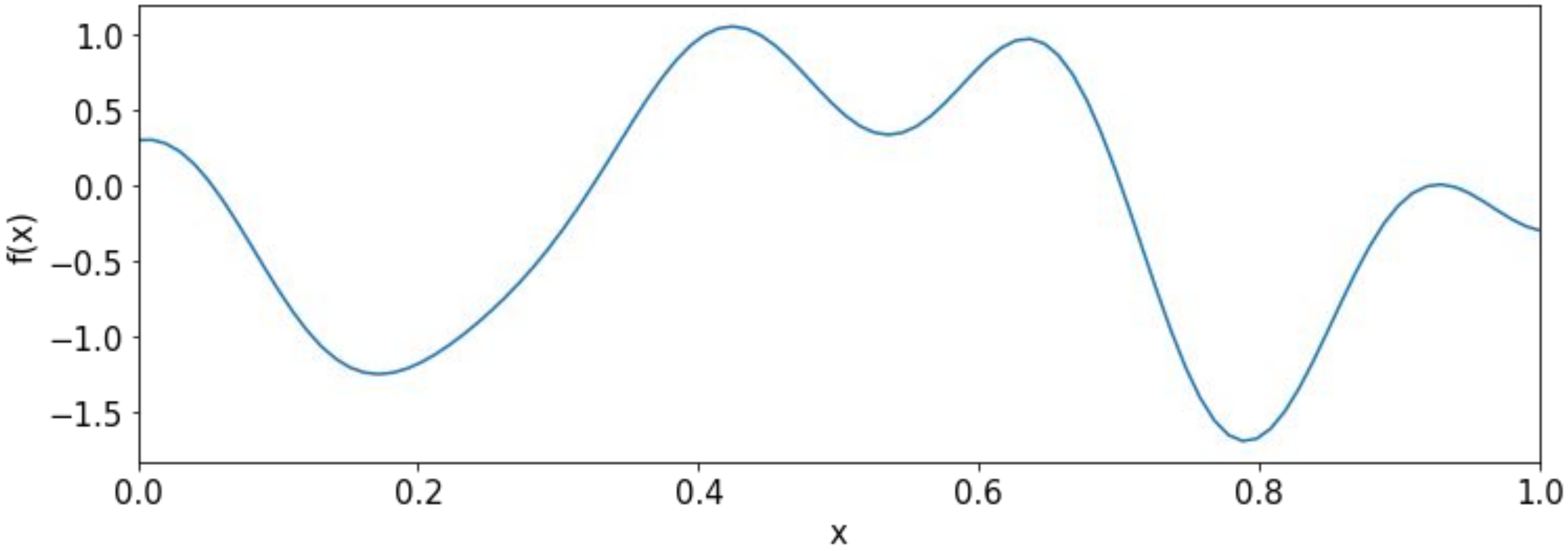

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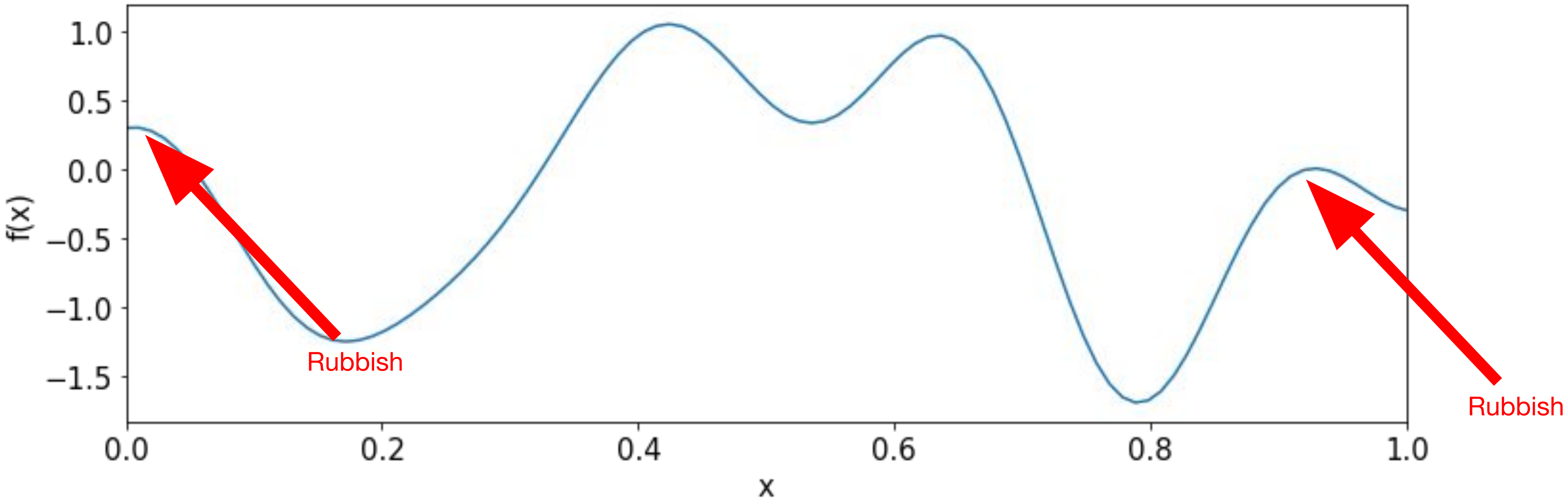

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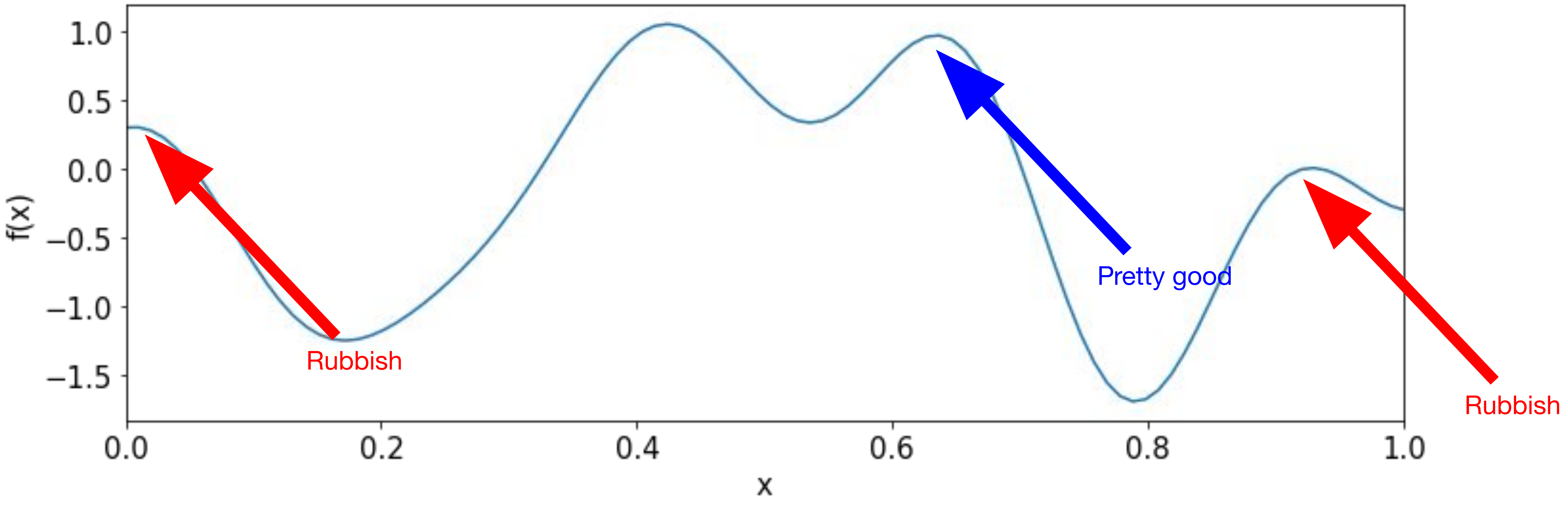

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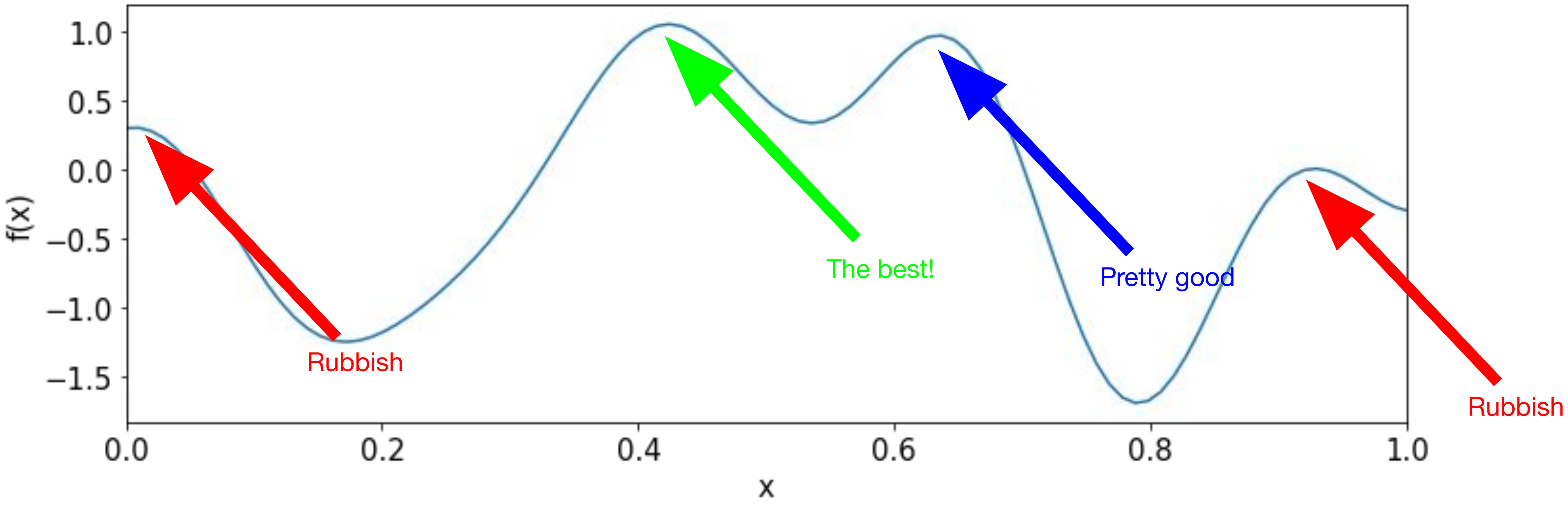
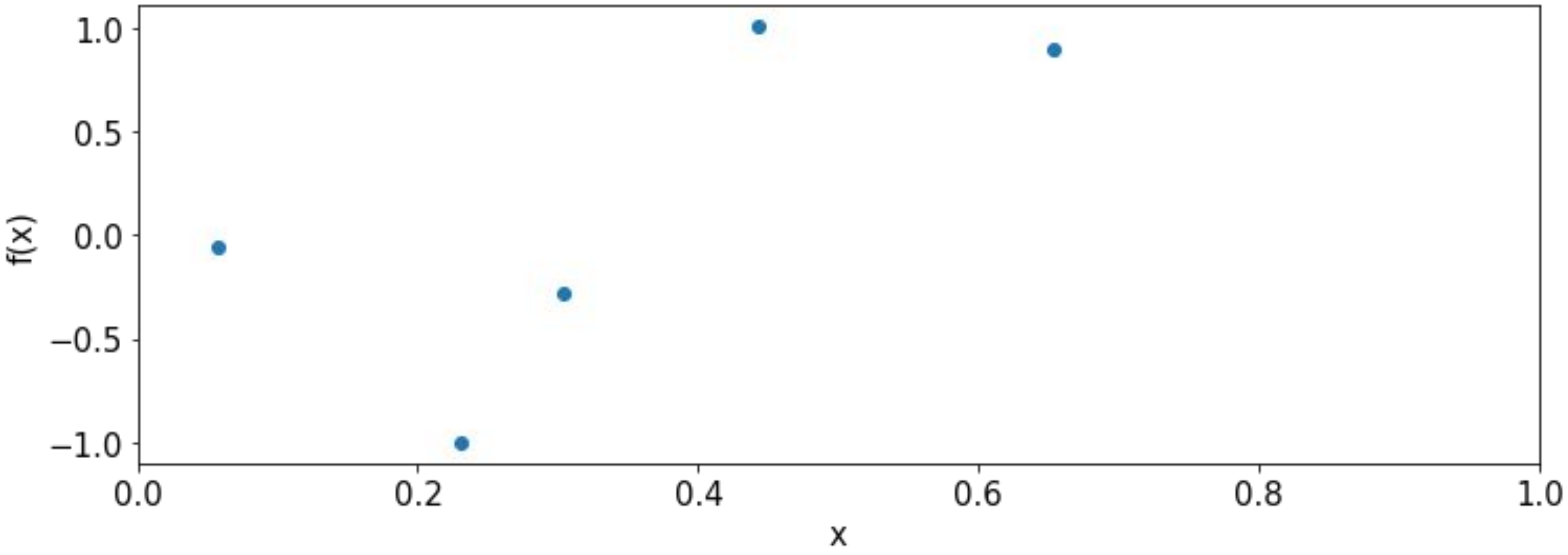


BO Demo

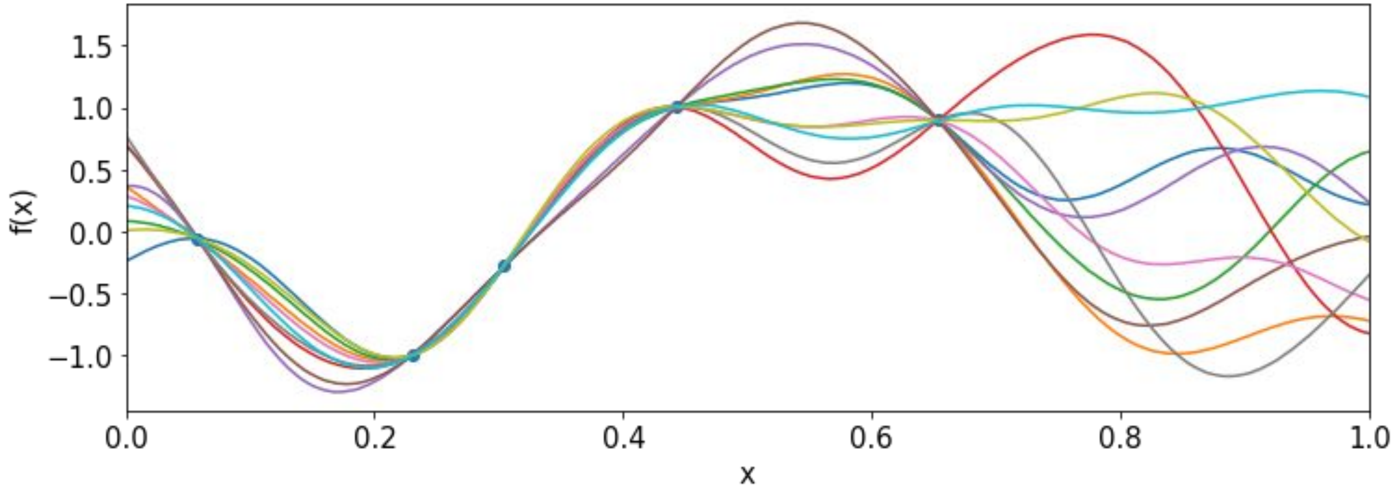
Suppose we make 5 evaluations

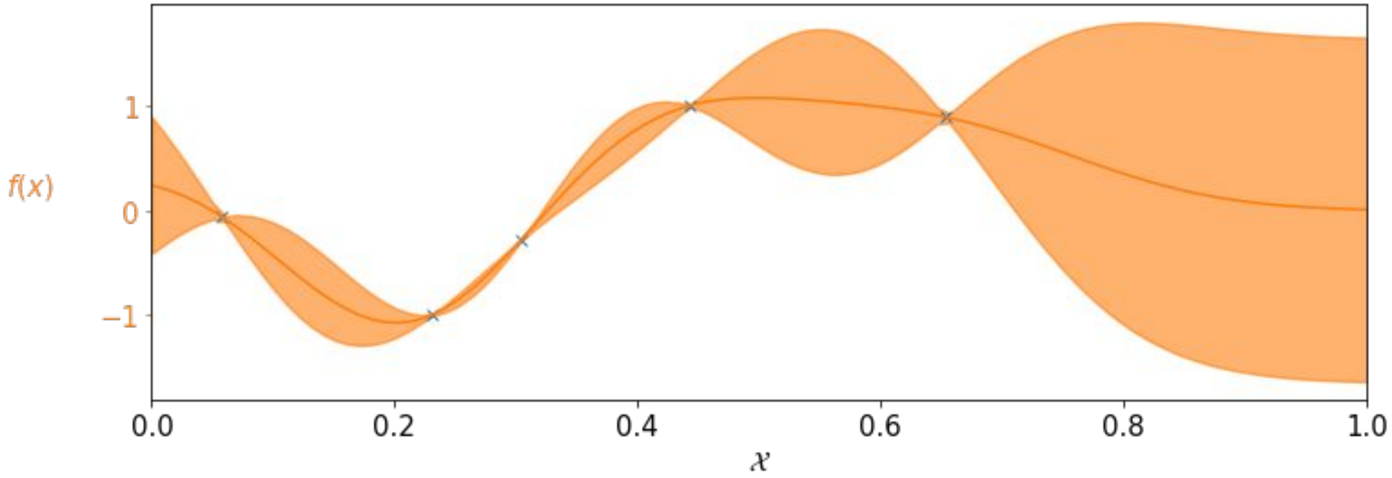


Where should we next evaluate? Explore/Exploit?

