Going Beyond Global Optima with **Bayesian Algorithm Execution**

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Stefano Ermon

Going Beyond Global Optima with **Bayesian Algorithm Execution**

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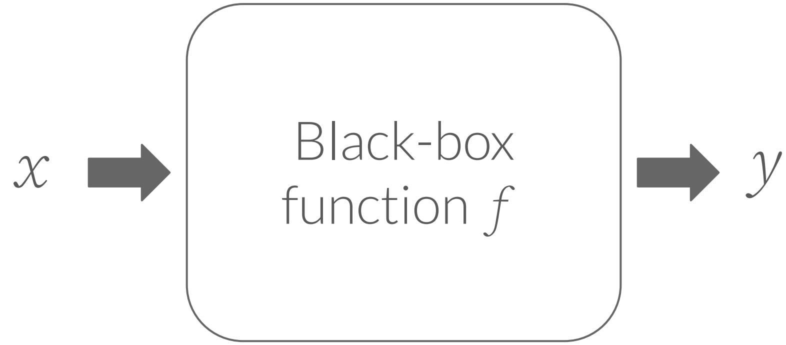
Extending Bayesian optimization from estimating *global optima* to estimating *other function properties defined by algorithms*

BACKGROUND

Background on *Black-box Global Optimization*

Suppose we have a noisy *"black-box"* function f.

Can ***query*** f:



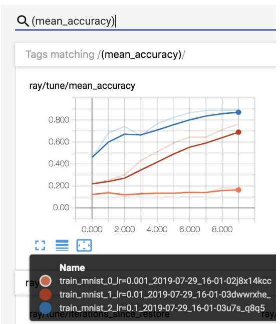
Assume:

- Observations are **noisy**: $y \sim f(x) + \varepsilon$
- Each function query is **costly**
  - E.g. in money, time, labor, etc.
- *Goal of this task*: estimate the location of **global optima** of f
- **Budget** of T queries

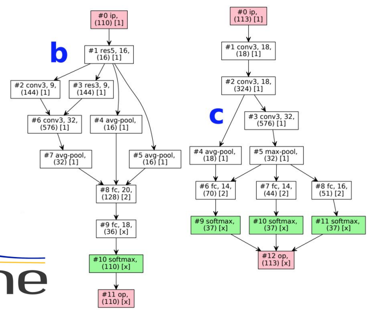
BACKGROUND

Black-box Global Optimization — many applications

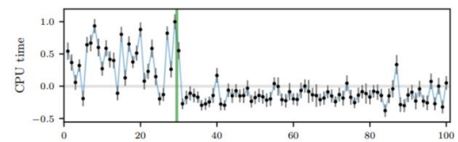
Hyperparameter Opt & Neural Architecture Search



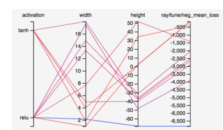
tune

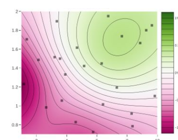


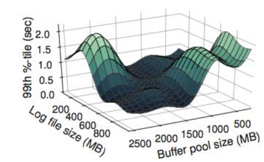
Systems Auto-tuning



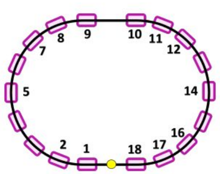
OTTER TUNE



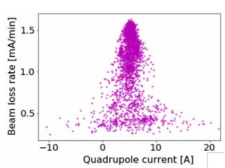




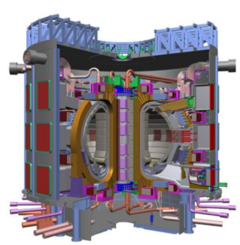
Optimizing Laboratory Equipment & Machines



(a) Layout of SPEAR3

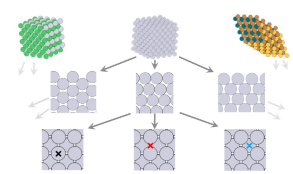


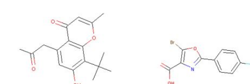
(b) Beam loss rate



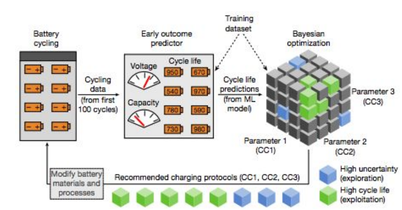
SLAC PPPL

Materials Discovery & Protocols





(a) QED 0.92083 (b) QED 0.92145



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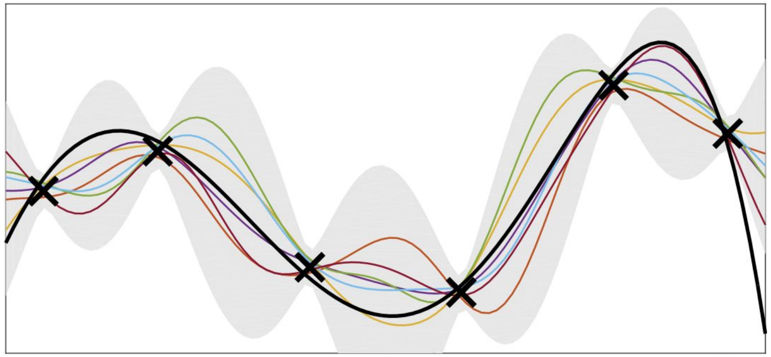
BACKGROUND

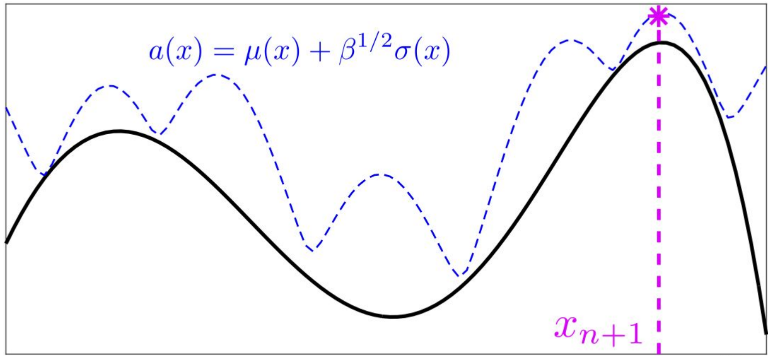
A popular method is **Bayesian optimization (BO)**

- Leverages a probabilistic model of f to sequentially choose queries.
- The model can:
  - incorporate prior beliefs about f (e.g. smoothness)
  - tell us where we are certain vs uncertain about f
- ⇒ Sample efficient optimization.

Probabilistic model of f



Use model to choose queries



Estimating other properties

In a variety of real-world tasks, there are **many other properties** of black-box functions that we also want to estimate:

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BEYOND GLOBAL OPTIMA

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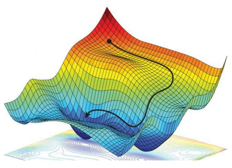
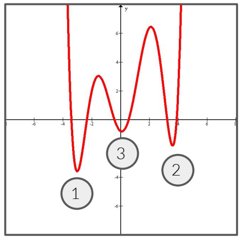


Local optima



Top-k optima

Applications

- *ML model training*
- *HPO / NAS*
- *Systems tuning*

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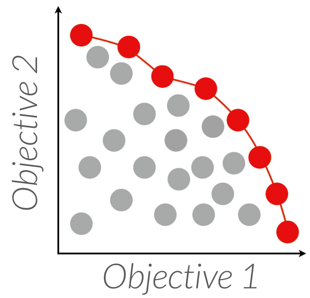

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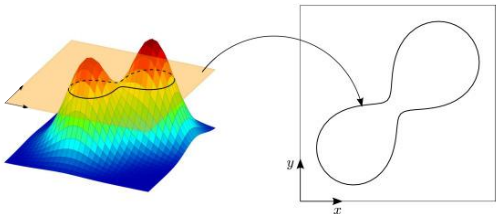

Applications

- *Catalyst design*
- *Active learning / weak supervision*
- *Environmental monitoring*

BEYOND GLOBAL OPTIMA

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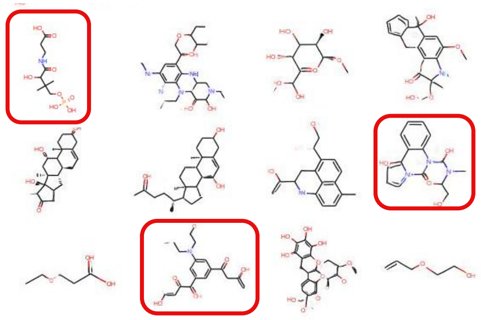
(molecules)



Applications

- *Drug discovery*
- *Fraud detection*
- *Targeted opinion polling*

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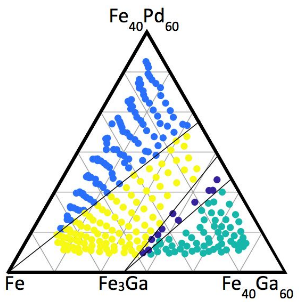
(compounds)



Applications

- High throughput materials design/discovery

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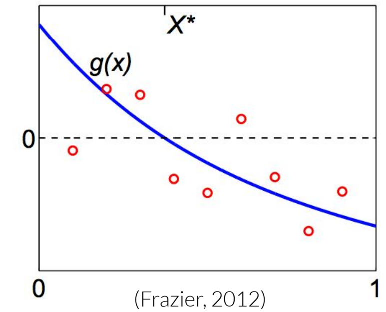

(Frazier, 2012)

Applications

- *Target localization* (airborne radar)
- *Edge detection* (computer vision)
- *Biology / microbiology* (phase shifts)