How to automate BO: step 1

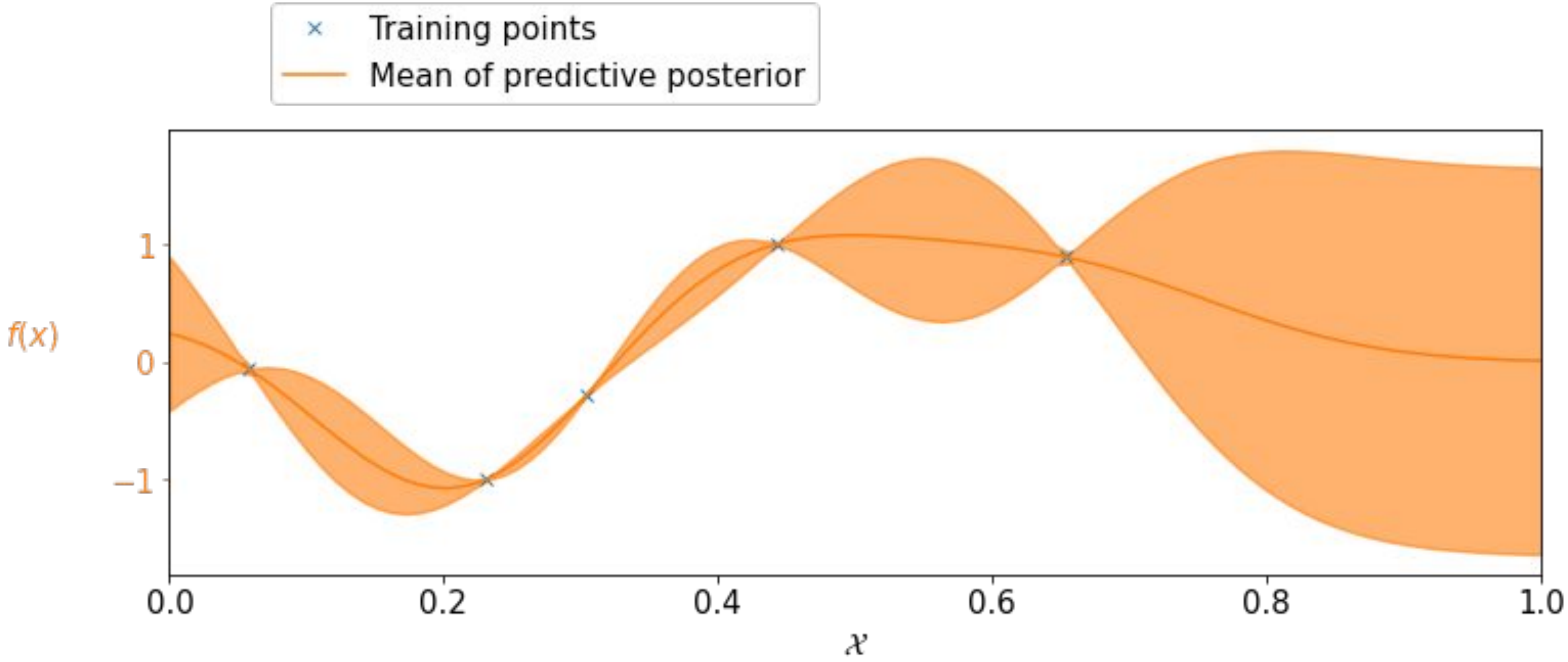
Use a statistical model like a Gaussian process





How to automate BO: step 2

Automated decision making via an acquisition function like expected improvement



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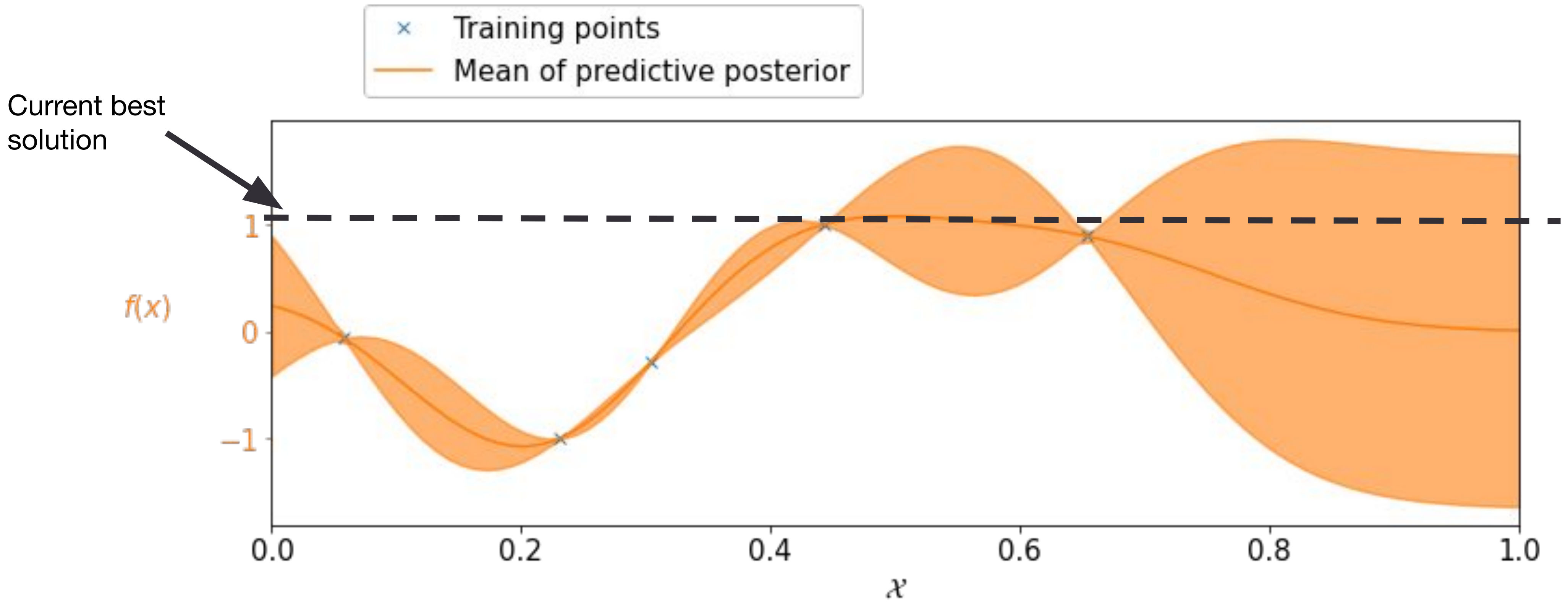

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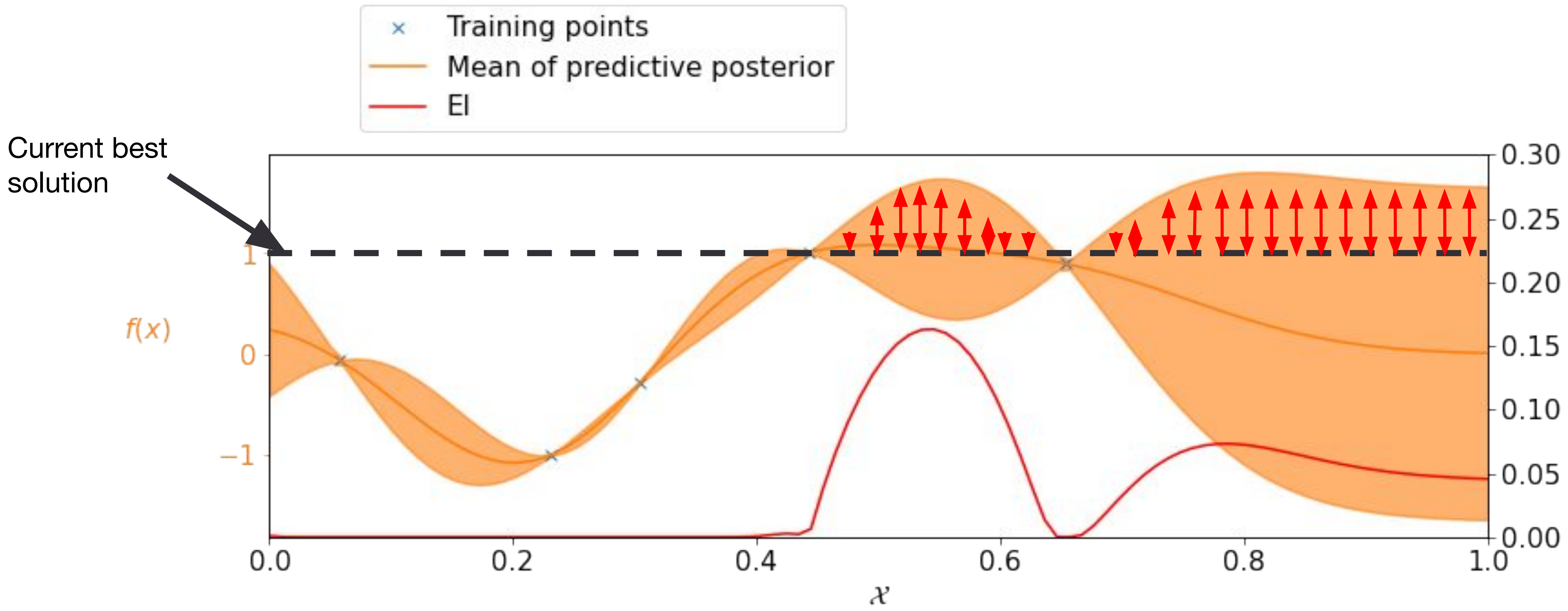

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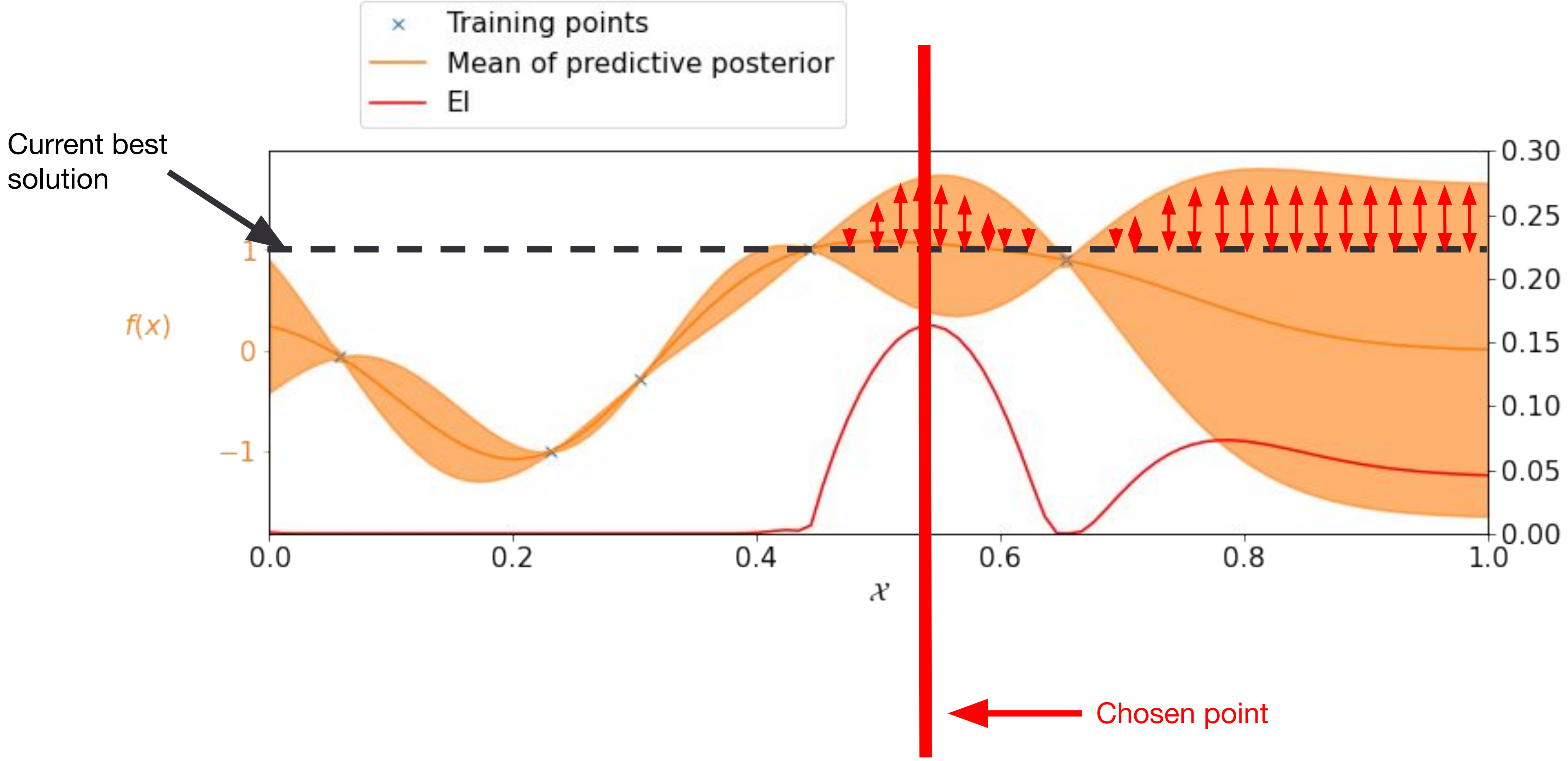
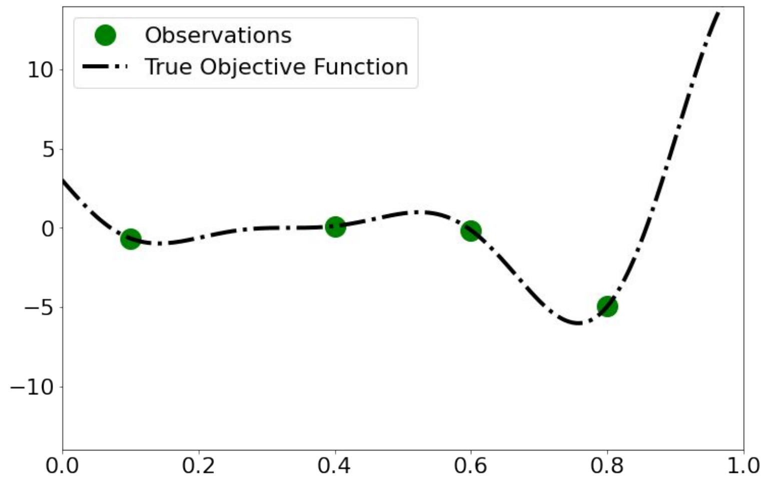


Expected Improvement

Demo BO loop



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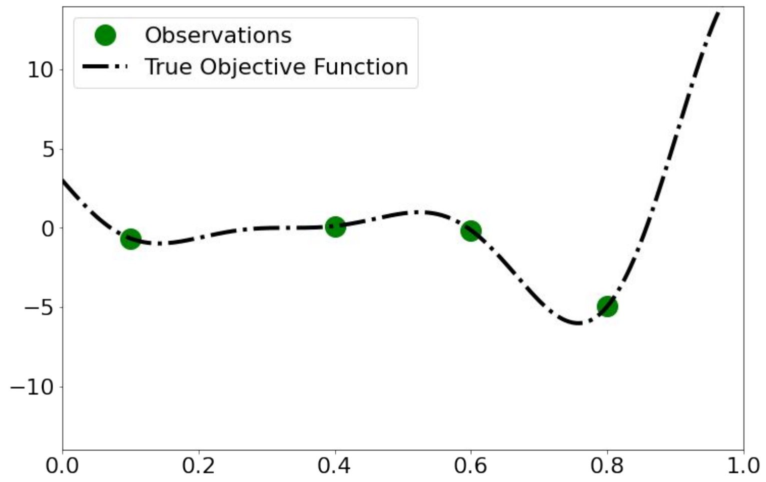

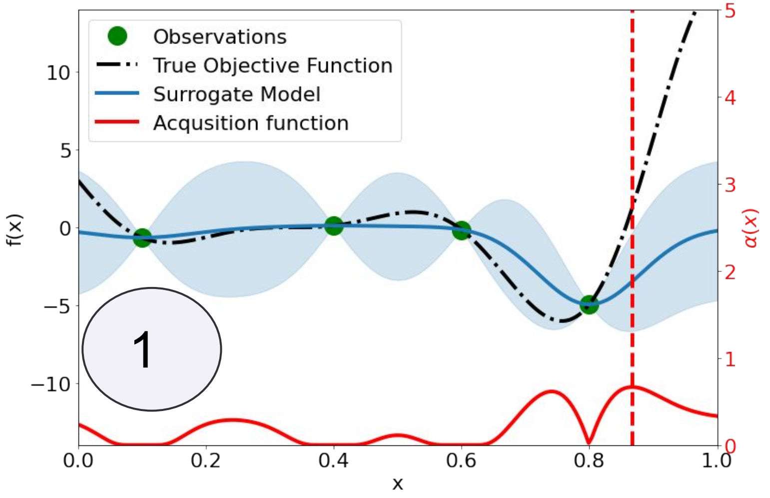

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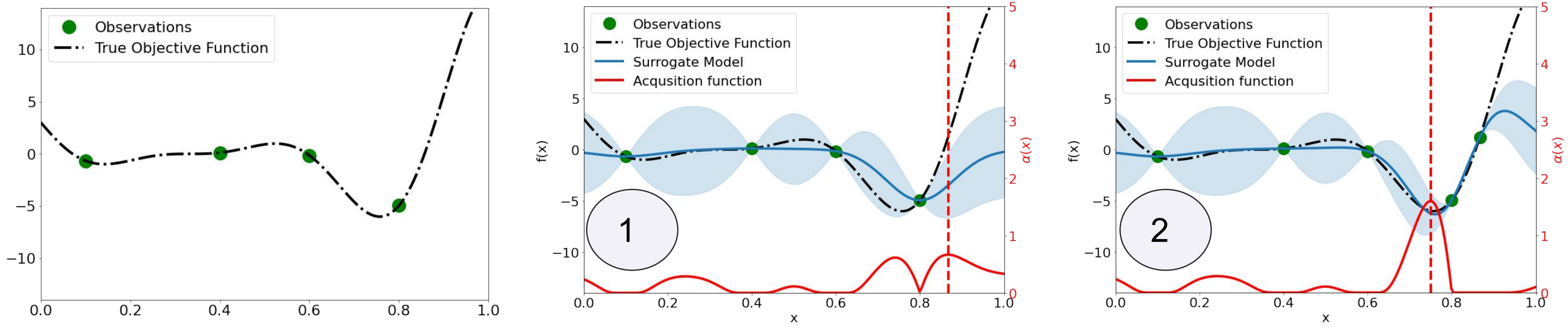

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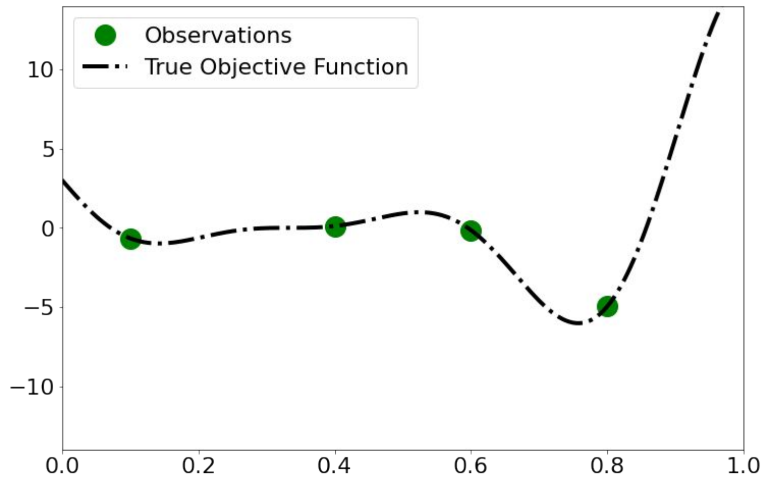