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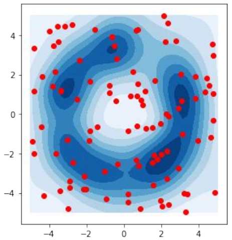
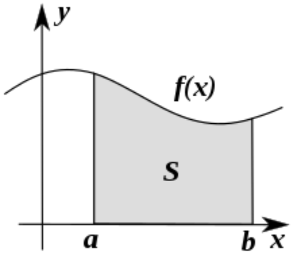


(Emukit, 2021)



Applications

- *Probabilistic modeling (marginal distributions, normalization constants)*
- *Estimating center of mass (and centroids)*

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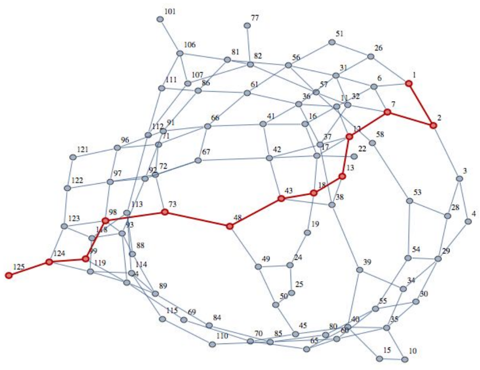

Applications

- *Transportation networks*
- *Shipping networks*
- *Social networks*

BEYOND GLOBAL OPTIMA

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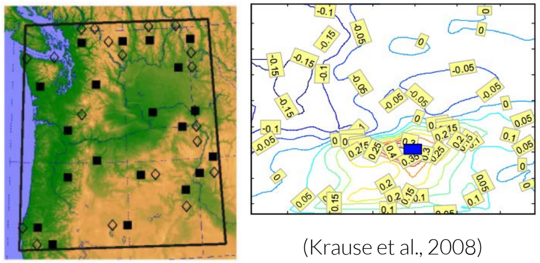

(Krause et al., 2008)

Applications

- *Water distribution systems*
- *Outbreak detection in networks*
- *Weather monitoring*

Our goal

To develop methods to estimate a broad set of function properties within a limited budget, using probabilistic models.

⇒ Can view this as a generalization of Bayesian optimization to other function properties... *beyond global optima*.

First question:

How do we formalize *"other function properties"*?

ALGORITHMS w/o BUDGET CONSTRAINTS

Note that, given a function property of interest...

Often exists effective algorithms for computing (or numerically approximating) the property, ***if you ignore budget constraint***

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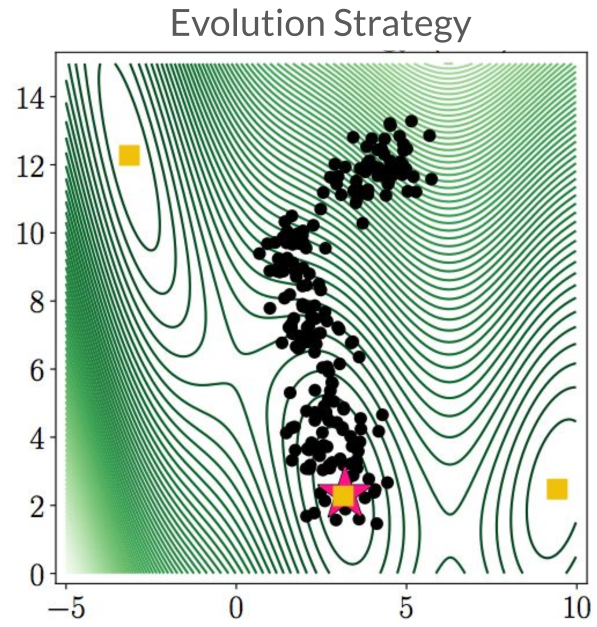
Algorithm: *local optimization algorithm* → e.g. gradient descent, Nelder-Mead method, evolutionary algorithm, etc.



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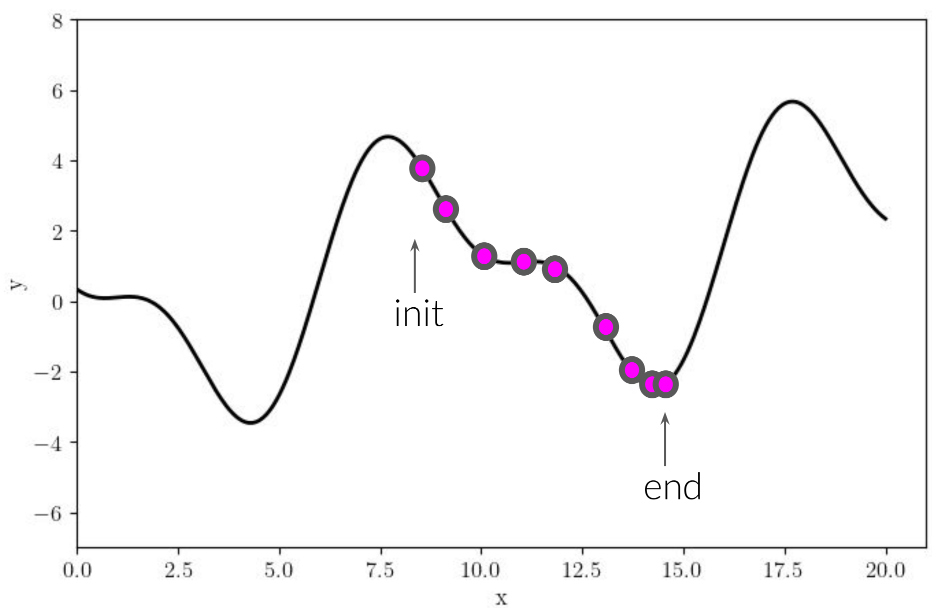
e.g. gradient descent, Nelder-Mead method, evolutionary algorithm, etc.

⇒ initialize at some location, then run local minimizer. Return final query as output.



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Property: *superlevel set of* f *(e.g. over a discrete space of items).*

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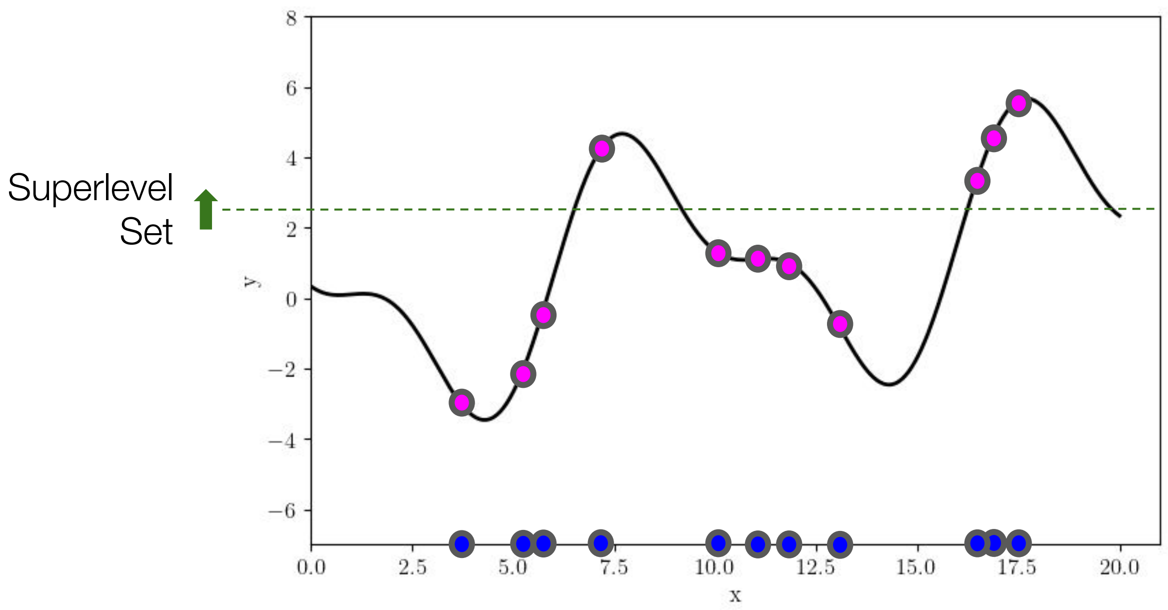
Often exists effective algorithms for computing (or numerically approximating) the property, ***if you ignore budget constraint***

Property: *superlevel set of f (e.g. over a discrete space of items).*

Algorithm: *scan and threshold.*

⇒ Scan through each item ● , query its value ● , return subset of items above threshold.



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Property: *integral or expectation of* f.

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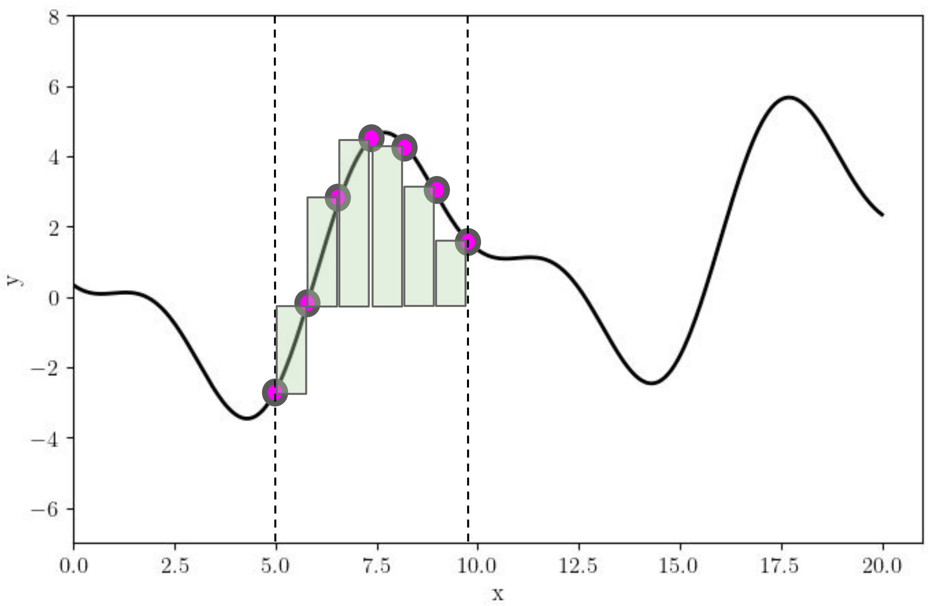
Often exists effective algorithms for computing (or numerically approximating) the property, ***if you ignore budget constraint***

Property: *integral or expectation of f.*

Algorithm: *numerical integration (e.g. rectangle/trapezoidal approximation).*

⇒ Run numerical integration *(e.g. rectangle/trapezoidal approximation)*. Return approximate integral over region.



Definition: *computable function property*

The output of a given algorithm A, if it were run on our black-box function f.

⇒ E.g. previous properties are all *computable function properties*:
local optima, integrals, level sets, Pareto frontiers, partitions — and many others, defined by an algorithm!

DEFINITIONS

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The task of estimating a *computable function property* (output of an algorithm A), using a budget of only T queries to f.

(Even if algorithm A requires far more than T queries.)

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Note: two main reasons to frame *function property* in terms of an algorithm:

(1) gives a flexible way to define function properties.

(2) we will use algorithm in our procedure to estimate these properties.

Methods for BAX

Information-based method for BAX

InfoBAX — an algorithm for BAX, based on info-theoretic methods for BO.

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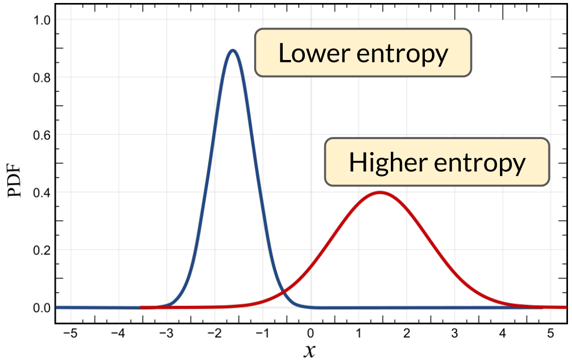
Some relevant background

There exist a few popular info-based methods for BO:

- E.g. entropy search (ES), predictive ES, max-value ES.
- Rooted in **Bayesian optimal experimental design (BOED).**

BOED: have model with an (unknown) parameter of interest.

- Choose experiments that most reduce uncertainty about parameter.
- *Uncertainty*: **entropy** of posterior distribution over parameter.



Some BOED History

Reducing theodolite measurements for surveying.

Information-based method for BAX

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To describe *InfoBAX*:

(1) Describe info-based BO.
(2) Extend it to info-based BAX.

Information-based Bayesian Optimization

Algorithm 1 BAYESIAN OPTIMIZATION

Information-based Bayesian Optimization

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Input: dataset $\mathcal{D}_1$, prior distribution $p(f)$ → Initial dataset of (x, y) pairs (function observations) — can be empty set.

Information-based Bayesian Optimization

Algorithm 1 BAYESIAN OPTIMIZATION

Input: dataset $\mathcal{D}_1$, prior distribution $p(f)$

1: **for** $t = 1, \ldots, T$ **do**

Over a sequence of T iterations:

Information-based Bayesian Optimization

Algorithm 1 BAYESIAN OPTIMIZATION

Input: dataset $\mathcal{D}_1$, prior distribution $p(f)$

1: **for** $t = 1, \ldots, T$ **do**

2: $\quad x_t \leftarrow \arg\max_{x \in \mathcal{X}} \alpha_t(x)$

Optimize an *acquisition function*.

- aims to capture value of querying f at an x.
- defined using our probabilistic model.

$\Rightarrow$ Chooses next x to query.

Information-based Bayesian Optimization

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2: $x_t \leftarrow \arg\max_{x \in \mathcal{X}} \alpha_t(x)$

3: $y_{x_t} \sim f(x_t) + \epsilon$

Query f on chosen x, observe y

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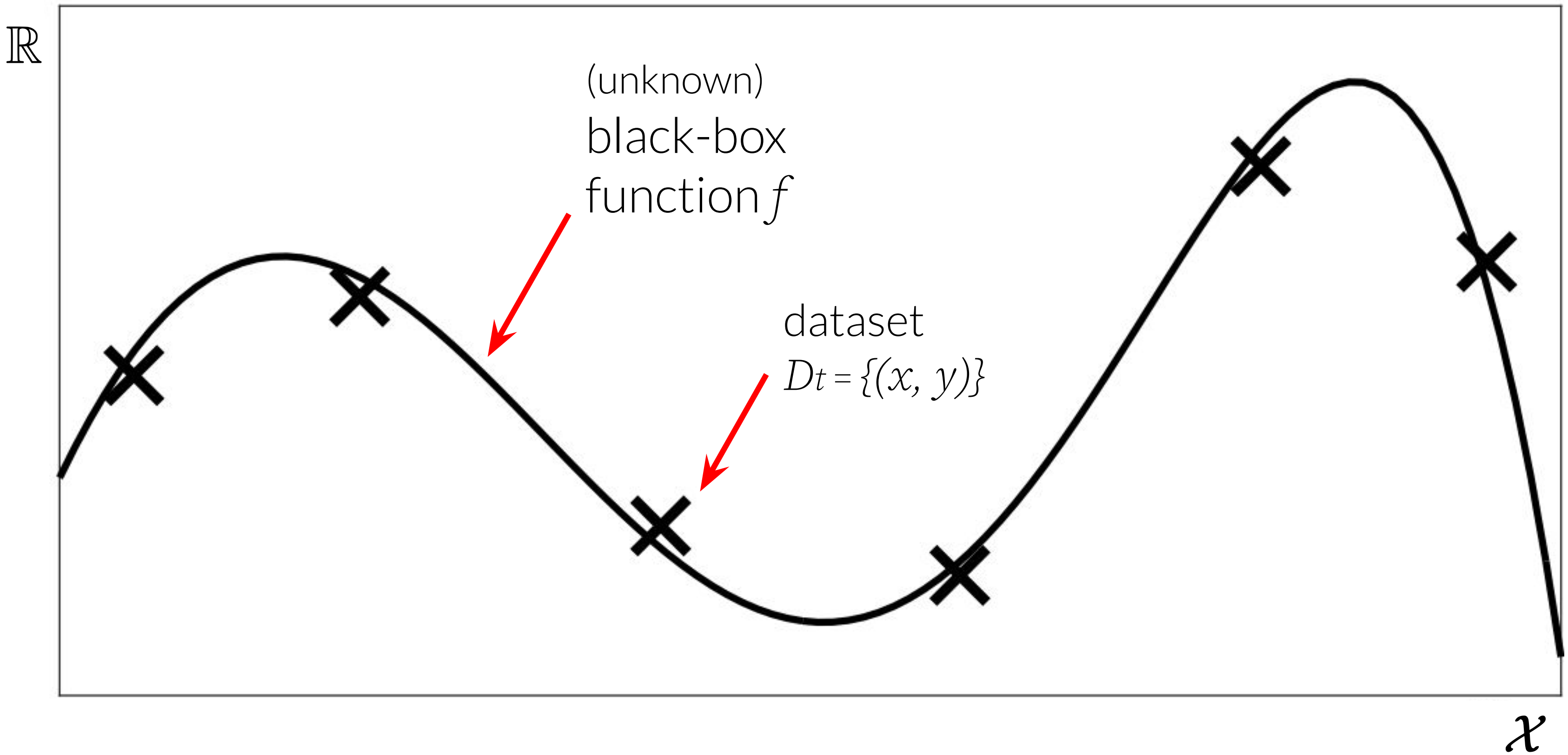
4: $\quad \mathcal{D}_{t+1} \leftarrow \mathcal{D}_t \cup \{(x_t, y_{x_t})\}$ → Update dataset with new *(x, y)* pair