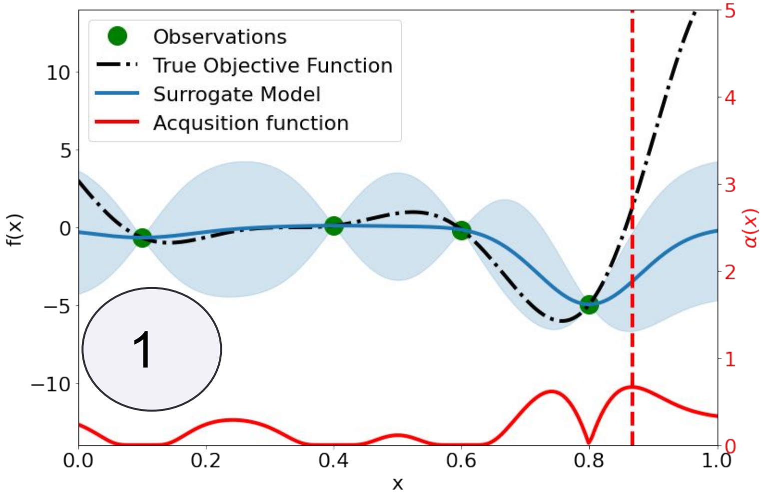

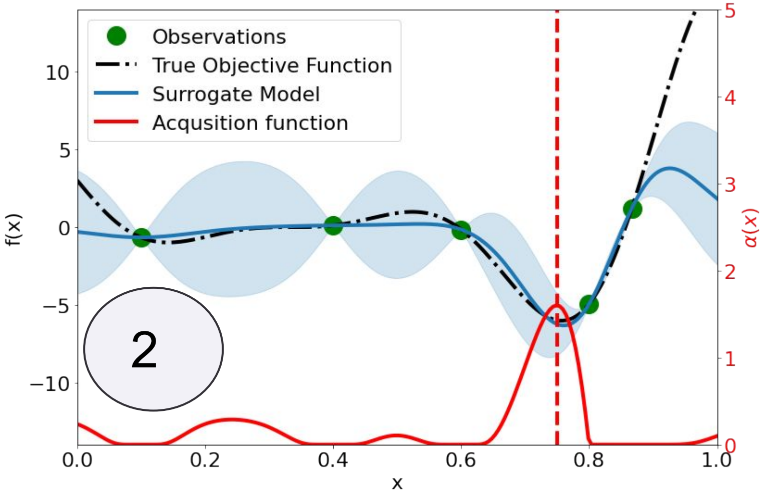

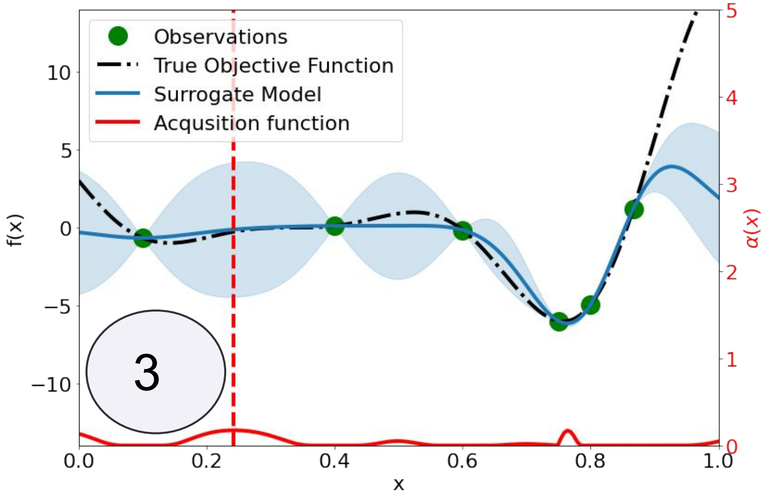

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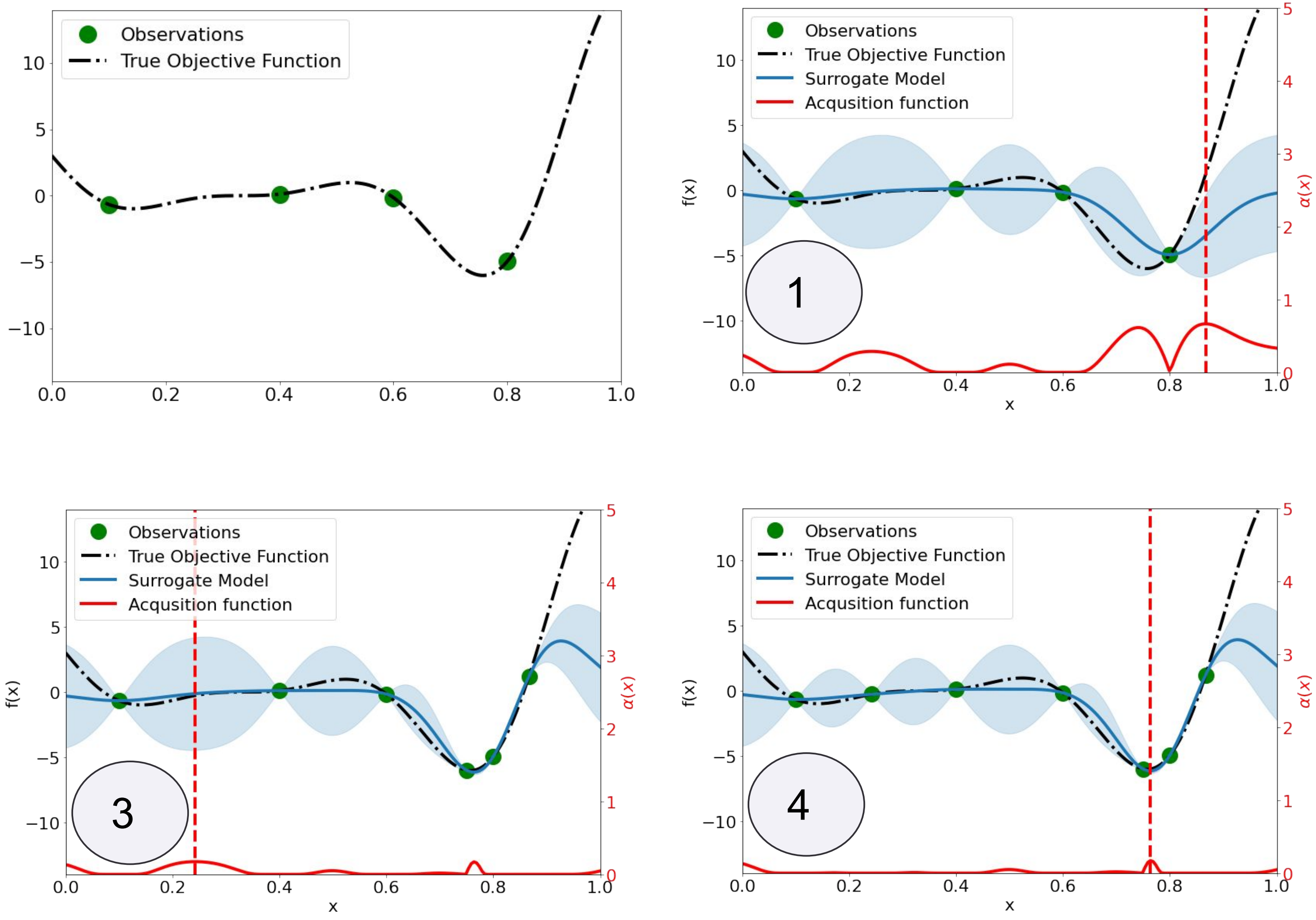

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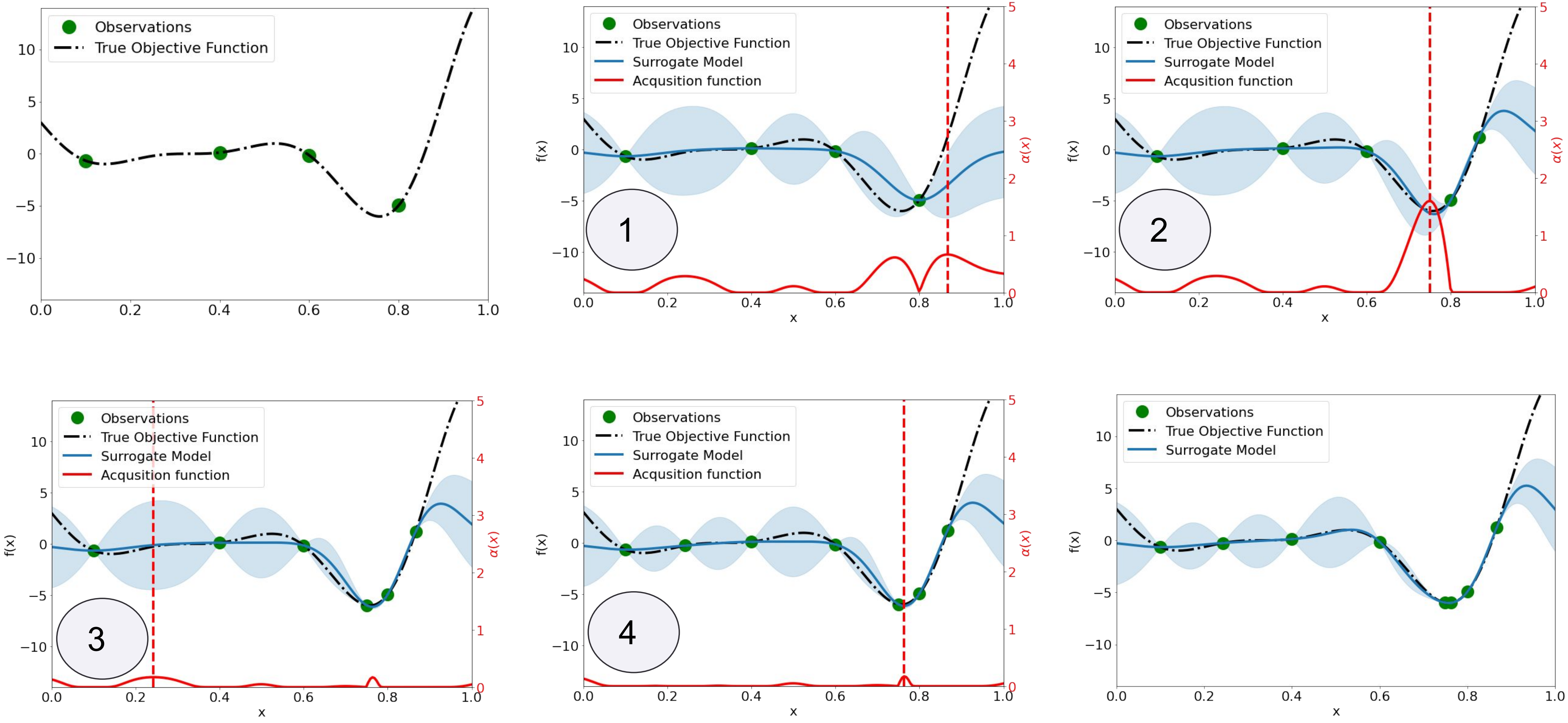
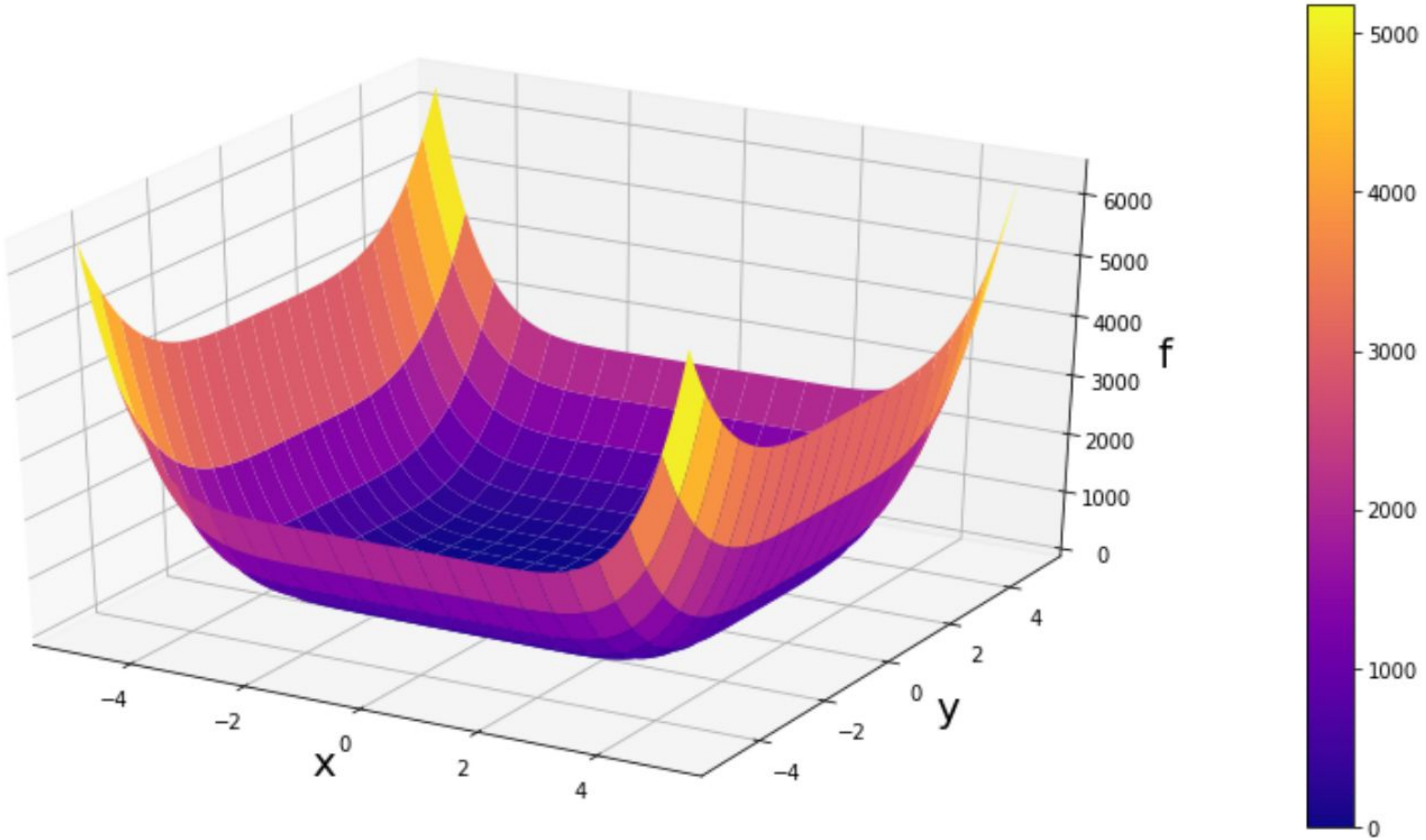


BO Demo 2

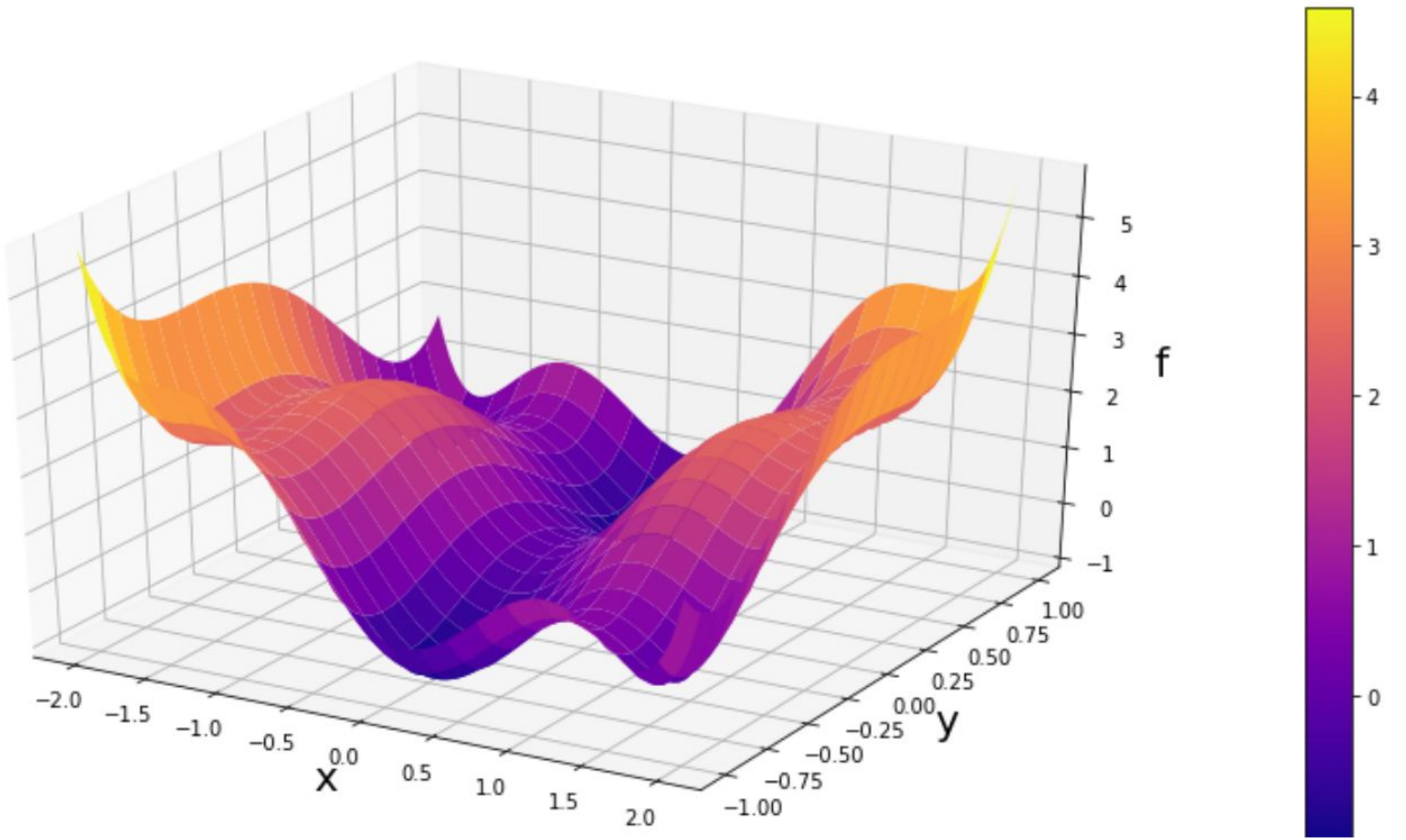
Let minimize the 6 Hump Camel function



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

BO Demo 2

Zoom in: Perhaps not quite as easy?



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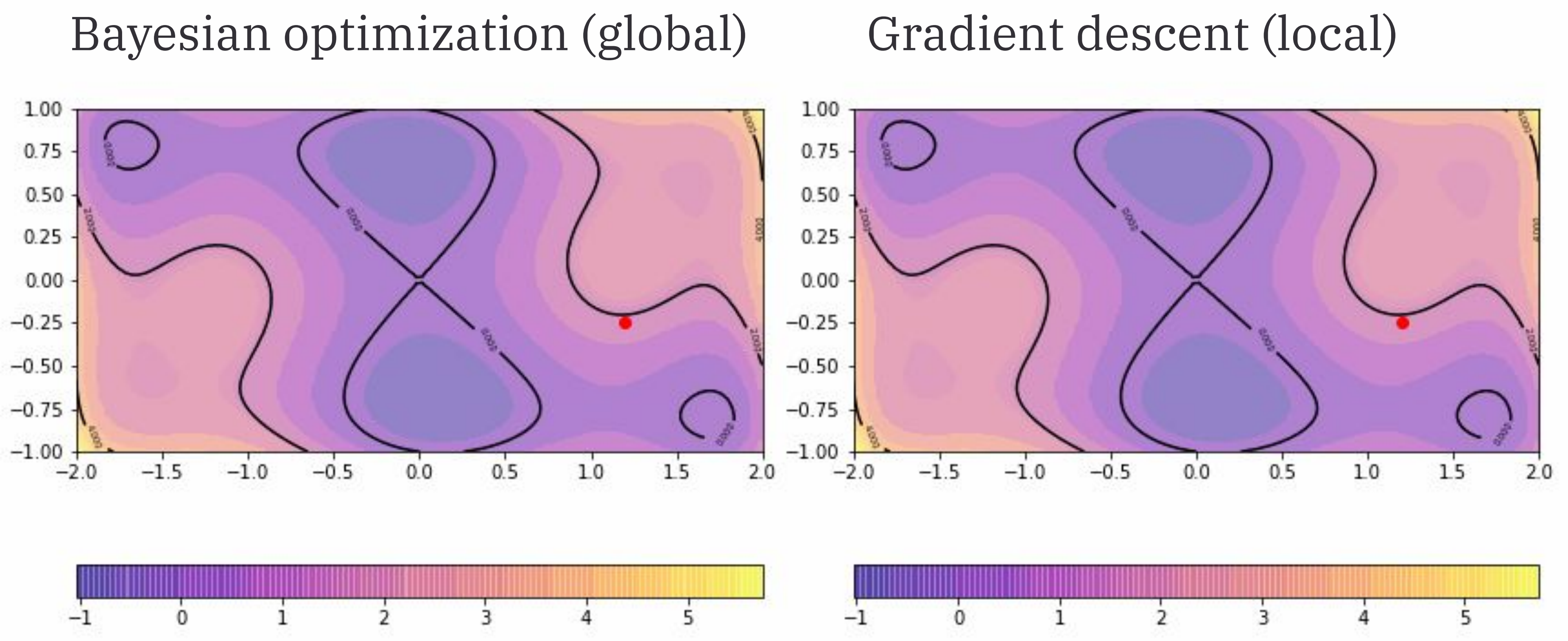
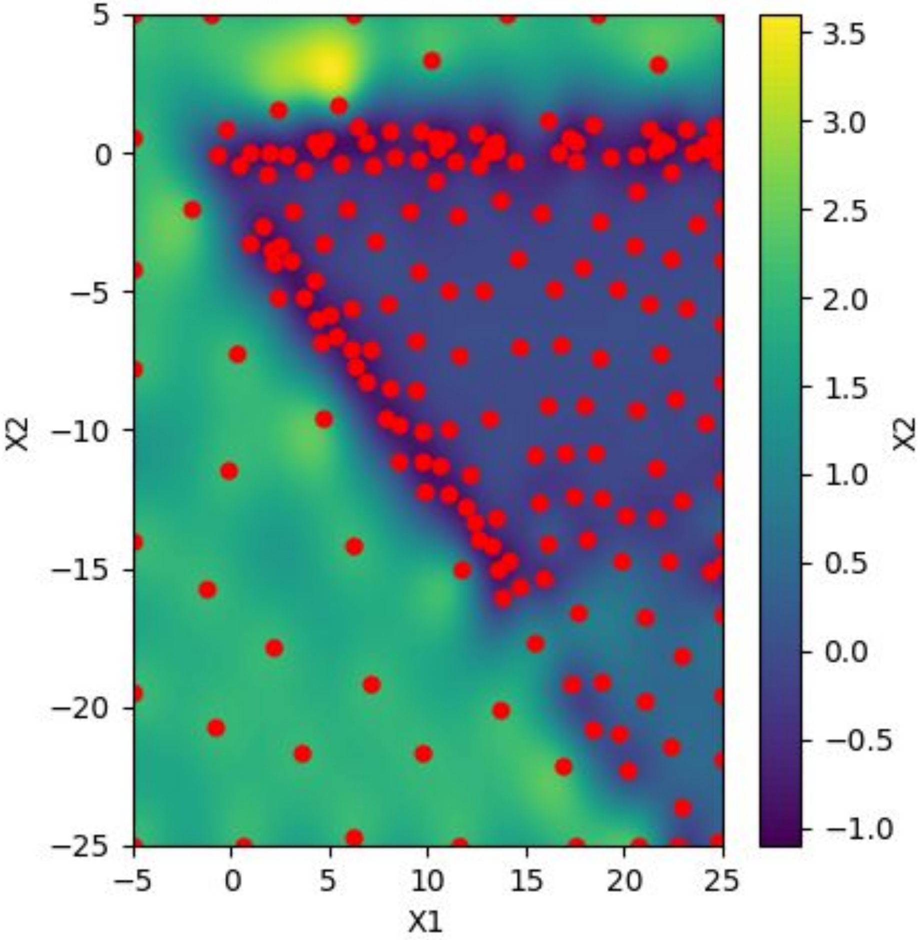
BO Demo 2

Bayesian optimization is a global optimizer



BO Demo 3

Efficient coverage of the search space



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BO: clever modelling rather than brute force!