Output: final dataset $\mathcal{D}_{T+1}$

Information-based Bayesian Optimization

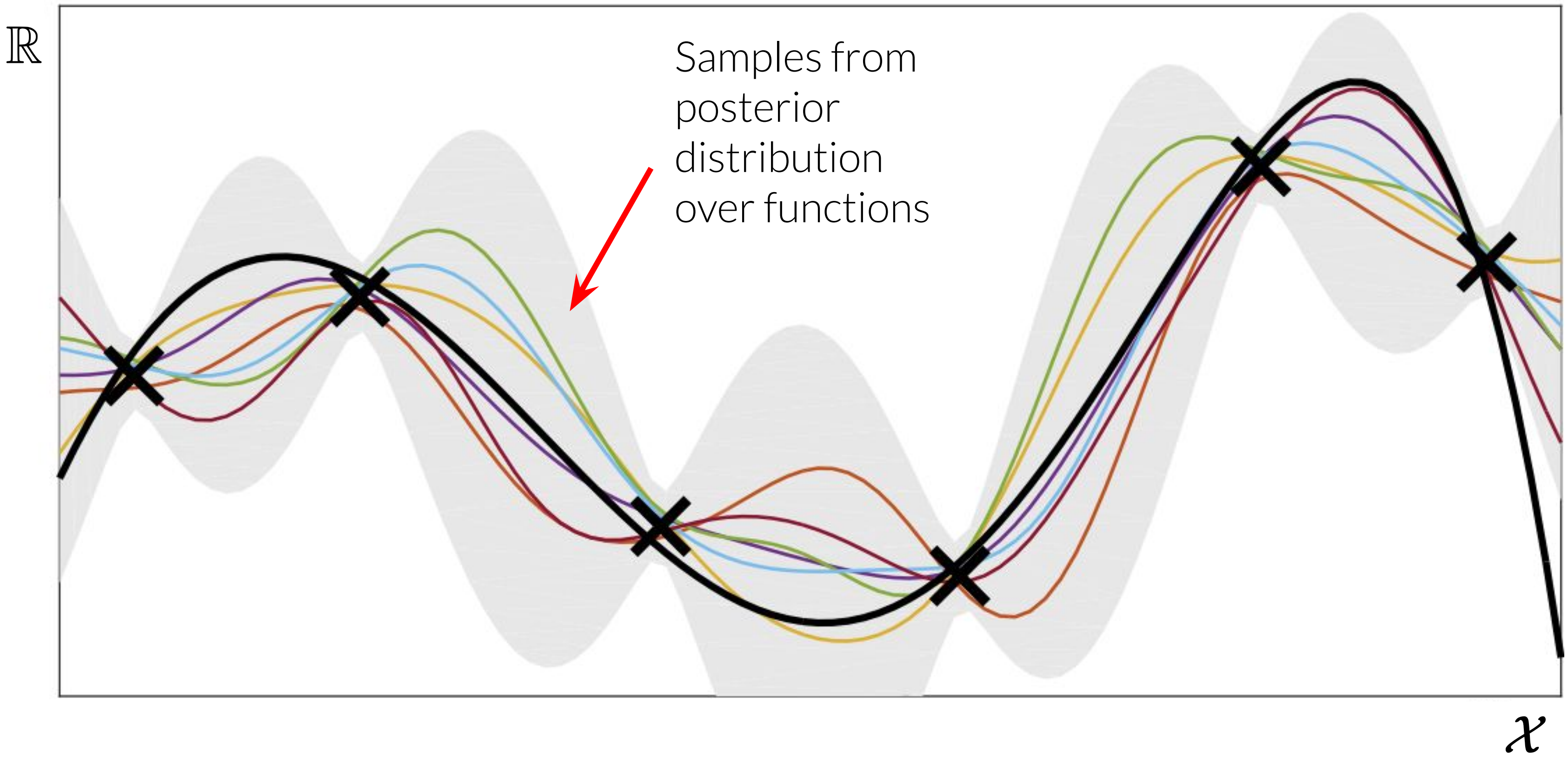
Visualizing this ...

BACKGROUND



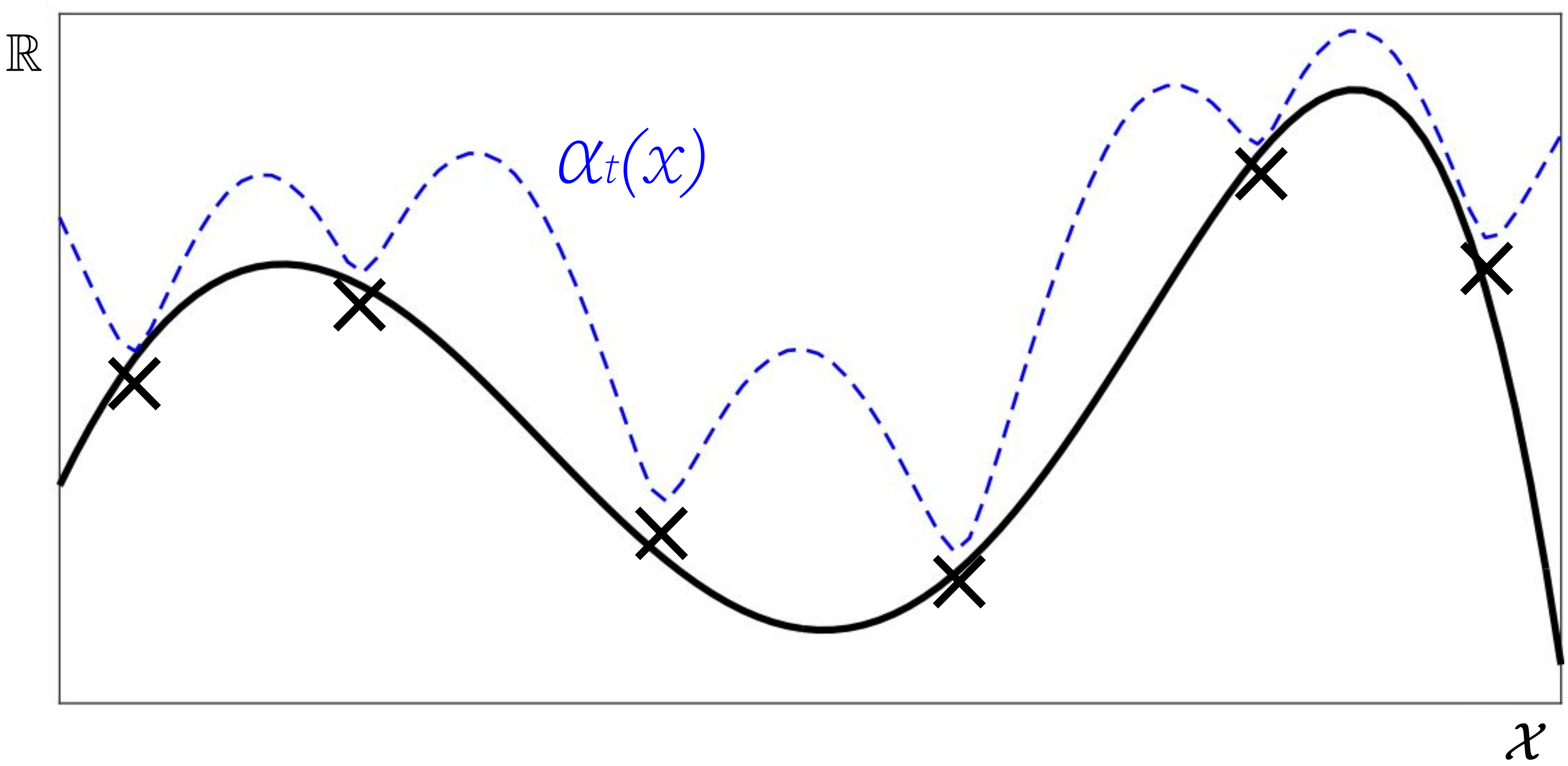
Unknown black-box f, and dataset of (x, y) pairs.

BACKGROUND

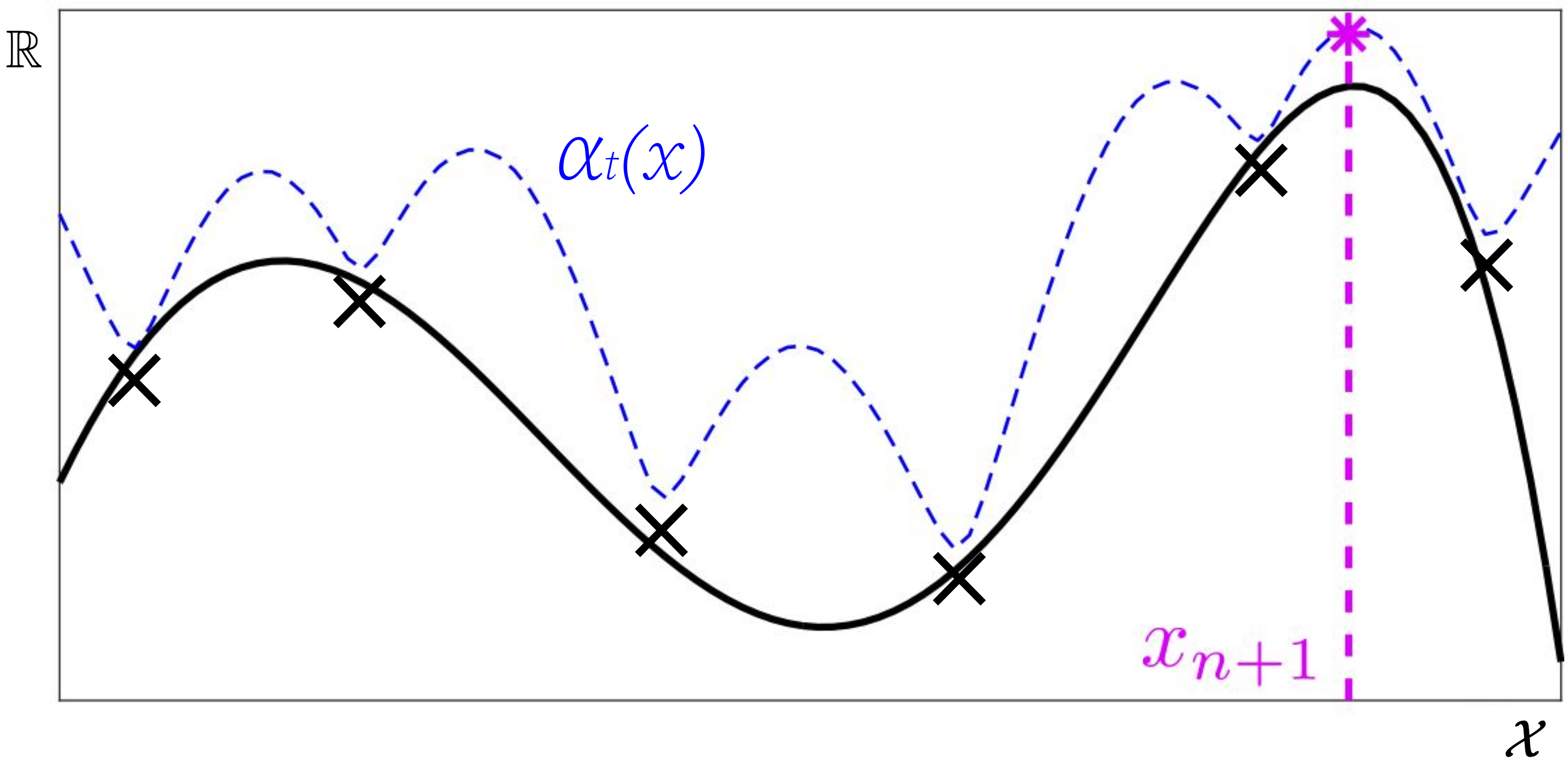


Given this dataset, can infer f using a probabilistic model.

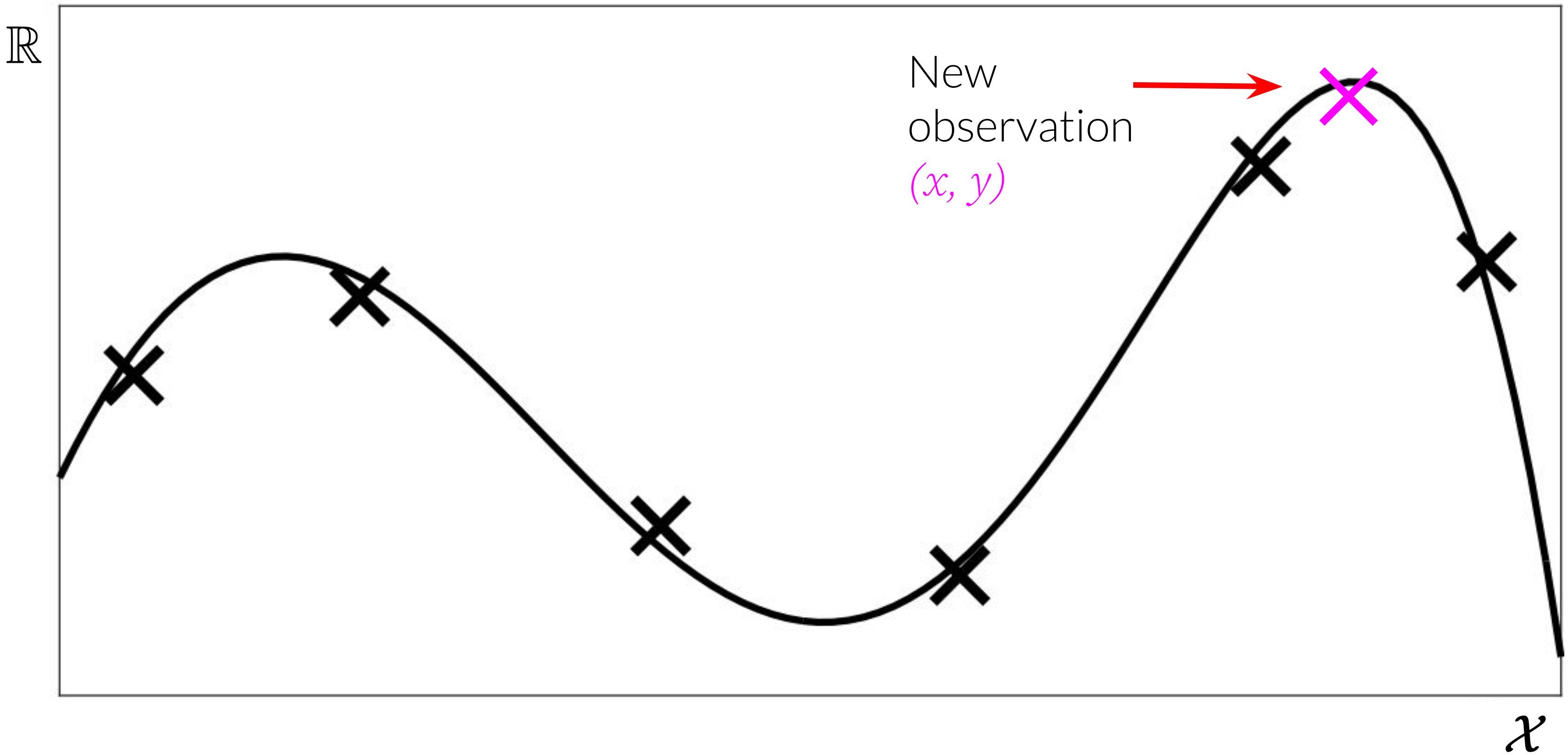
BACKGROUND



Define acquisition function using probabilistic model.



Optimize acquisition function ⇒ yields next point to query.



Query black-box f at x, observe y, and update dataset.

Information-based Bayesian Optimization

… Key step is line 2: *defining and optimizing acquisition function.*

Algorithm 1 BAYESIAN OPTIMIZATION

Input: dataset $\mathcal{D}_1$, prior distribution $p(f)$, algorithm $\mathcal{A}$

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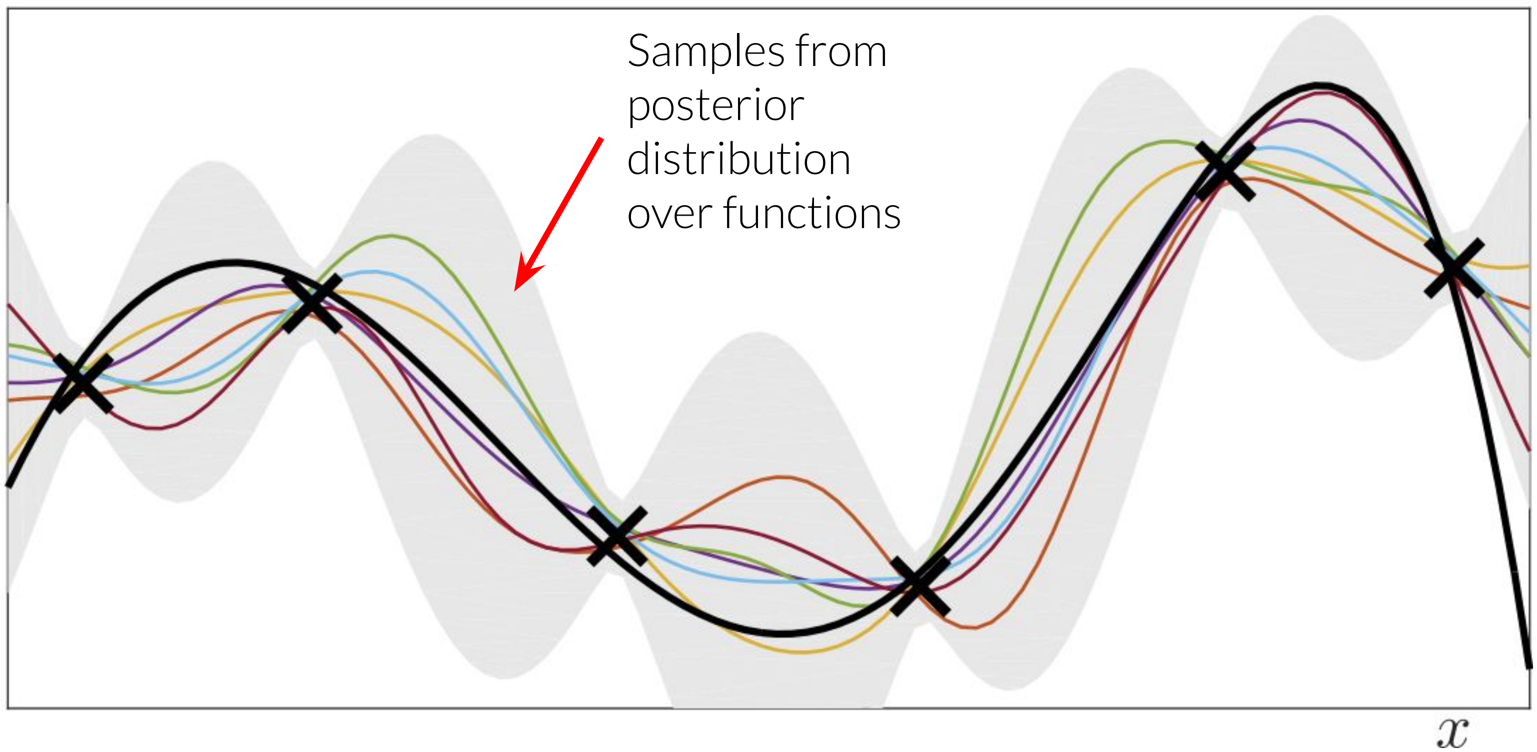
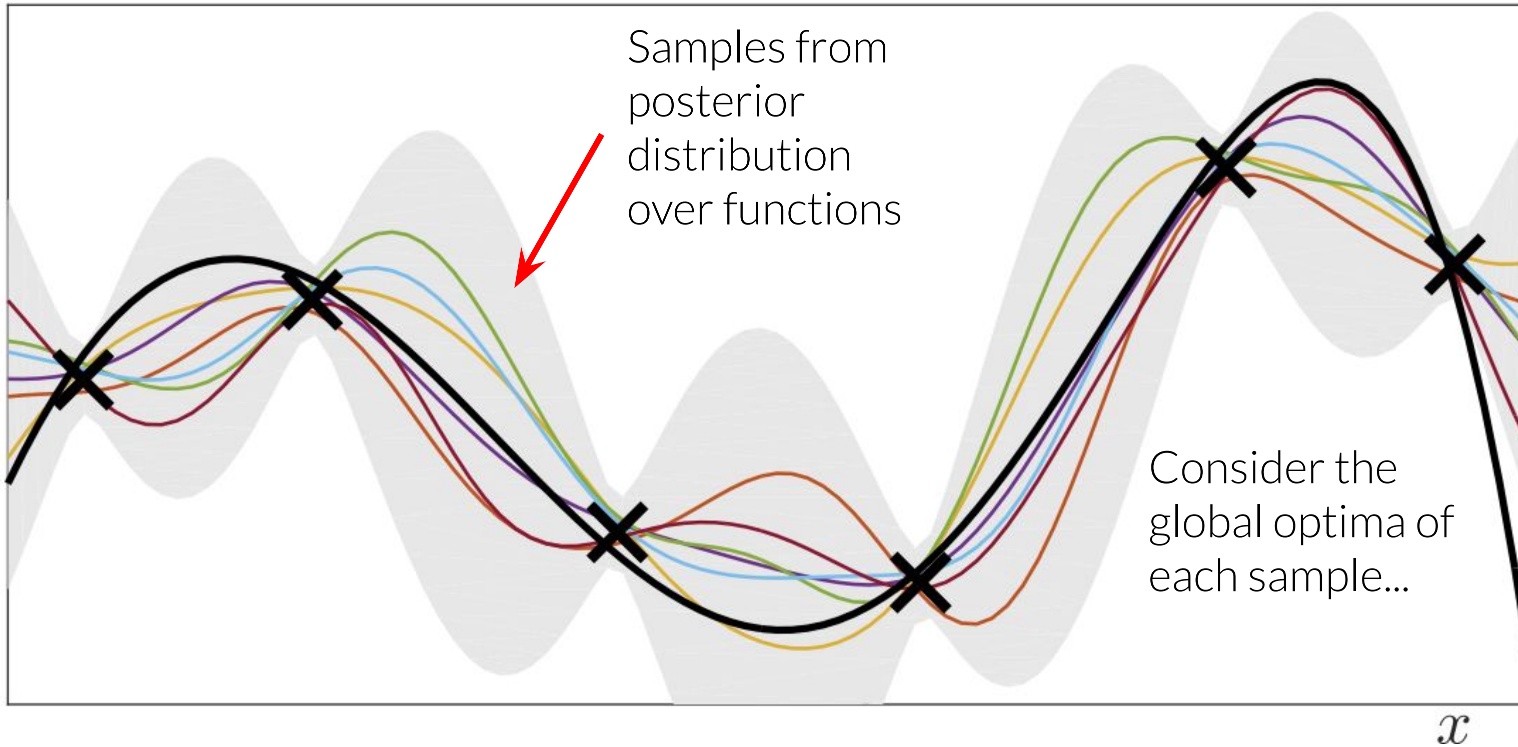
Acquisition function — info-based BO