Cool things that you can do with BO

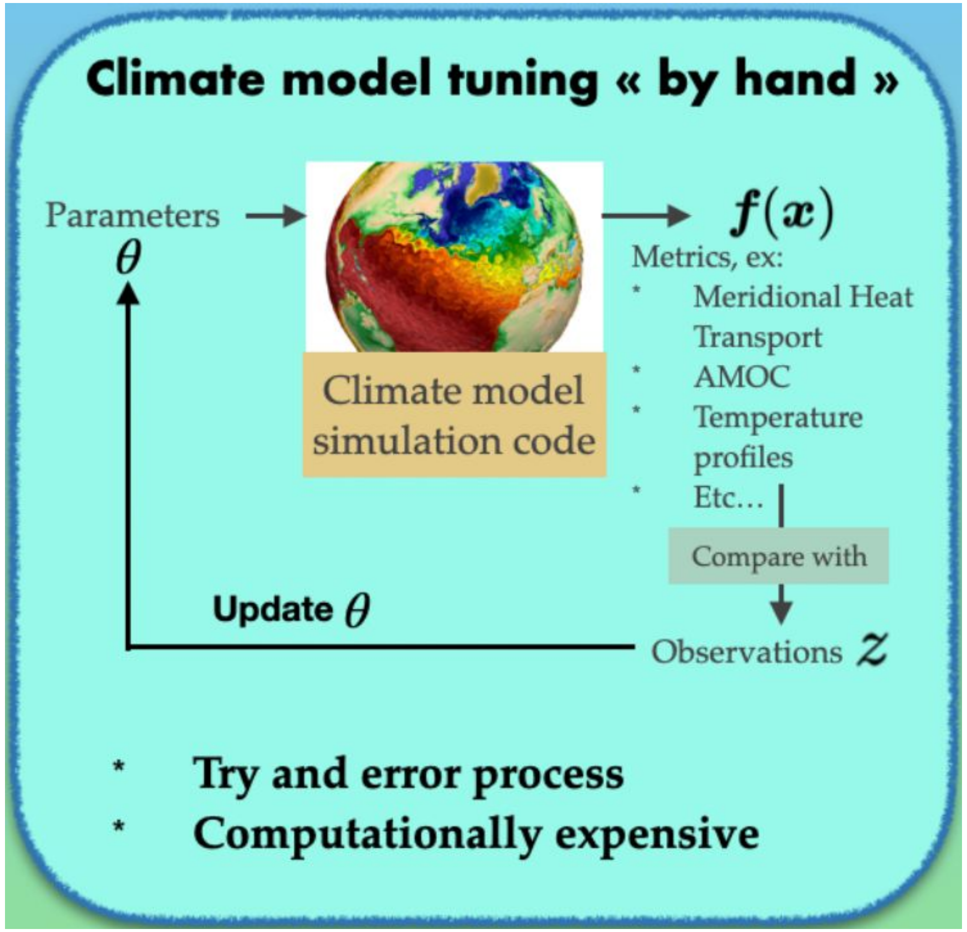
- Fine-tune the performance of AlphaGO (https://arxiv.org/abs/1812.06855)
- Allow Amazon Alexa learn how to speak with new voices (https://arxiv.org/abs/2002.01953)
- Efficiently find new molecules / genes (https://arxiv.org/abs/2010.00979)
- Fine-tune electric car engines
- Optimize large climate models

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

So, Climate model calibration?

Climate model calibration

Identifying reasonable values for model parameters



Lguensat et al. 2022.

Climate model calibration

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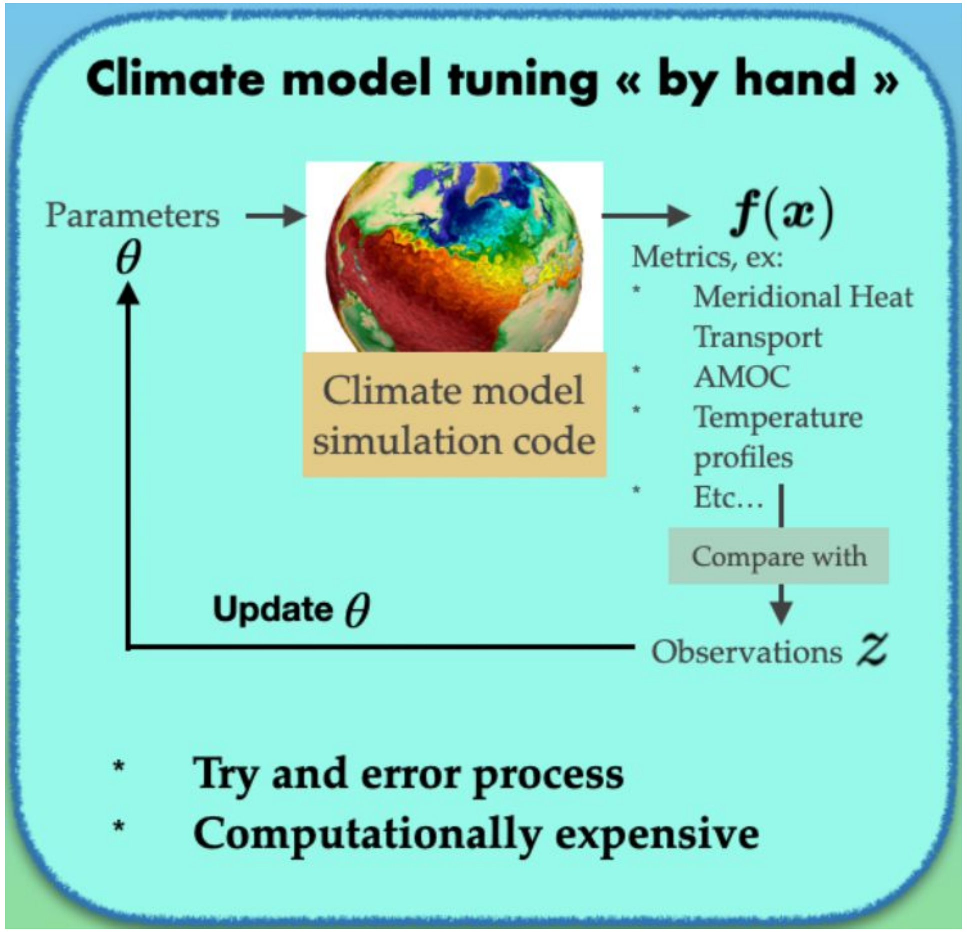

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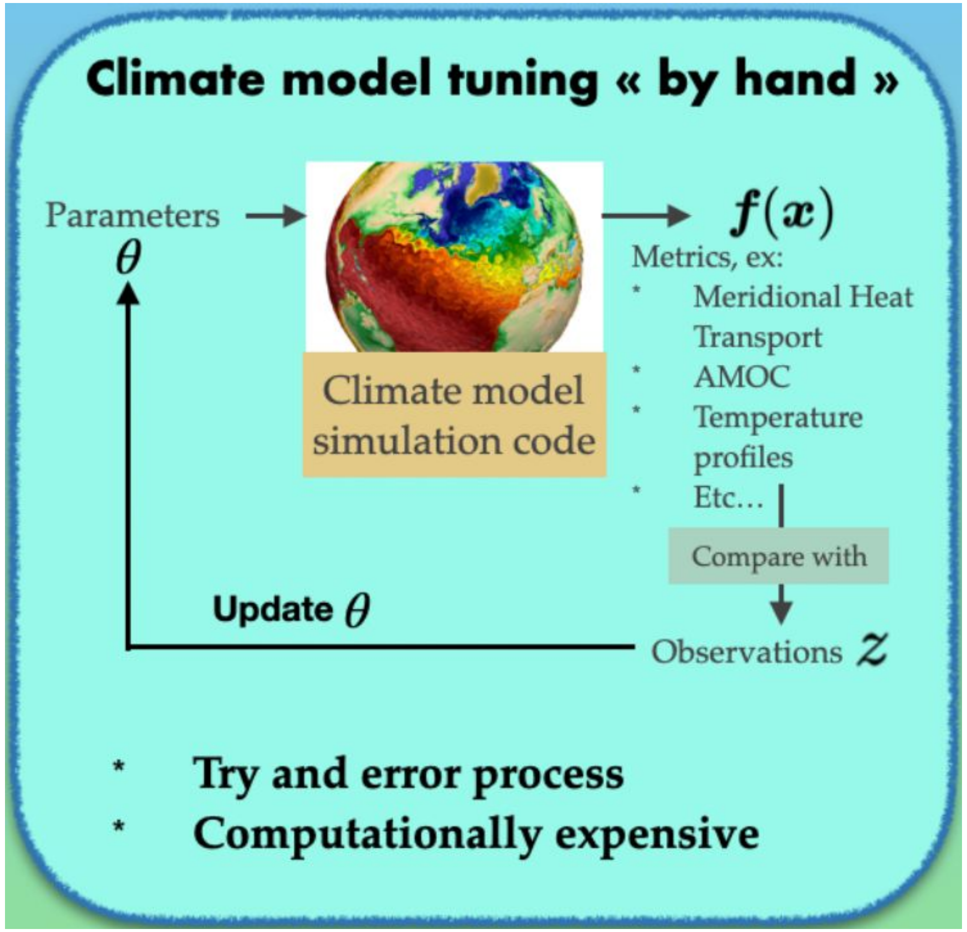

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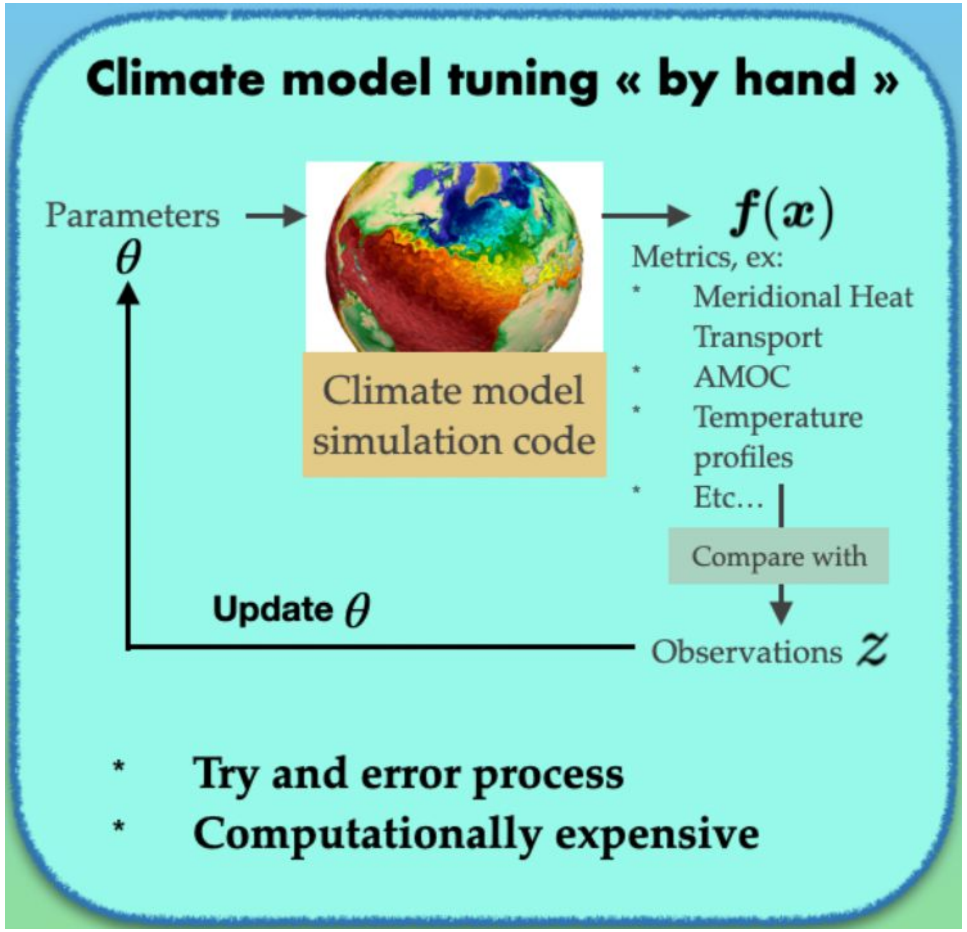

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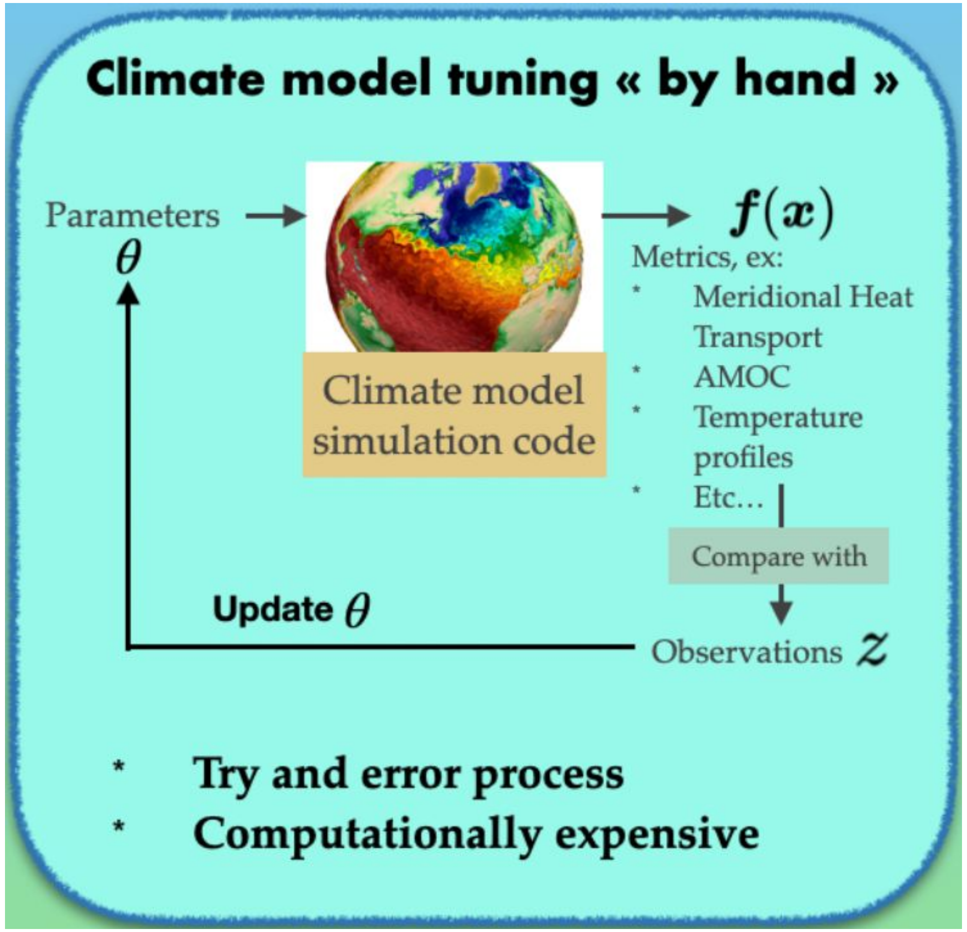
Climate model calibration

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.

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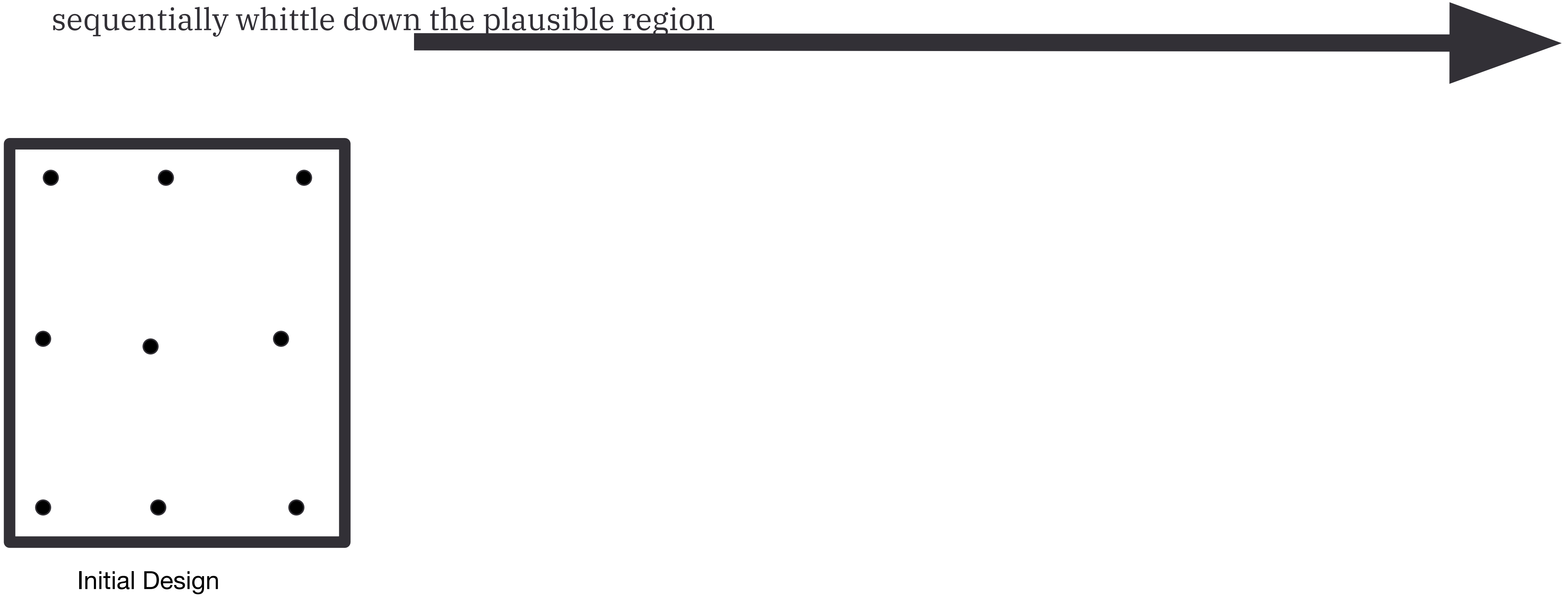

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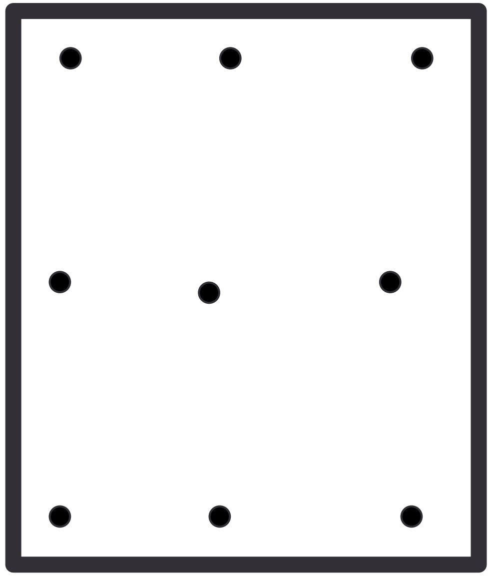
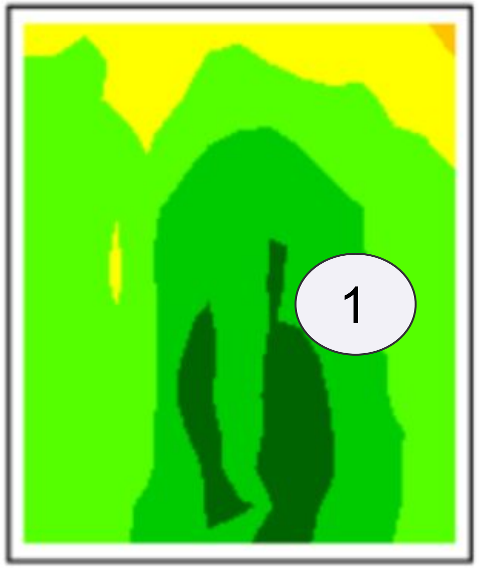


Initial Design



Predicted implausibility

Based on Lguensat et al. 2022.