Probabilistic model of f, given dataset.

Acquisition function — info-based BO



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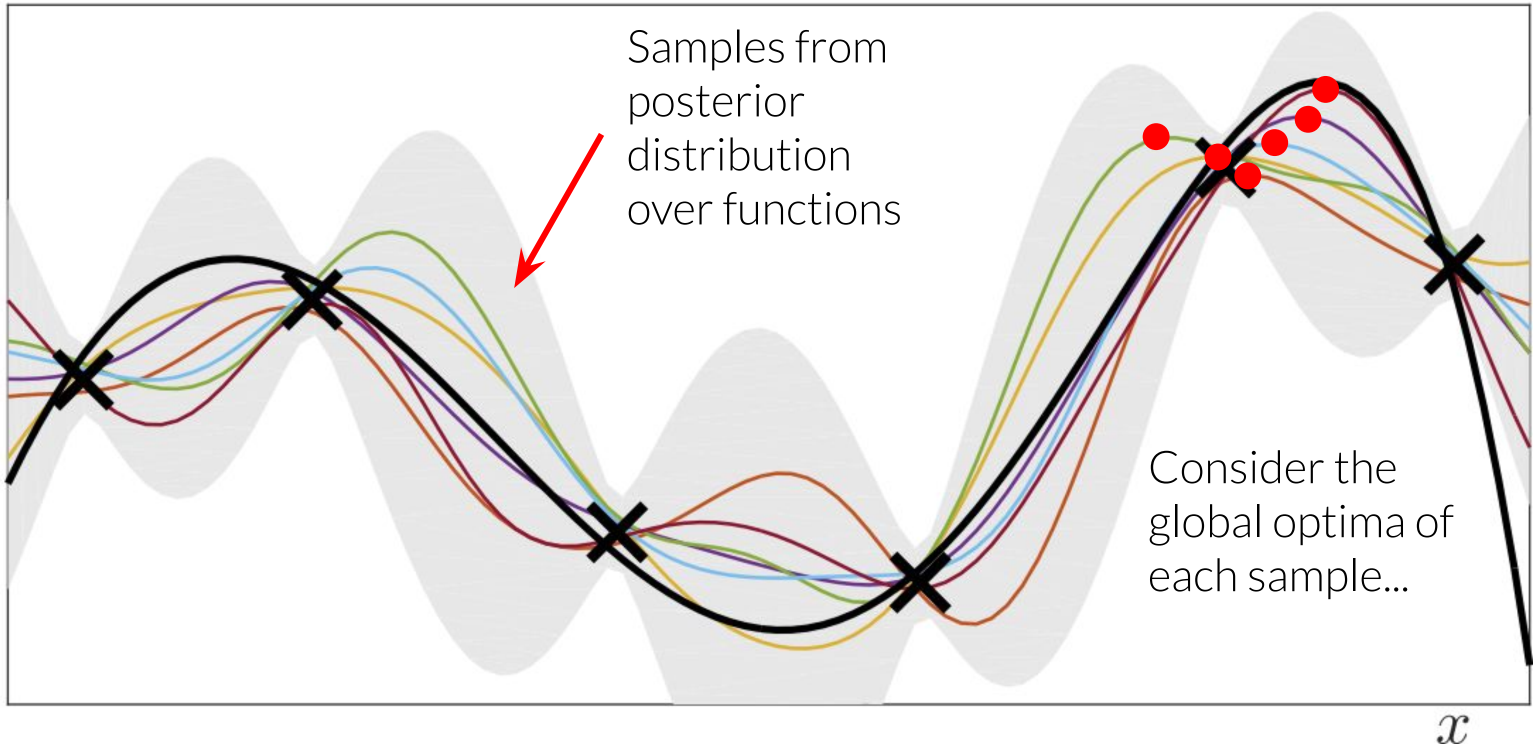
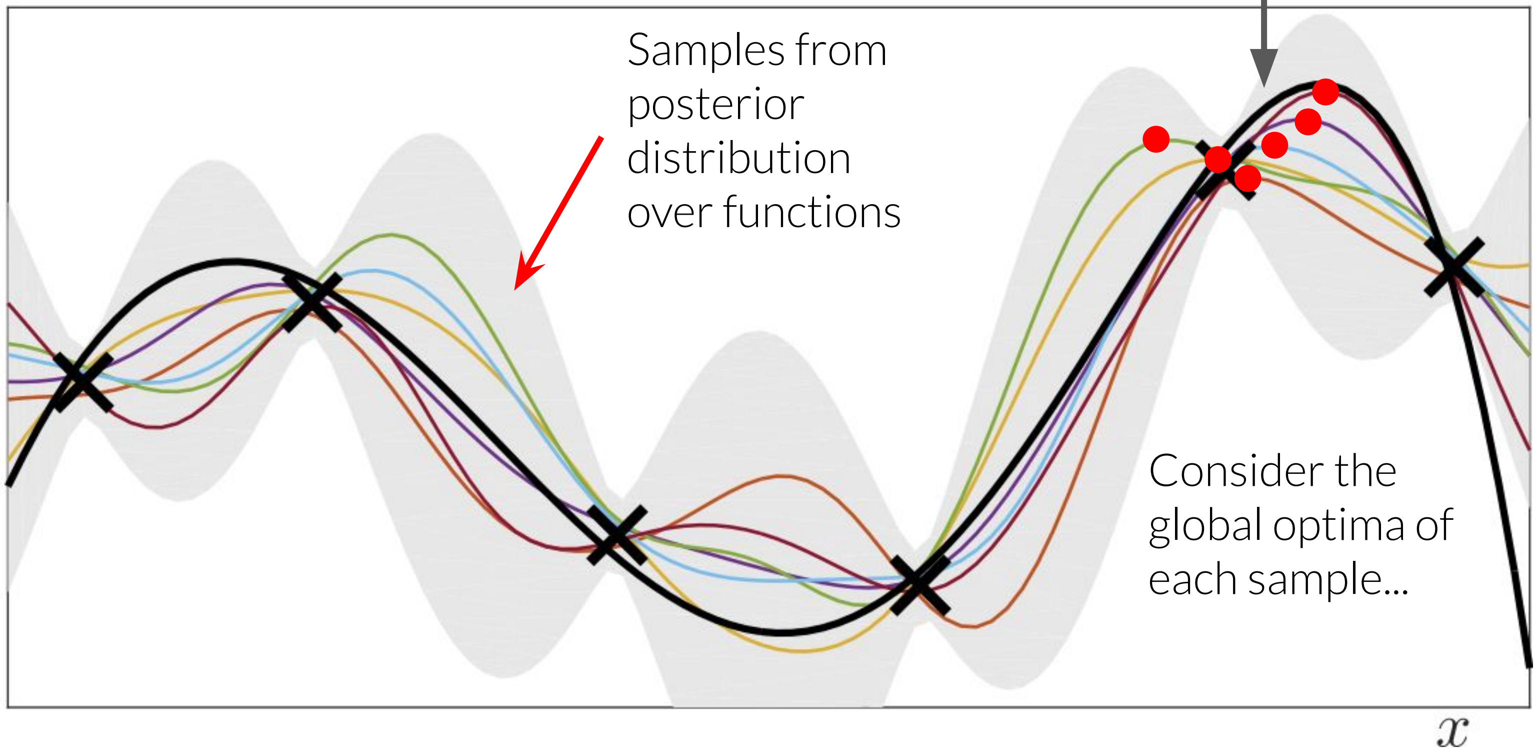


Probabilistic model of f, given dataset.