Climate model calibration by iteratively refocusing

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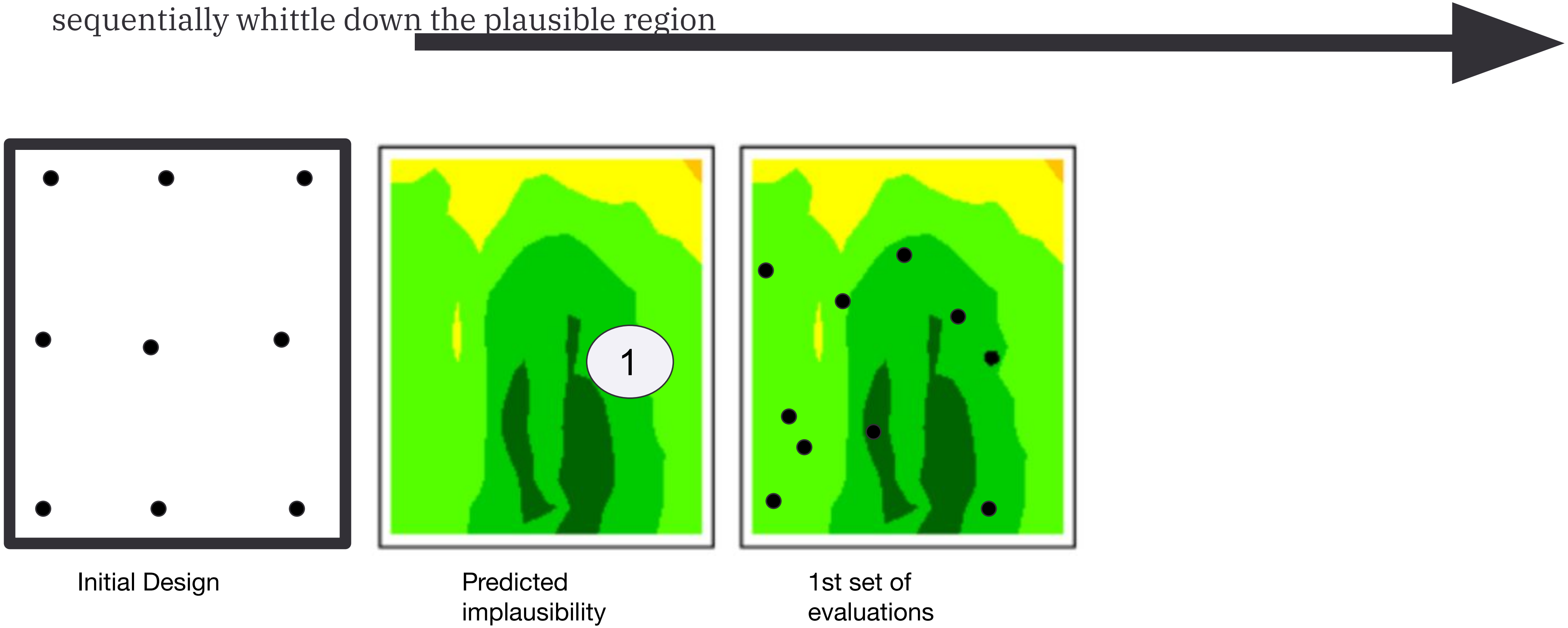

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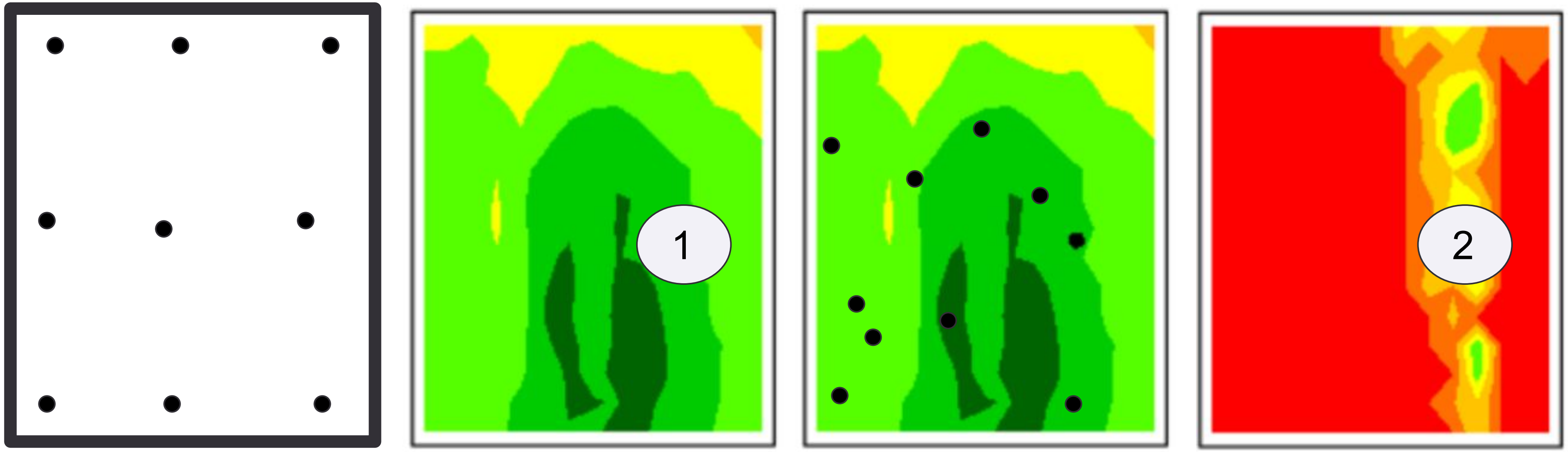

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1st set of evaluations

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Climate model calibration by iteratively refocusing

sequentially whittle down the plausible region

Initial Design

Predicted implausibility

1st set of evaluations

Predicted implausibility

2nd set of evaluations

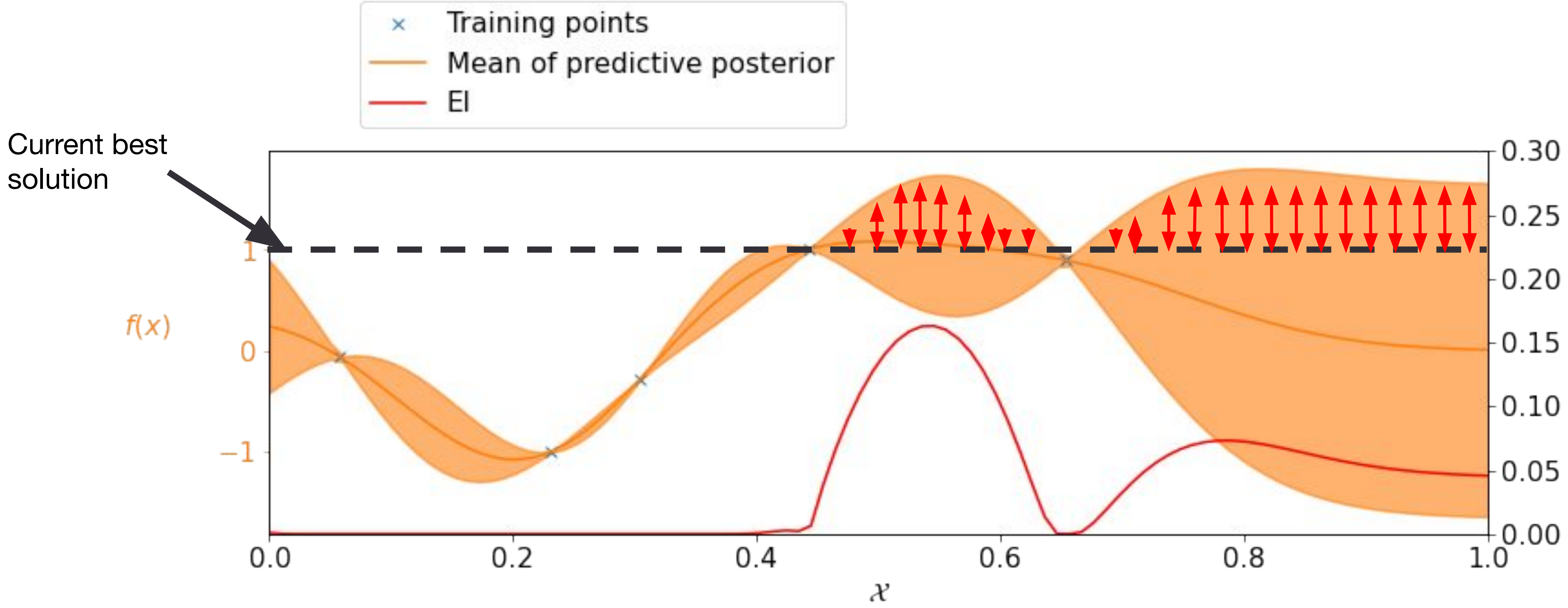
Based on Lguensat et al. 2022.

Back to molecular design

Large batches

Automatically choosing batches of points

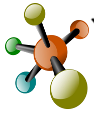
Using GP posteriors and utility functions



How to pick **3** points ?

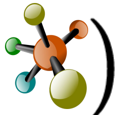
Automatically choosing batches of molecules

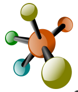
Using GP posteriors and utility functions

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

Automatically choosing batches of molecules

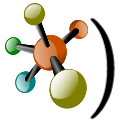
Using GP posteriors and utility functions

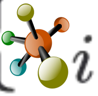
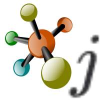
- $\alpha_{\mathrm{EI}}($$) = \mathbb{E}_f[\max(f - f^\star, 0)]$

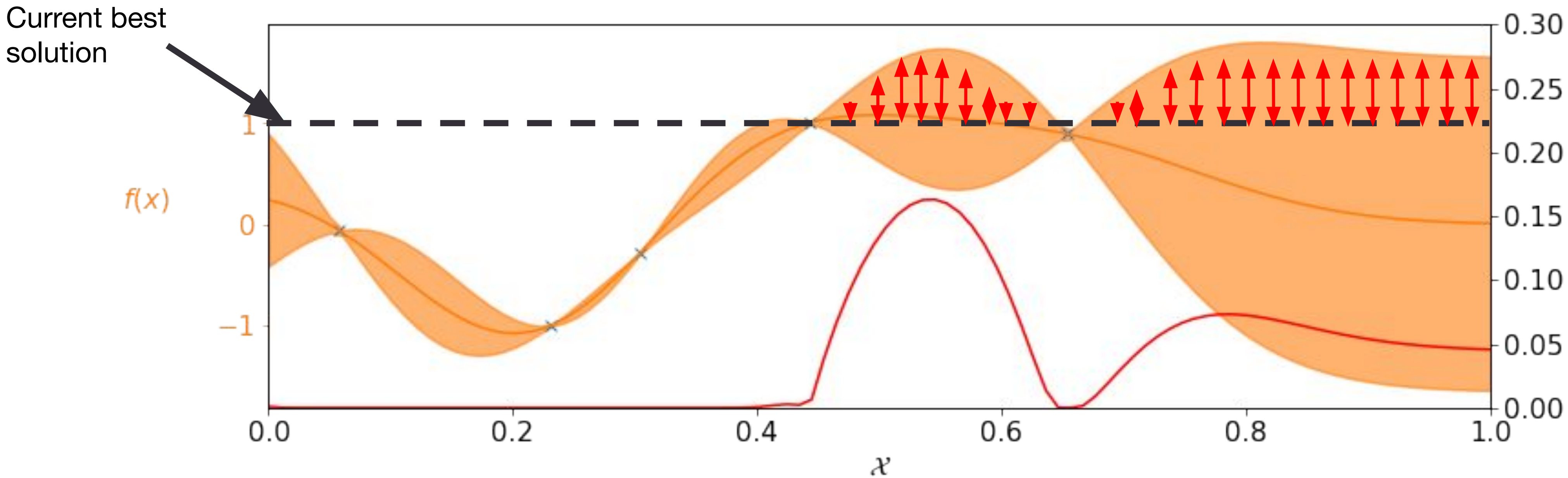
- $\alpha_{\mathrm{EI}}(\{$$_i,$$_j\}) = ???$

Automatically choosing batches of molecules

Using GP posteriors and utility functions

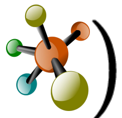
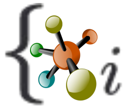
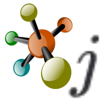
- $\alpha_{\mathrm{EI}}($  $) = \mathbb{E}_f[\max(f - f^\star, 0)]$

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



Automatically choosing batches of molecules

Using GP posteriors and utility functions

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

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

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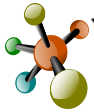
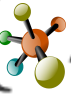
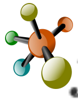
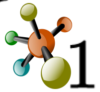
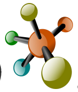
Automatically choosing batches of molecules

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)]$

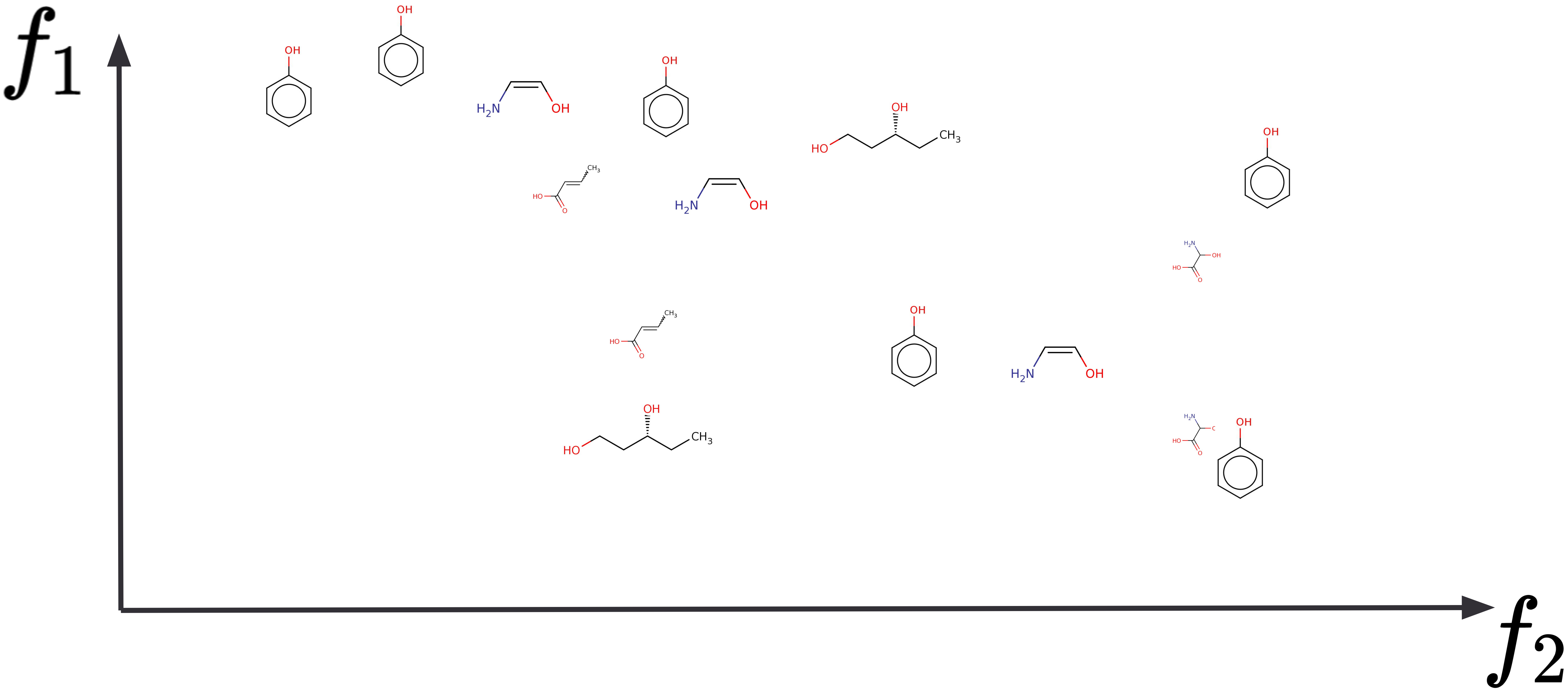
- $\alpha_{\mathrm{EI}}(\{$$_1, \ldots,$$_B\}) = ???$

Back to molecular design

Multiple objectives

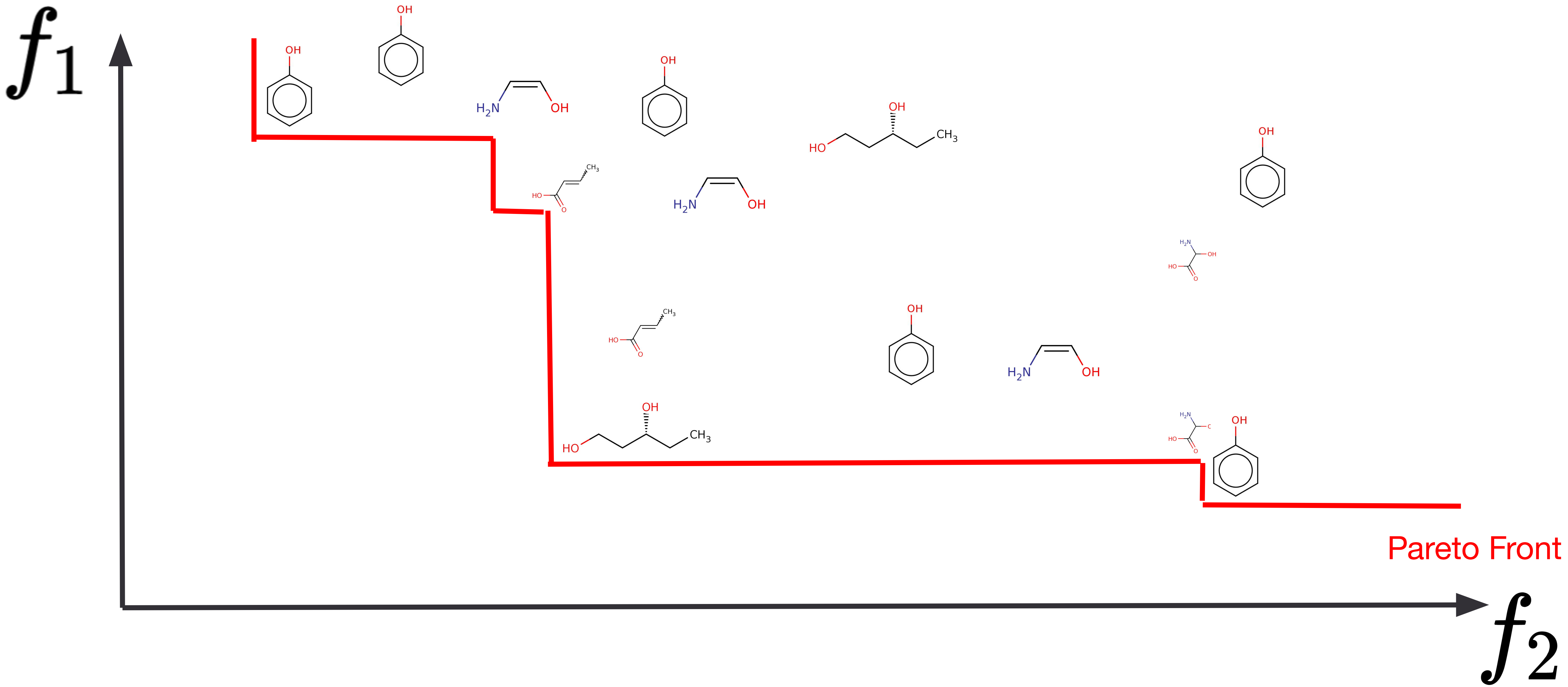
Multi-objective Optimisation

>1 competing objectives



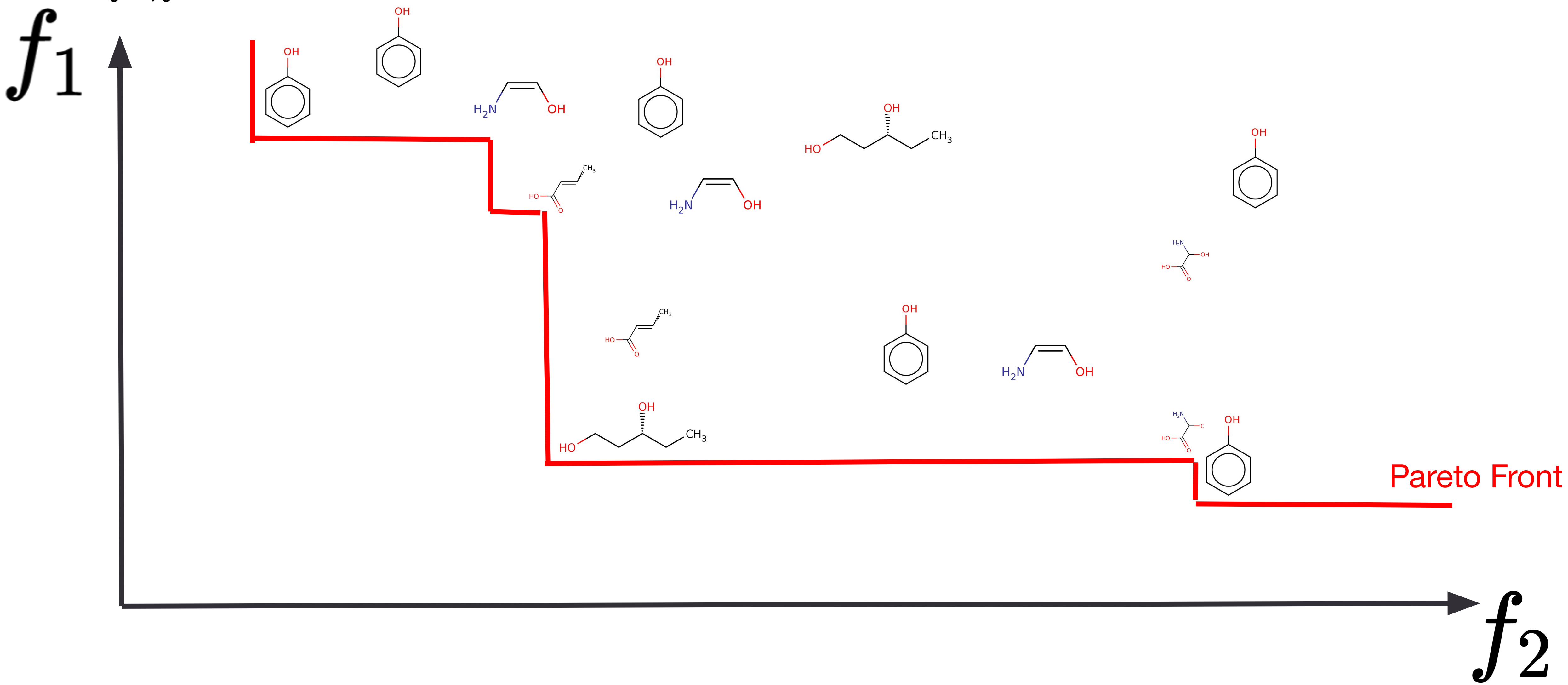
Multi-objective Optimisation

>1 competing objectives

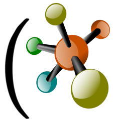
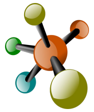