Acquisition function — info-based BO

There is a posterior distribution over global optima induced by probabilistic model: $p(x^* \mid \mathcal{D}_t)$



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This leads us to the acquisition function:

e.g. used in entropy search (ES), predictive entropy search (PES)

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$$\alpha_t(x) = H[p(x^* \mid \mathcal{D}_t)] - \mathbb{E}_{p(y_x \mid \mathcal{D}_t)}[H[p(x^* \mid \mathcal{D}_t \cup \{(x, y_x)\})]]$$

entropy of posterior distribution over global optima x^*

minus

expected entropy of posterior distribution over global optima x^*, *... if we were to make a query at x*

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"*Expected information gain*" (EIG) — expected decrease in entropy if we were to query f at x.

There exists a clever way to compute/optimize this (from work on PES)…

Acquisition function — info-based BO

How to compute and optimize it? **Two stages:**

Acquisition function — info-based BO

How to compute and optimize it? **Two stages:**

1) Before acquisition optimization:

- Generate posterior samples of global optima x^*.
- (⇒ run optimization algorithm on function samples to get optima).

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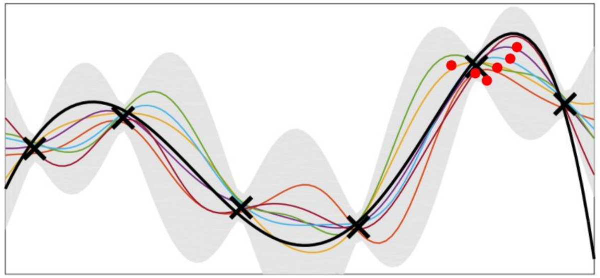
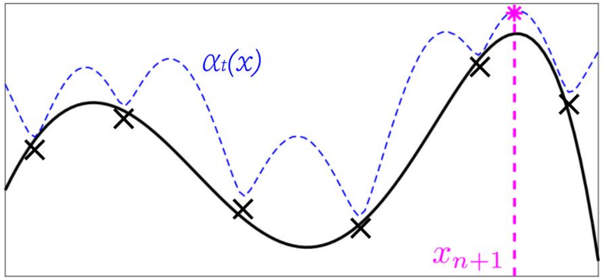
- For any x, approximate EIG $\alpha_t(x)$ using these samples.
- Allows us to optimize acquisition function.





Benefits: generate samples (of x^*) only once. Then cheaper during iterative acquisition opt.

(*previous was existing work, following is new*)

What acquisition function do we use for *InfoBAX*?

Recall goal of BAX:

- Estimate a computable function property using a limited budget of queries.
- (*equivalently:* Estimate output of algorithm $\mathcal{A}$.)

(previous was existing work, following is new)

What acquisition function do we use for *InfoBAX*?

Recall goal of BAX:

- Estimate a computable function property using a limited budget of queries.
- (*equivalently*: Estimate output of algorithm A.)

Similar to info-based BO, *take a BOED strategy*:

- Denote the output of algorithm A (computable function property): $O_{\mathcal{A}}$
- We care about posterior over output: $p(O_{\mathcal{A}} \mid \mathcal{D}_t)$
- And its entropy: $H[p(O_{\mathcal{A}} \mid \mathcal{D}_t)]$

Want to make queries to best reduce this uncertainty over algorithm output.

InfoBAX acquisition function

Can also define an expected information gain (EIG) acquisition function:

InfoBAX acquisition function

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$$\alpha_t(x) = H[p(O_{\mathcal{A}} \mid \mathcal{D}_t)] - \mathbb{E}_{p(y_x \mid \mathcal{D}_t)}[H[p(O_{\mathcal{A}} \mid \mathcal{D}_t \cup \{(x, y_x)\})]]$$

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"Expected decrease in entropy on the ***algorithm output****, if we were to query f at x."*

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expected entropy of posterior distribution over algorithm output,
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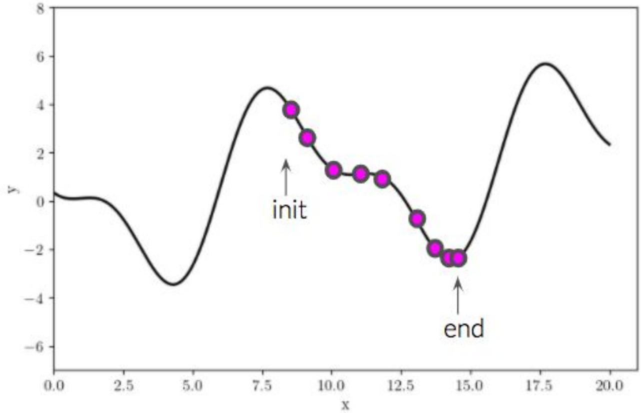
"Expected decrease in entropy on the ***algorithm output****, if we were to query f at x."*

… how can we compute (and optimize) this?

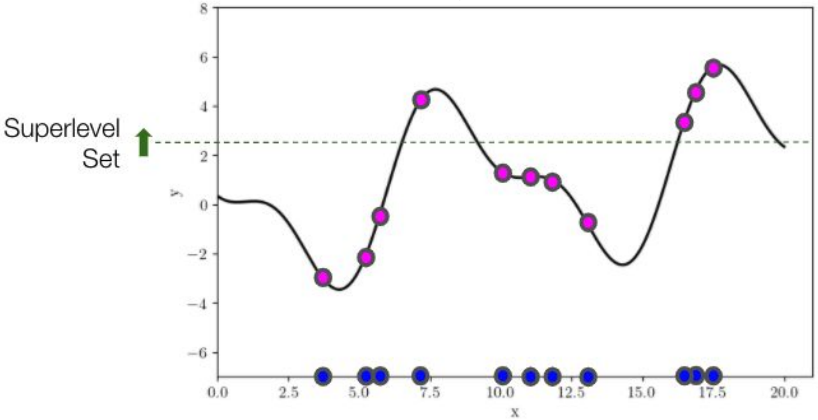
Definition:

Define the ***execution path of algorithm*** A as the sequence of queries ((x, y) pairs) that A would make on the black-box function f.

Local Optima



Superlevel Set



BAYESIAN ALGORITHM EXECUTION

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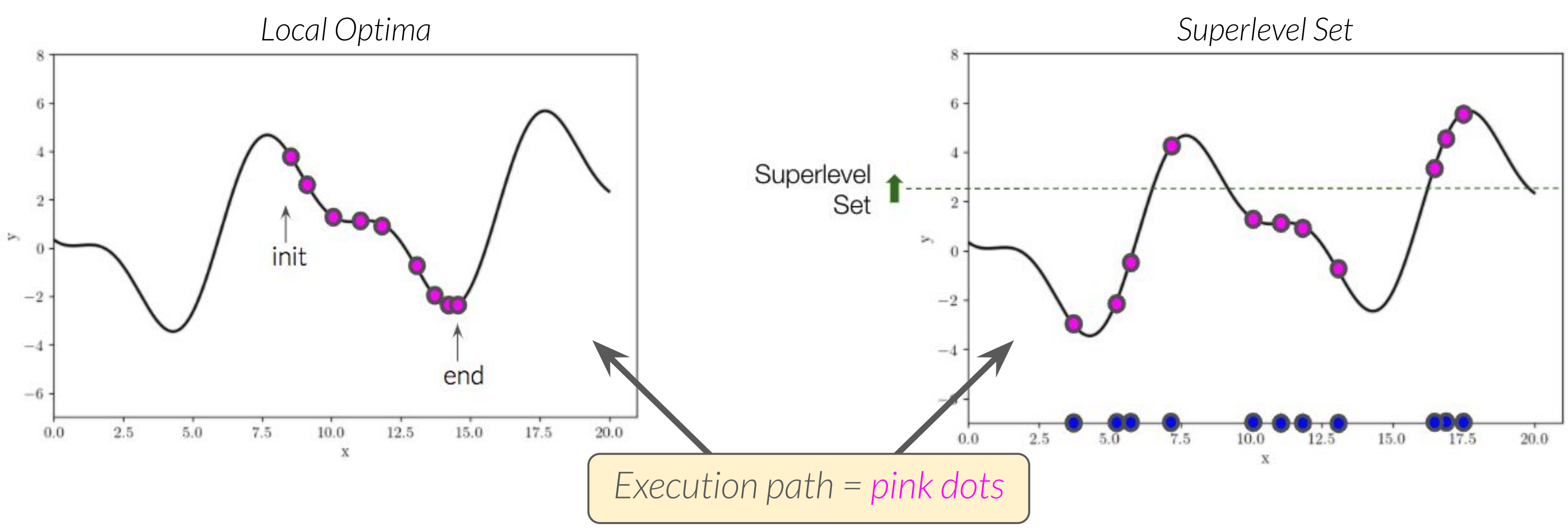