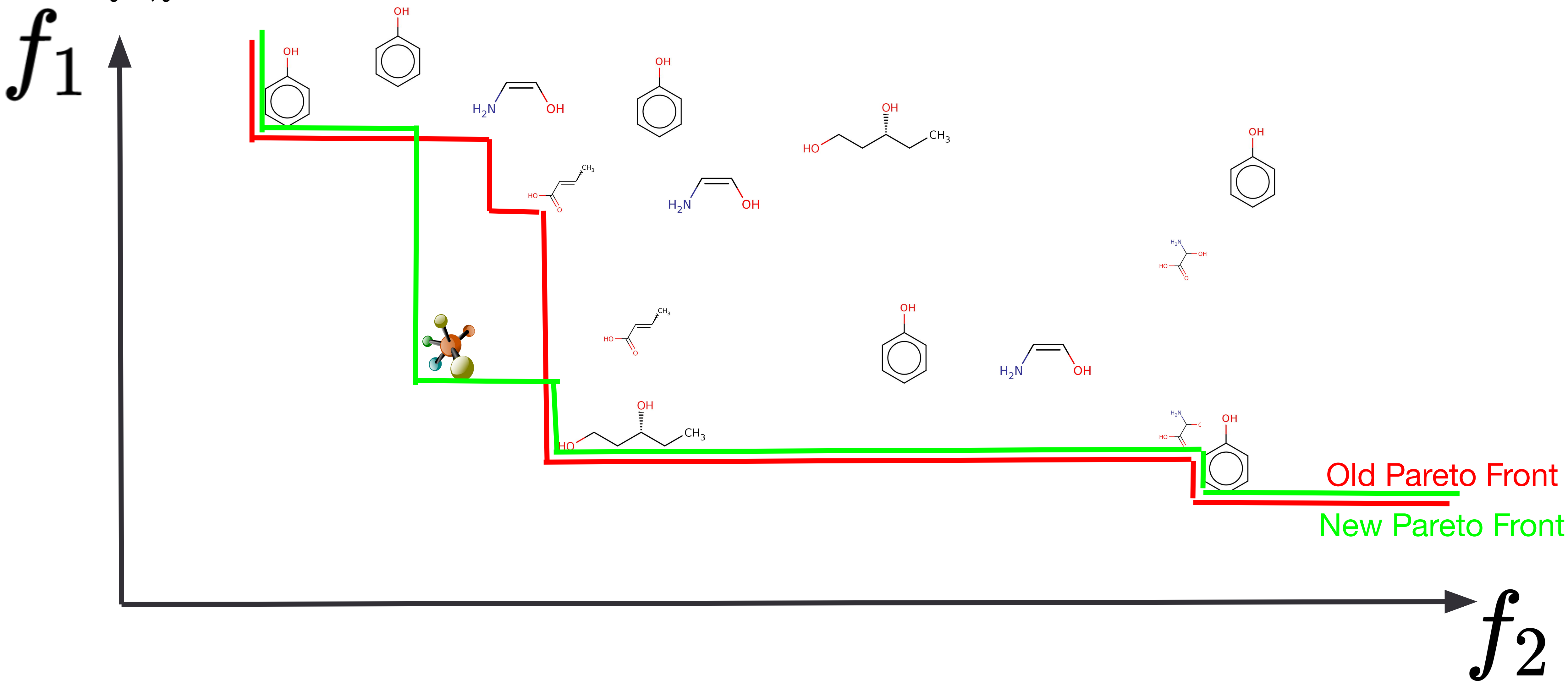
Multi-objective Optimisation

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



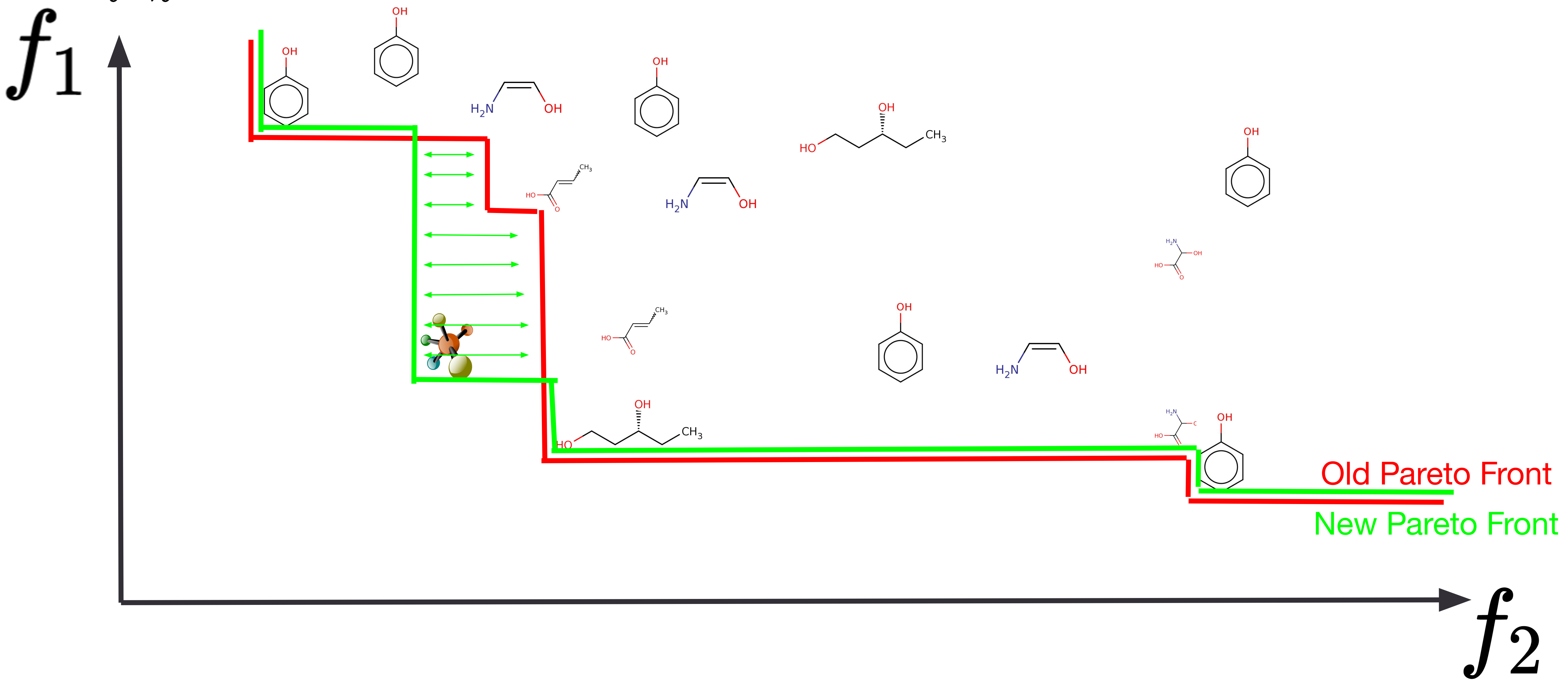
Multi-objective Optimisation

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)



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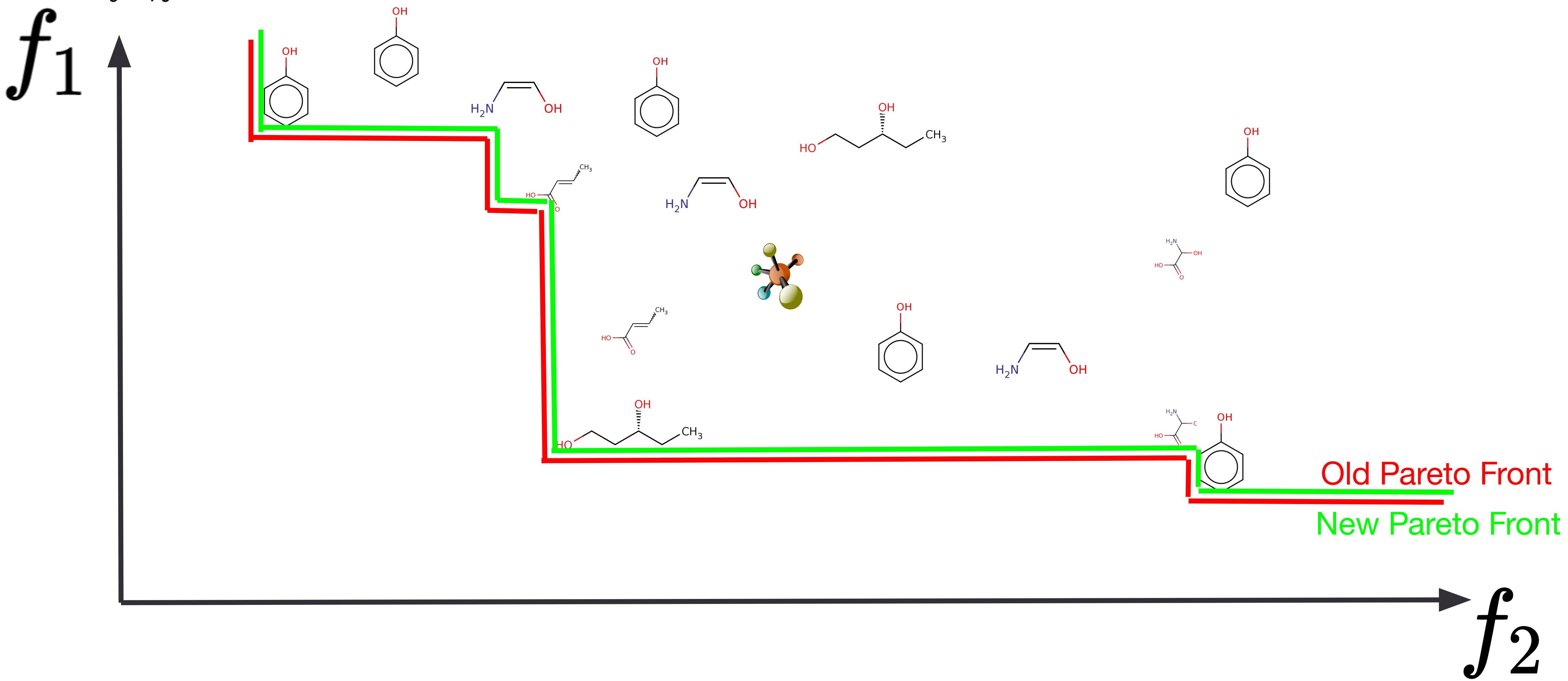
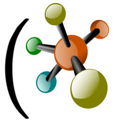
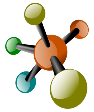
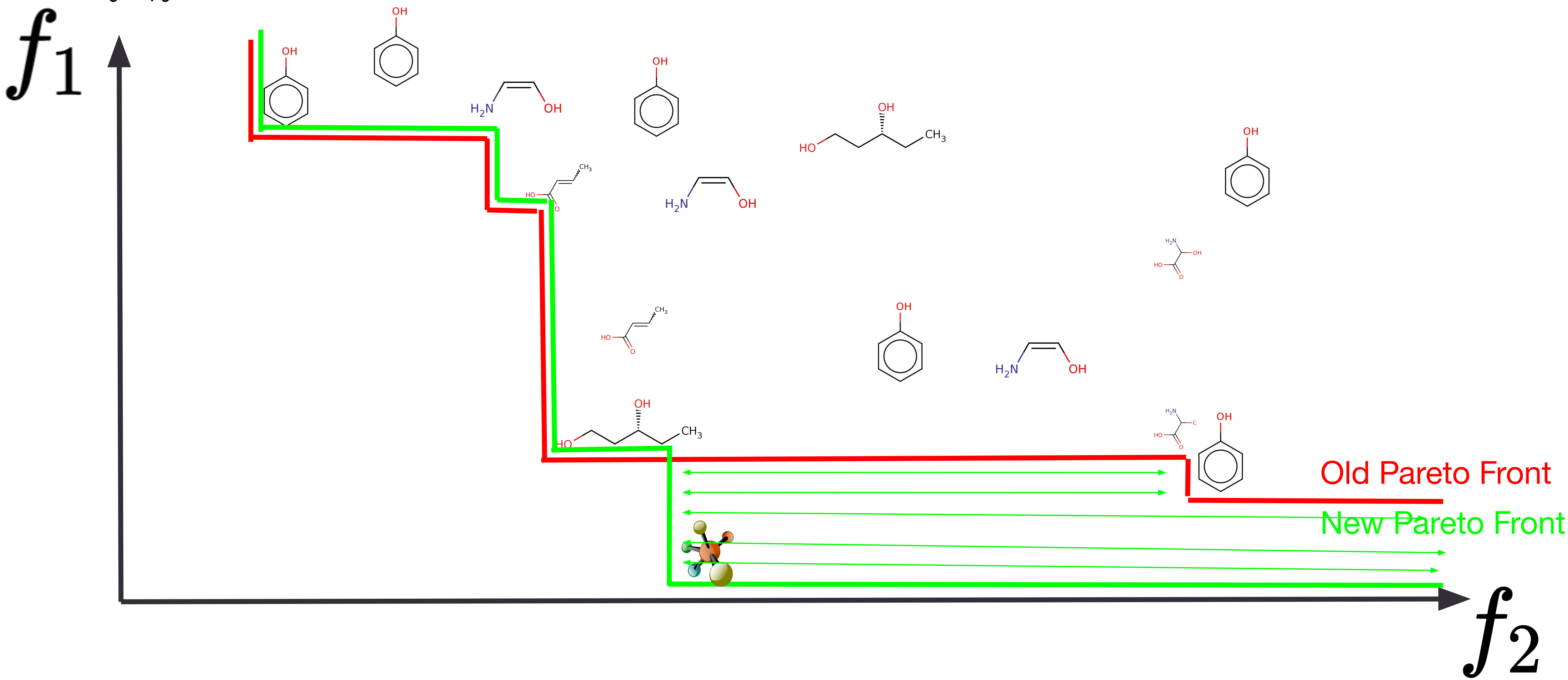
Multi-objective Optimisation

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

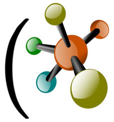
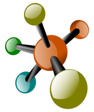


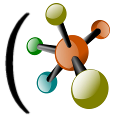
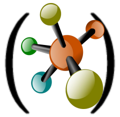
Multi-objective Optimisation

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

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

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

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

$$\alpha_{\mathrm{EHVI}}(\{\cdot_i, \cdot_j\}) = ???$$

What the haters say .....

What the haters say .....

They can't handle large data volumes

They can’t handle large data volumes

aters say .....

Only for Gaussian data.......

They can’t handle large data volumes

They can’t handle high-dimensional data

haters say .....

Only for Gaussian data.......

They can't handle large data volumes

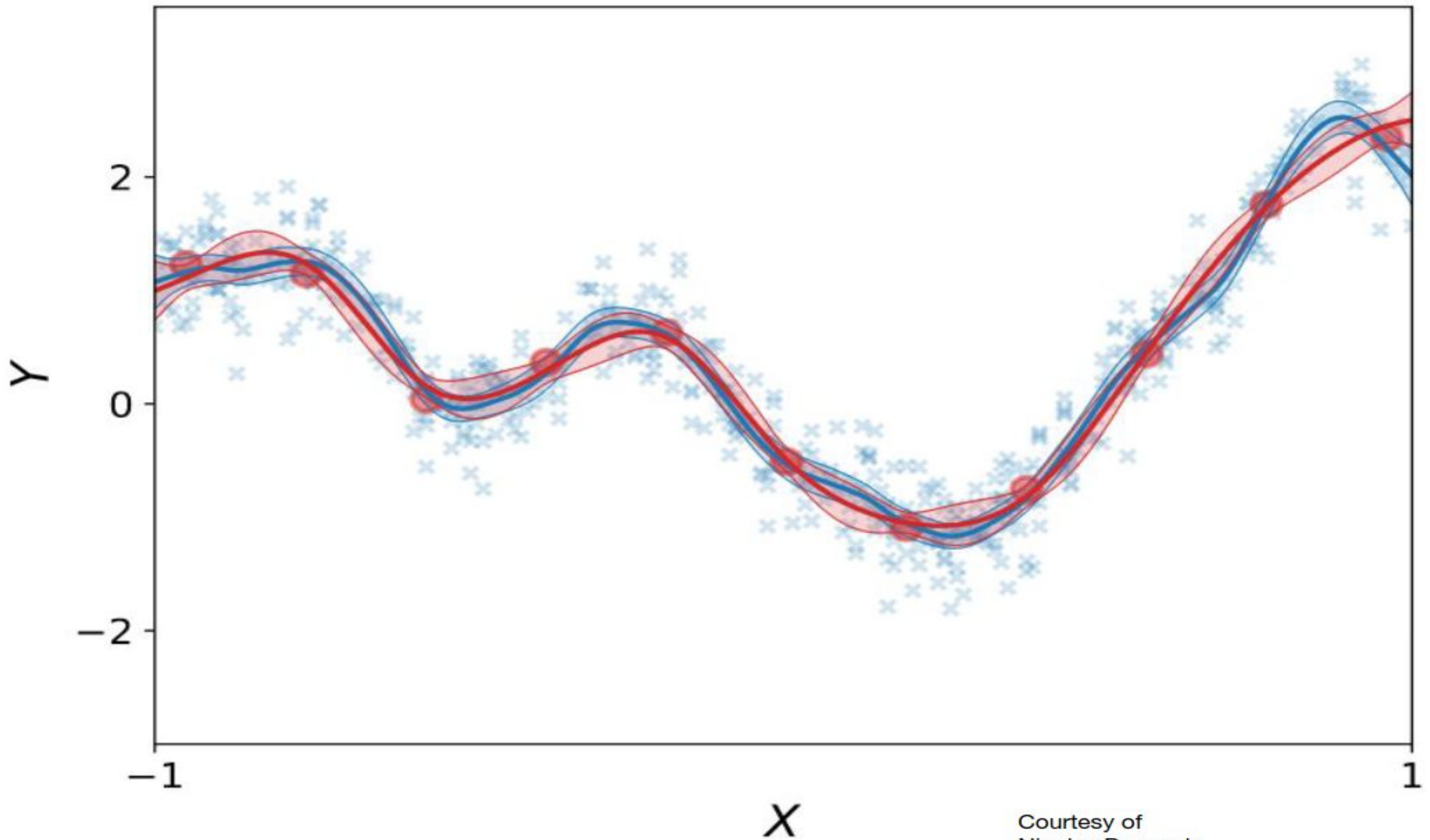
They can't handle high-dimensional data

Only for Gaussian data.......

They are not interpretable

GPs for big data?

- Use Sparse variational GP
- Replace with M (<<N) representative points

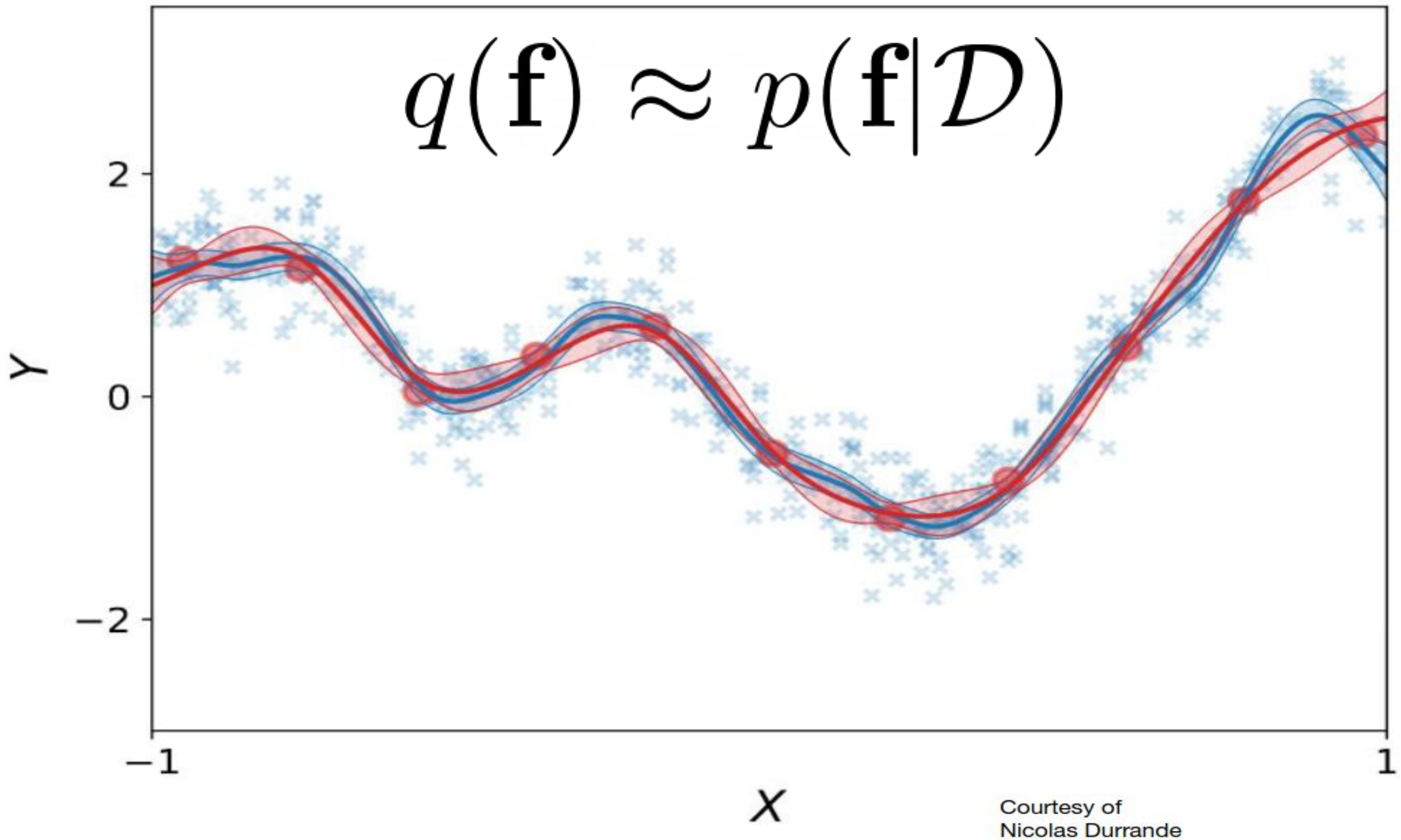


Courtesy of
Nicolas Durrande

GPs for big data?

- Use Sparse variational GP
- Replace with M (<<N)

  representative points



Courtesy of
Nicolas Durrande

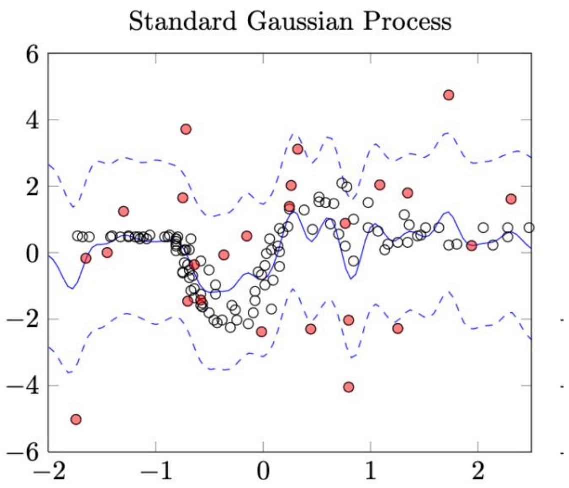
$$\text{ELBO}(q(\mathbf{f})) = \int q(\mathbf{f}) \log p(\mathbf{y}|\mathbf{f}) d\mathbf{f} - \mathcal{KL}(q(\mathbf{f}), p(\mathbf{f}))$$

$$= \sum_{i=1}^{N} \int q(f_i) \log p(y_i|f_i) d\mathbf{f} - \mathcal{KL}(q(\mathbf{f}), p(\mathbf{f}))$$

$$y_i \sim \mathcal{N}(f(\mathbf{x}_i), \sigma^2)$$

SVGPs for non-Gaussian data?

(Hensman et al. 2015, Saul et al. 2016)

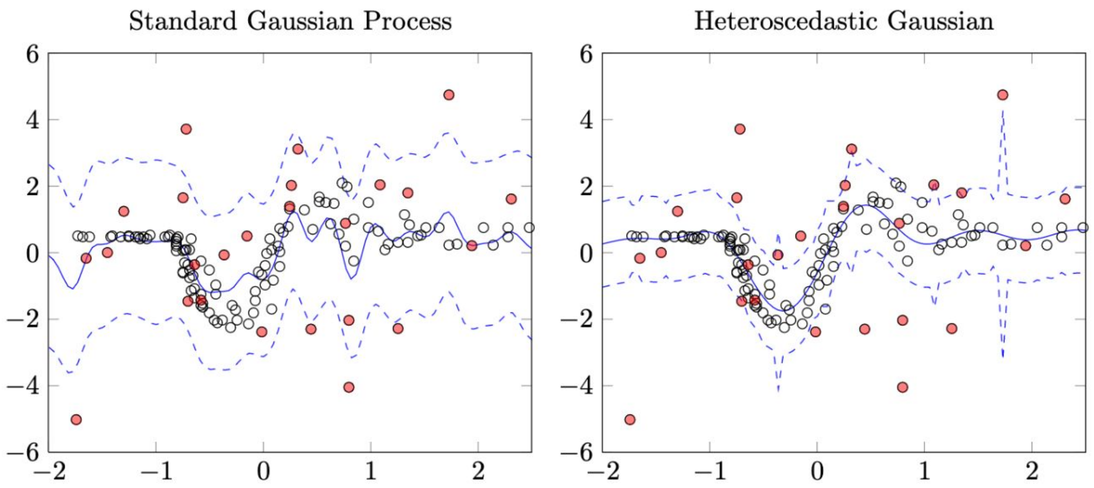


SVGPs for non-Gaussian data?

(Hensman et al. 2015, Saul et al. 2016)

~~$y_i \sim \mathcal{N}(f(\mathbf{x}_i), \sigma^2)$~~

$$y_i \sim \mathcal{N}(f_0(\mathbf{x}_i), e^{f_1(\mathbf{x}_i)})$$



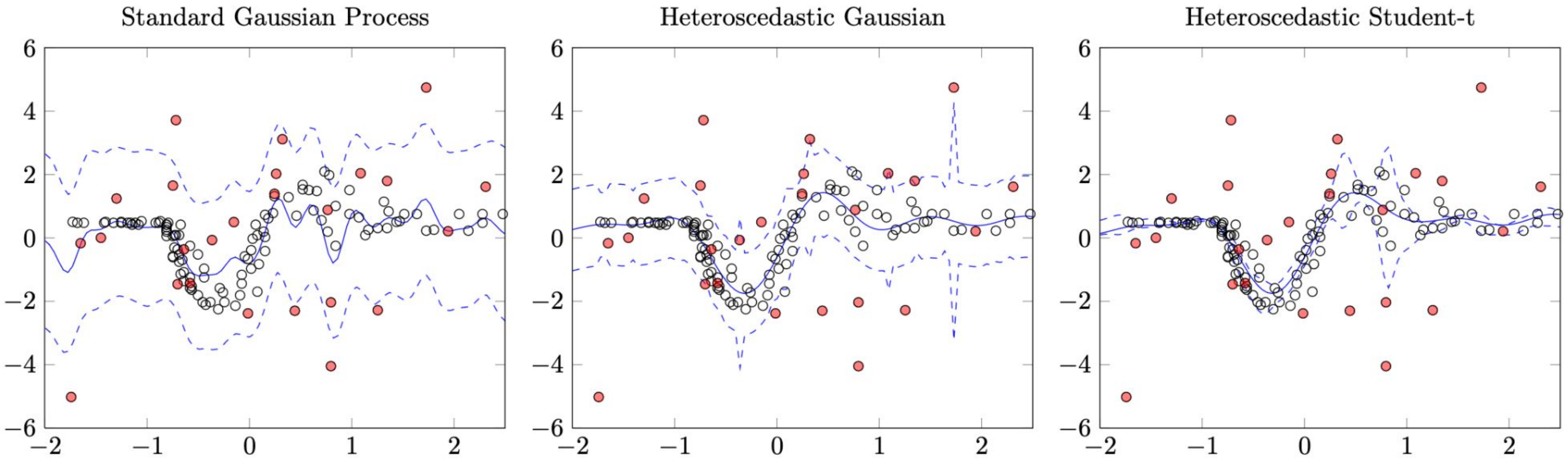
SVGPs for non-Gaussian data?

(Hensman et al. 2015, Saul et al. 2016)

$$y_i \sim \mathcal{N}(f(\mathbf{x}_i), \sigma^2)$$

$$y_i \sim \mathcal{N}(f_0(\mathbf{x}_i), e^{f_1(\mathbf{x}_i)})$$

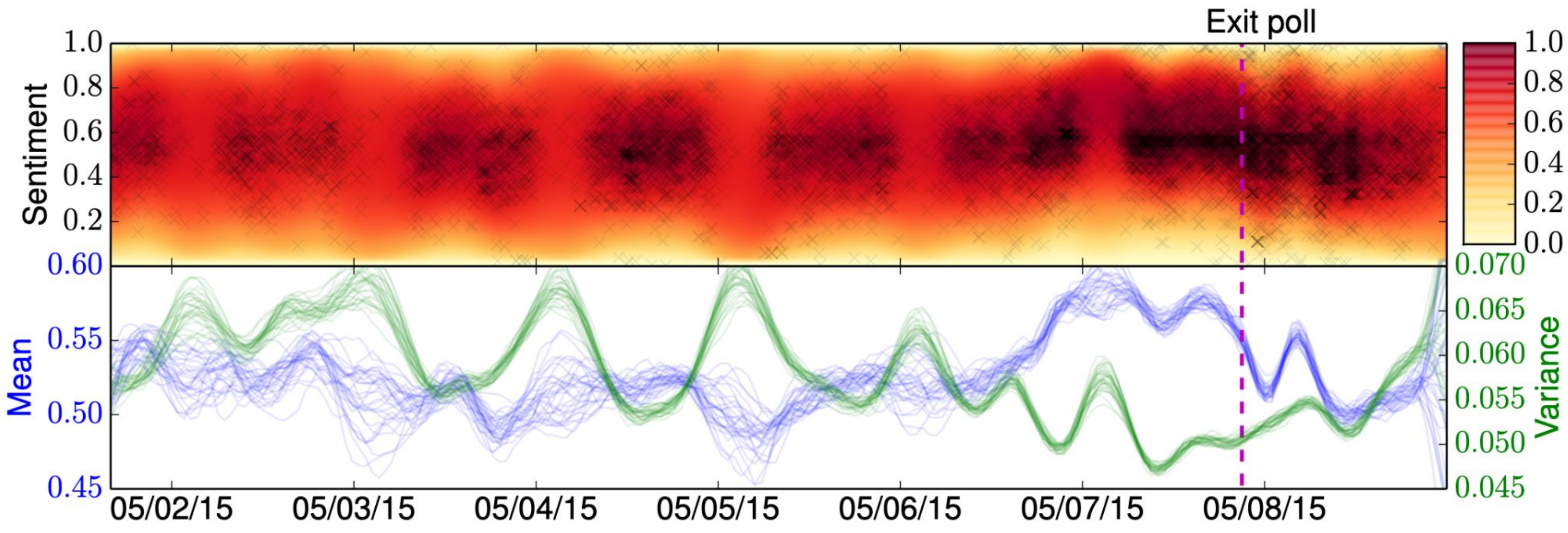
$$y_i \sim \mathcal{S}t(f_0(\mathbf{x}_i), e^{f_1(\mathbf{x}_i)}, \nu)$$



SVGPs for non-Gaussian data?

(Hensman et al. 2015, Saul et al. 2016)

$$y_i \sim \mathcal{B}(\alpha = f_0(\mathbf{x}_i), \beta = e^{f_1(\mathbf{x}_i)})$$



GPs for high-dim data?

Beware the curse of dimensionality ....

$$k(\mathbf{x}, \mathbf{y}) = e^{-\frac{||\mathbf{x}-\mathbf{y}||^2}{2l^2}}$$

GPs for high-dim data?

- GPs are great in high-dim
- RBF kernels are not……
- $l_i \propto \sqrt{D}$

GPs for high-dim data?

$$k(\mathbf{x}, \mathbf{y}) = e^{-\frac{||\mathbf{x}-\mathbf{y}||^2}{2l^2}}$$

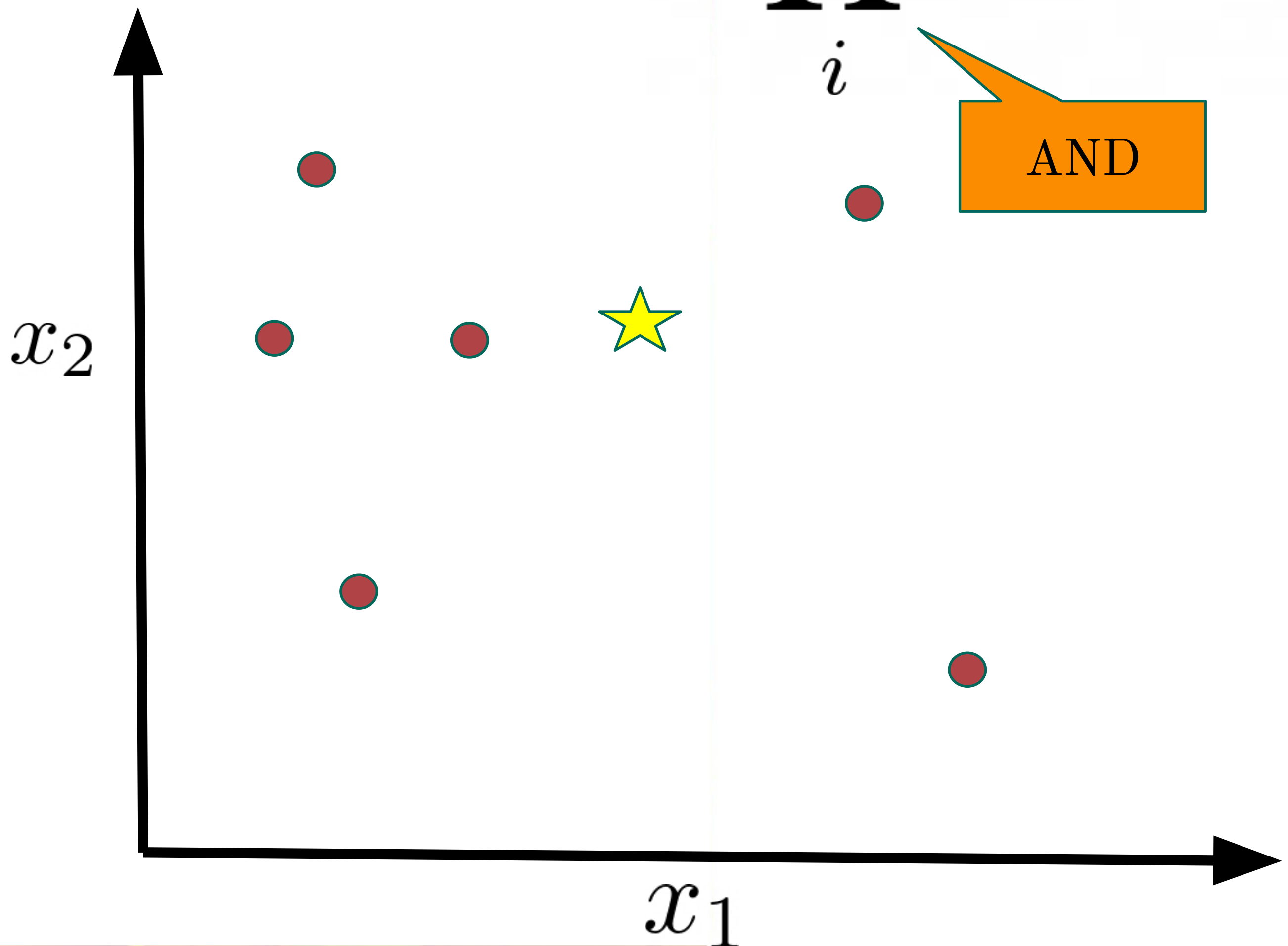
$$= \prod_i^d k_i(x_i, y_i)$$

AND

GPs for high-dim data?

$$k(\mathbf{x}, \mathbf{y}) = e^{-\frac{||\mathbf{x}-\mathbf{y}||^2}{2l^2}}$$

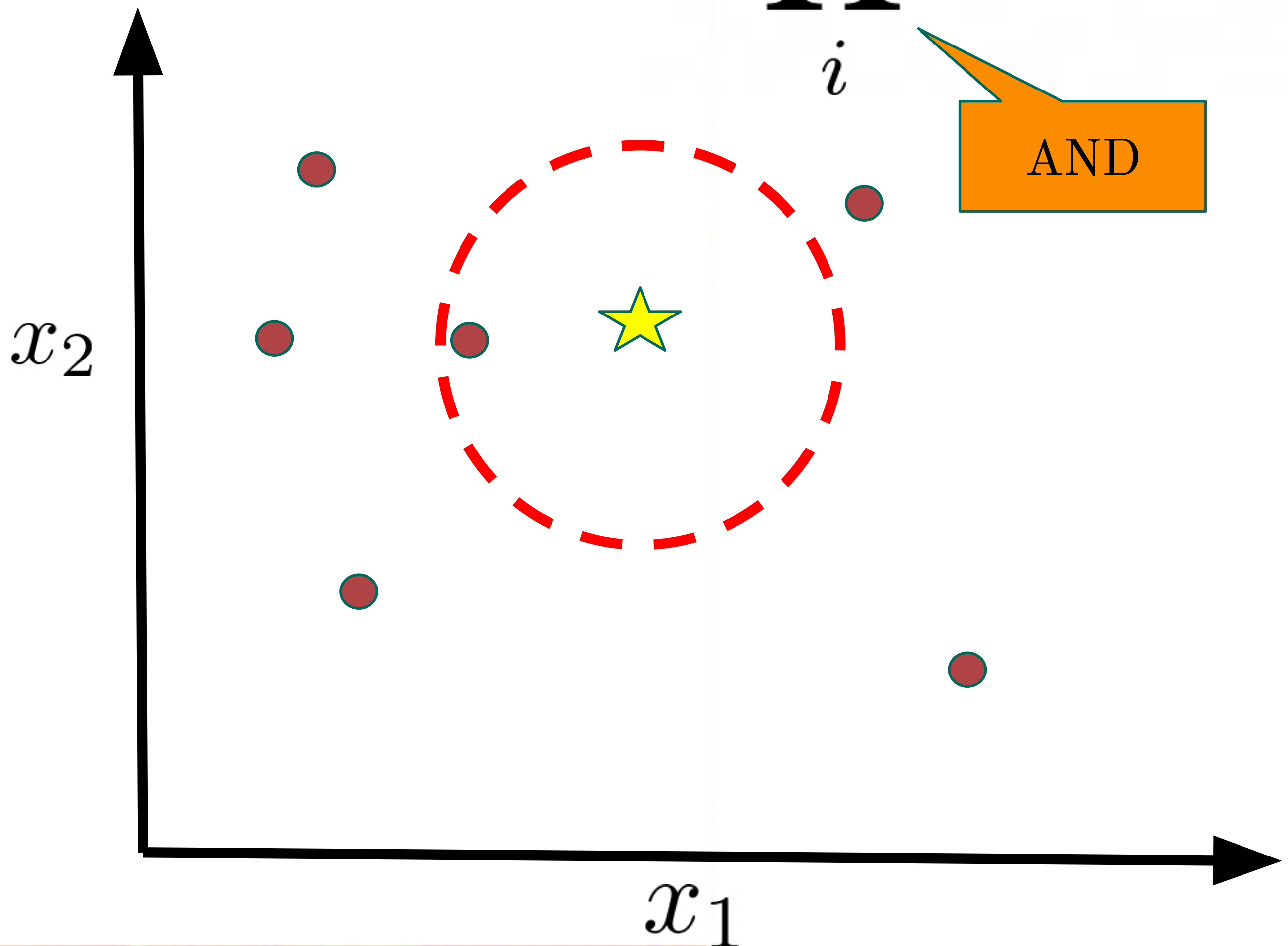
$$= \prod_i^d k_i(x_i, y_i)$$



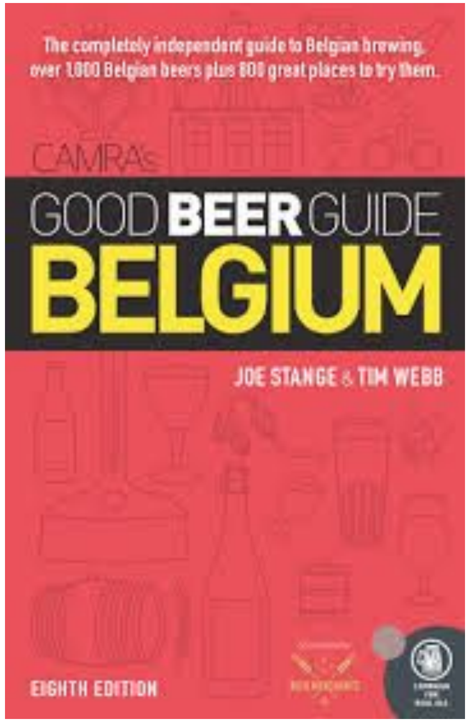
GPs for high-dim data?

$$k(\mathbf{x}, \mathbf{y}) = e^{-\frac{||\mathbf{x}-\mathbf{y}||^2}{2l^2}}$$

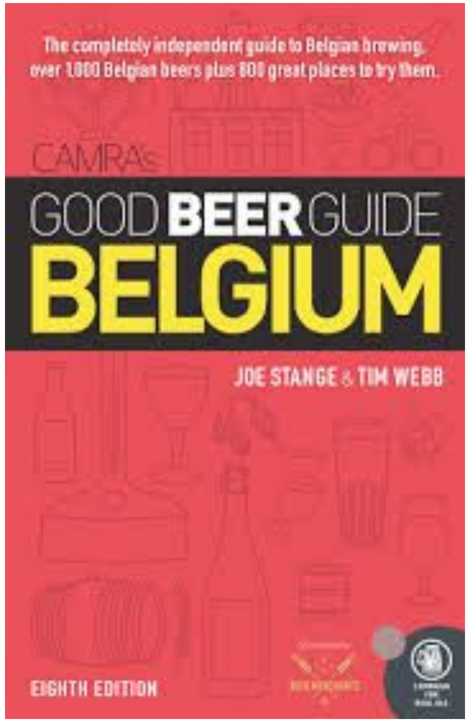
$$= \prod_i^d k_i(x_i, y_i)$$



GPs for high-dim data?

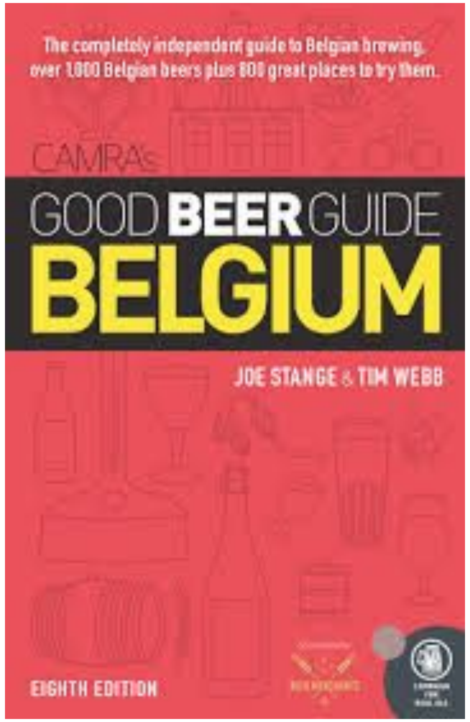


GPs for high-dim data?



GPs for high-dim data?

- Type of fermentation (wild yeast?)
- Ingredients (orange peel?, coriander??????)
- Strength
- Brewed by a monk?
- Barrel-aged?



GPs for high-dim data?

$$k(\mathbf{x}, \mathbf{y}) = e^{-\frac{||\mathbf{x}-\mathbf{y}||^2}{2l^2}}$$

$$= \prod_i^d k_i(x_i, y_i)$$

AND

GPs for high-dim data?

$$k(\mathbf{x}, \mathbf{y}) = e^{-\frac{||\mathbf{x}-\mathbf{y}||^2}{2l^2}}$$

$$= \prod_i^d k_i(x_i, y_i)$$

AND

$$k_1(\mathbf{x}, \mathbf{y}) = \sum_i^d k_i(x_i, y_i)$$

OR

$$k_2(\mathbf{x}, \mathbf{y}) = \sum_{i<j}^d k_i(x_i, y_i) k_j(x_j, y_j)$$

Additive Gaussian Processes

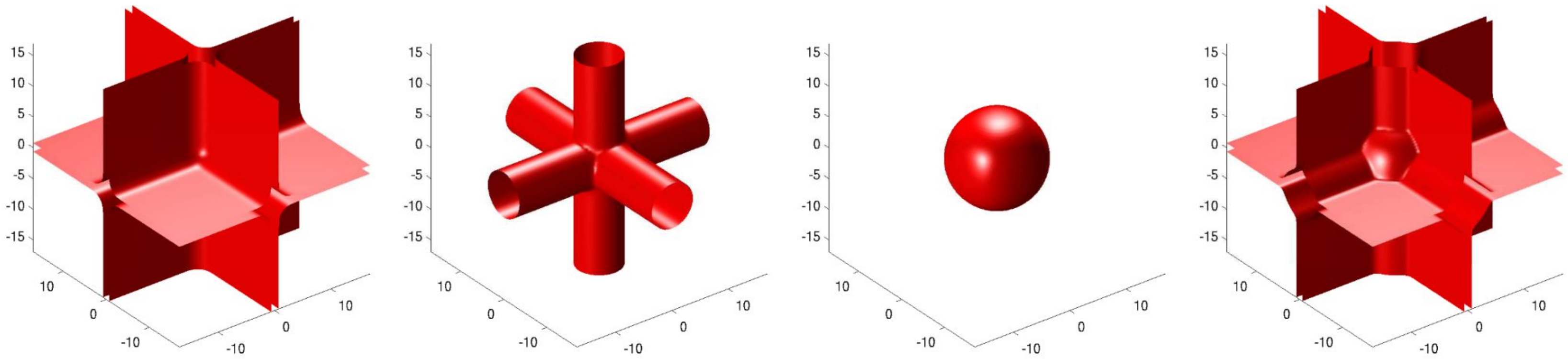
$$k(x, y) = \overset{0}{k_0} + \overset{1}{\sum k_i(x_i, y_i)} + \overset{2}{\sum_{i<j} k_i(x_i, y_i) k_j(x_j . y_j)}$$

Additive Gaussian Processes

0 1 2

$$k(x, y) = k_0 + \sum k_i(x_i, y_i) + \sum_{i<j} k_i(x_i, y_i)k_j(x_j.y_j)$$

(Duvenaud et al 2011)



1st order interactions
$k_1 + k_2 + k_3$

2nd order interactions
$k_1k_2 + k_2k_3 + k_1k_3$

3rd order interactions
$k_1k_2k_3$
(Squared-exp kernel)

All interactions

(Additive kernel)

Additive Gaussian Processes

0 1 2

$$k(x,y) = k_0 + \sum k_i(x_i, y_i) + \sum_{i<j} k_i(x_i, y_i) k_j(x_j . y_j)$$

$$\Updownarrow$$

Ginsbourger et al. (2016)

$$f(\mathbf{x}) = f_0 + \sum f_i(x_i) + \sum_{i<j} f_{ij}(x_i, x_j)$$

Additive Gaussian Processes

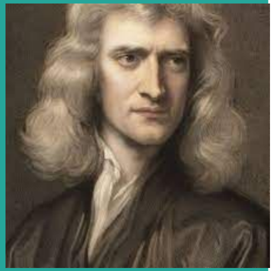
0 1 2

$$k(x,y) = k_0 + \sum k_i(x_i, y_i) + \sum_{i<j} k_i(x_i, y_i) k_j(x_j . y_j)$$

$$\Updownarrow$$

$$f(\mathbf{x}) = f_0 + \sum f_i(x_i) + \sum_{i<j} f_{ij}(x_i, x_j)$$

- Standard RBF -> $O(d(N^2 + NM))$
- d additive RBF -> $O(2^d(N^2 + NM))$



Additive Gaussian Processes

- Newton Girard (Duvenaud et al 2011)

$$\overset{0}{} \quad \overset{1}{} \quad \overset{2}{}$$

$$k(x,y) = k_0 + \sum k_i(x_i, y_i) + \sum_{i<j} k_i(x_i, y_i) k_j(x_j . y_j)$$

$$\Updownarrow$$

$$f(\mathbf{x}) = f_0 + \sum f_i(x_i) + \sum_{i<j} f_{ij}(x_i, x_j)$$

- Standard RBF -> $O(d(N^2 + NM))$
- d additive RBF -> $O(2^d(N^2 + NM))$
- d additive BBF (NG) -> $O(d^2(N^2 + NM))$

Additive Gaussian Processes

0 1 2

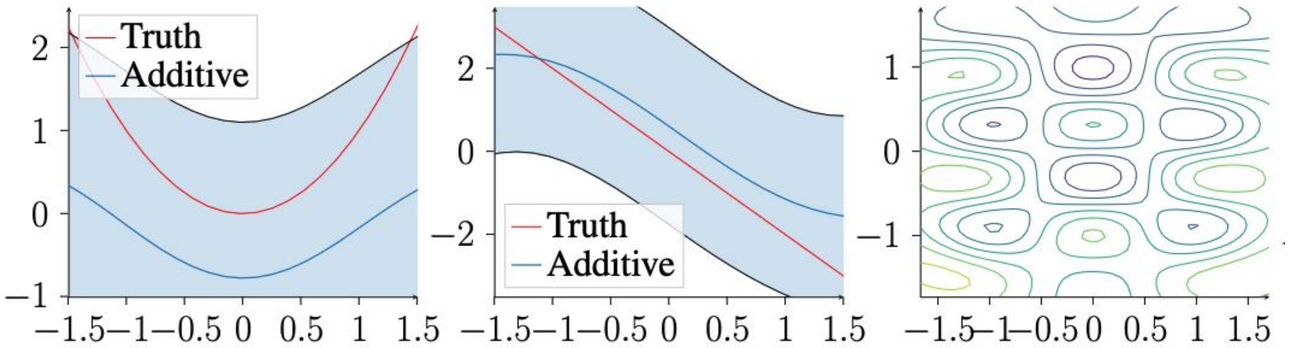
$$k(x,y) = k_0 + \sum k_i(x_i,y_i) + \sum_{i<j} k_i(x_i,y_i)k_j(x_j.y_j)$$

$$\Updownarrow$$

Ginsbourger et al. (2016)

$$f(\mathbf{x}) = f_0 + \sum f_i(x_i) + \sum_{i<j} f_{ij}(x_i,x_j)$$

$$f(x_1,x_2) = x_1^2 - 2x_2 + cos(3x_1)sin(5x_2)$$



(a) f_1 (b) f_2 (c) Interaction

$$E[f_i(x_i)|\mathcal{D}] = k_i(x_i,X)K(X,X)^{-1}\mathbf{y}$$

Lu et al. 2022

Additive Gaussian Processes

- Orthogonalise (Durrande et al 2012)

$$f(x_1, x_2) = (f_1(x_1) + \delta) + (f_2(x_2) - \delta)$$

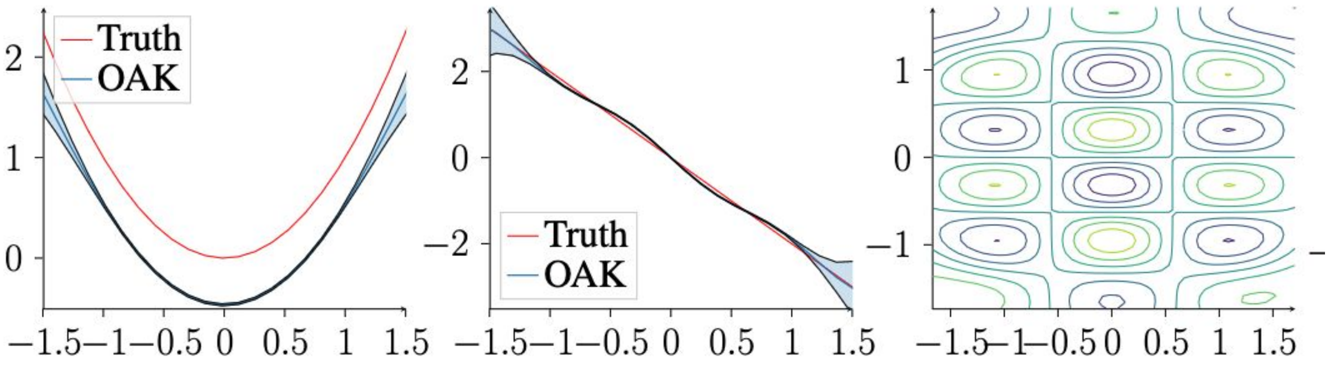
0 1 2

$$k(x, y) = k_0 + \sum k_i(x_i, y_i) + \sum_{i<j} k_i(x_i, y_i) k_j(x_j . y_j)$$

$$\Updownarrow$$

$$f(\mathbf{x}) = f_0 + \sum f_i(x_i) + \sum_{i<j} f_{ij}(x_i, x_j)$$

$$f(x_1, x_2) = x_1^2 - 2x_2 + cos(3x_1) sin(5x_2)$$



(f) f_1 (g) f_2 (h) Interaction

Lu et al. 2022

Additive Gaussian Processes

- Orthogonalise (Durrande et al 2012)

$$f(x_1, x_2) = (f_1(x_1) + \delta) + (f_2(x_2) - \delta)$$

- By conditioning

$$f_i(x_i) \Bigg| \int f_i(x_i) p(x_i) dx_i = 0$$

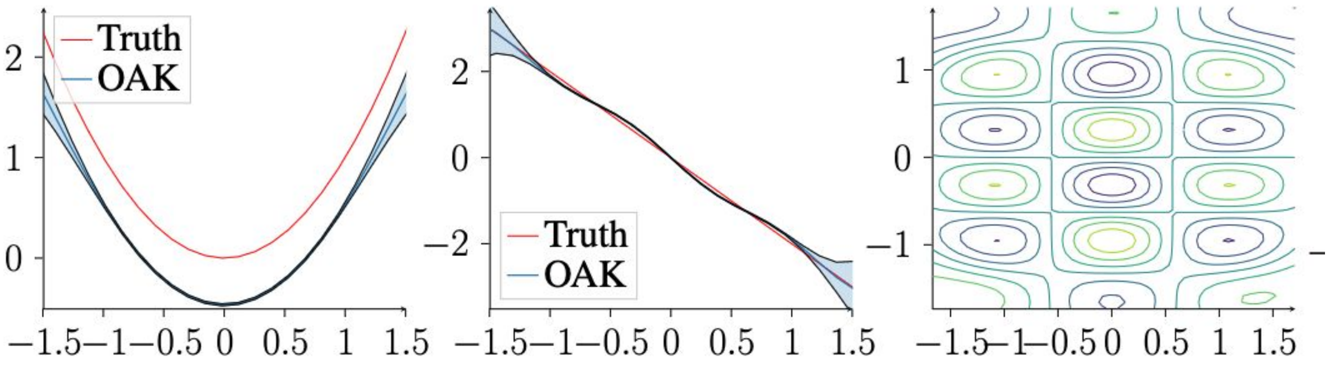
0 1 2

$$k(x, y) = k_0 + \sum k_i(x_i, y_i) + \sum_{i<j} k_i(x_i, y_i) k_j(x_j . y_j)$$

$$\Updownarrow$$

$$f(\mathbf{x}) = f_0 + \sum f_i(x_i) + \sum_{i<j} f_{ij}(x_i, x_j)$$

$$f(x_1, x_2) = x_1^2 - 2x_2 + cos(3x_1) sin(5x_2)$$



(f) f_1 (g) f_2 (h) Interaction

Lu et al. 2022

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This model is quite interpretable......

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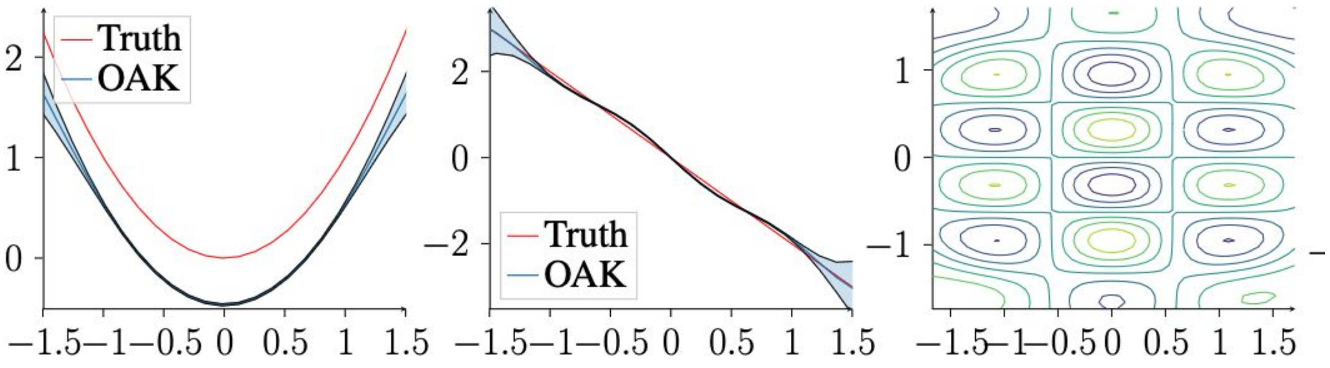

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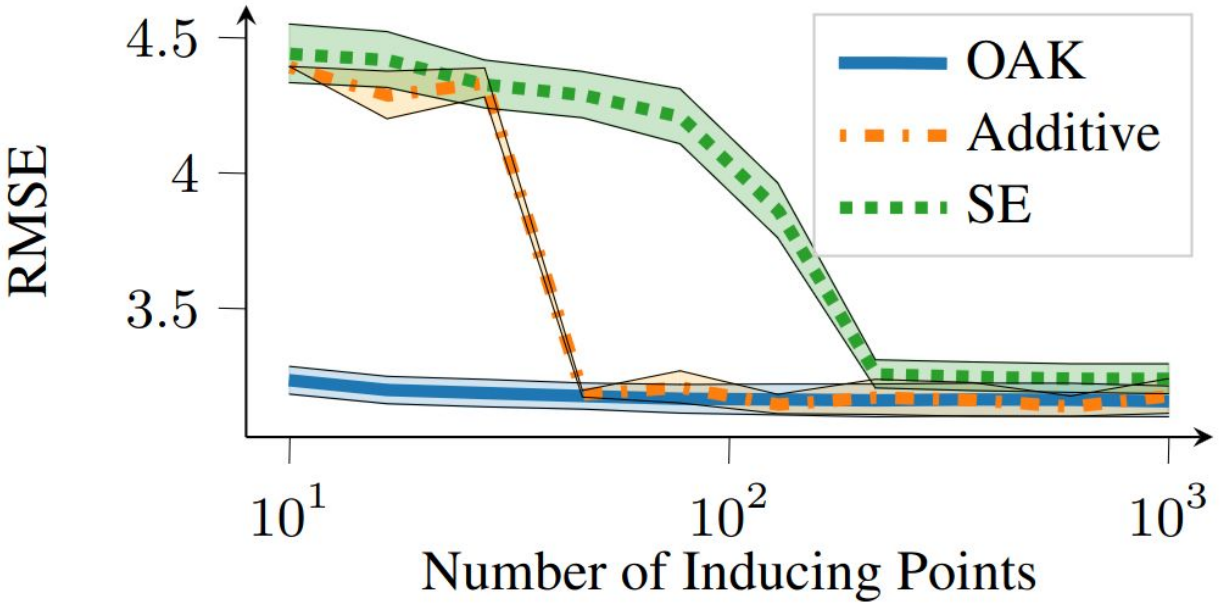

Thanks for listening

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