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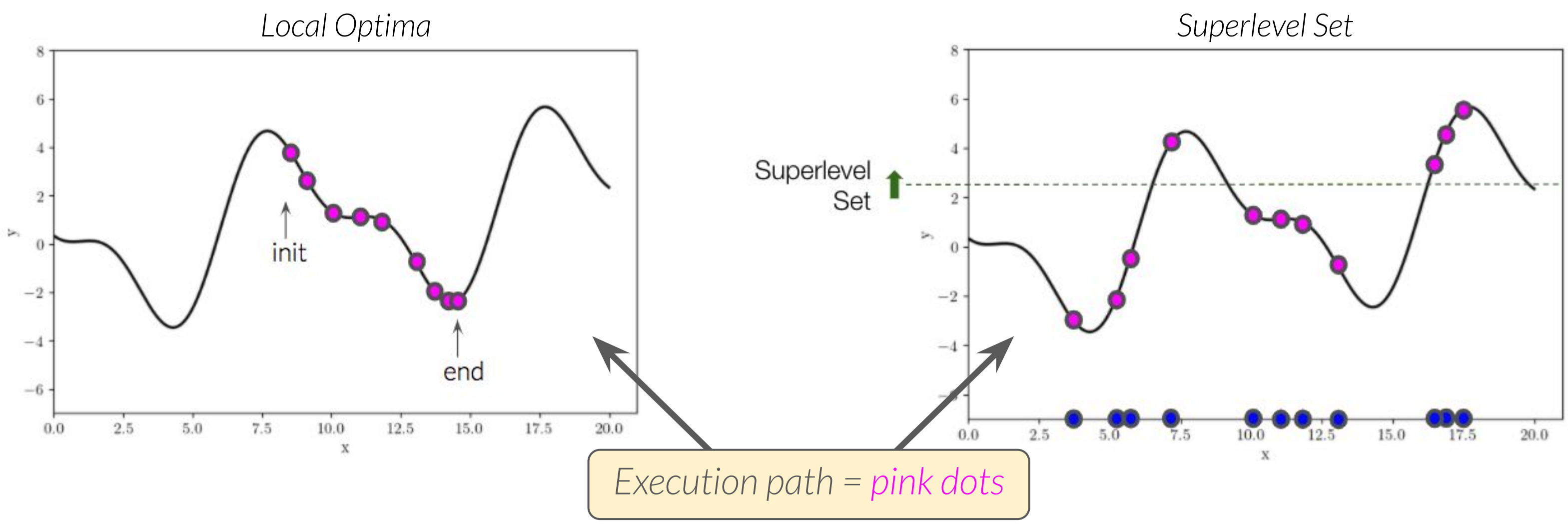
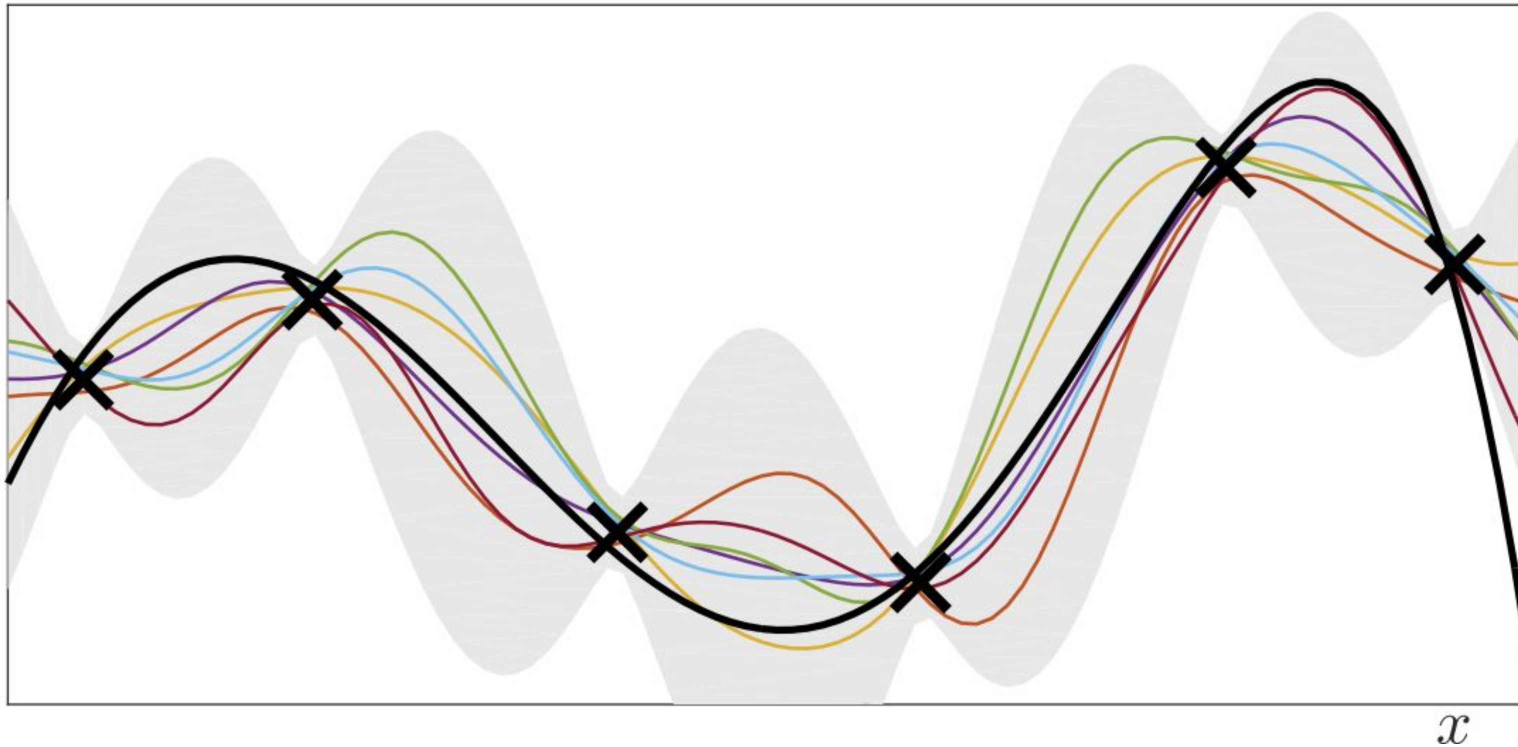


Note: we don't know true execution path.

- (Since we are not running A on $f \Rightarrow$ this require too many queries)
- But given a model for f, we have a *posterior distribution over execution paths*

InfoBAX acquisition function



Probabilistic model of f, given dataset.

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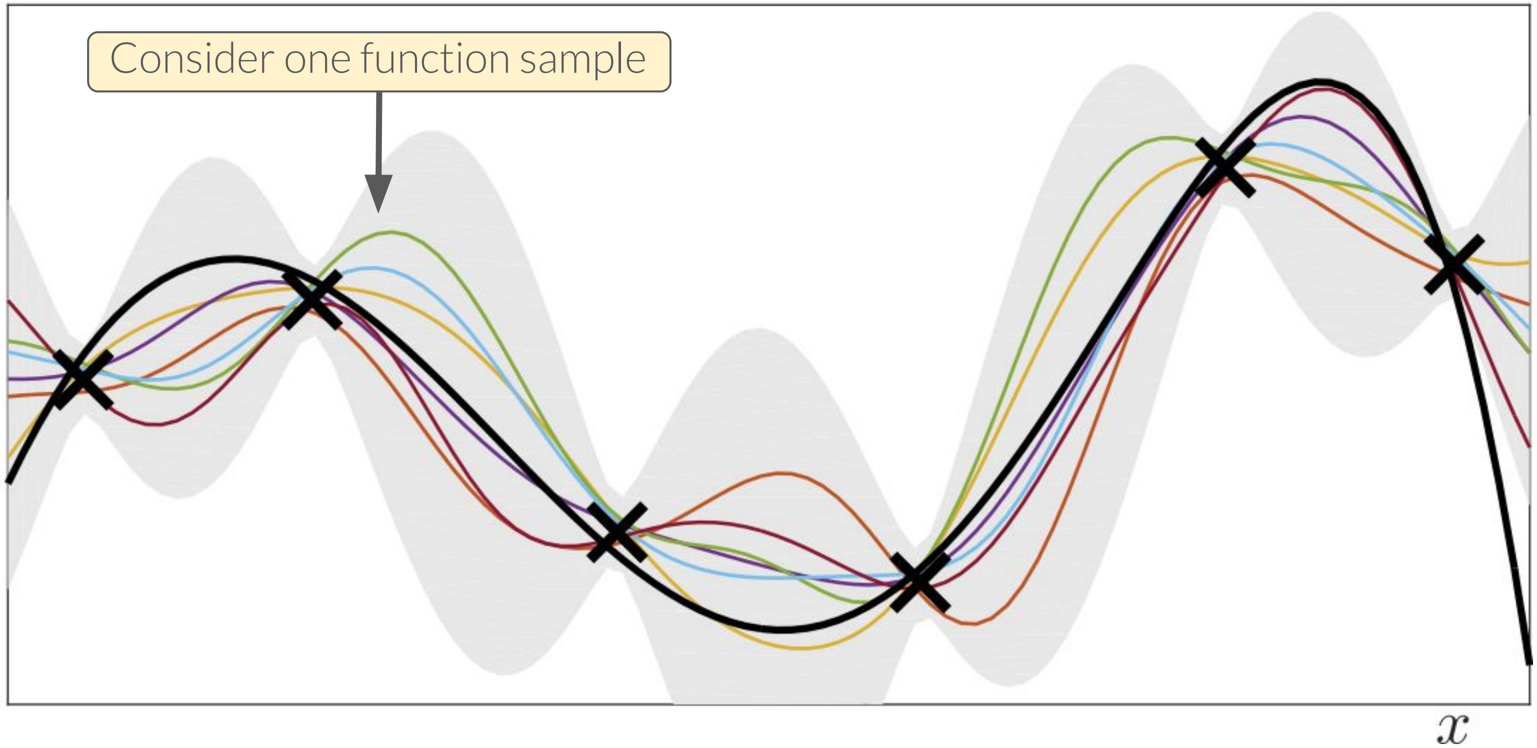

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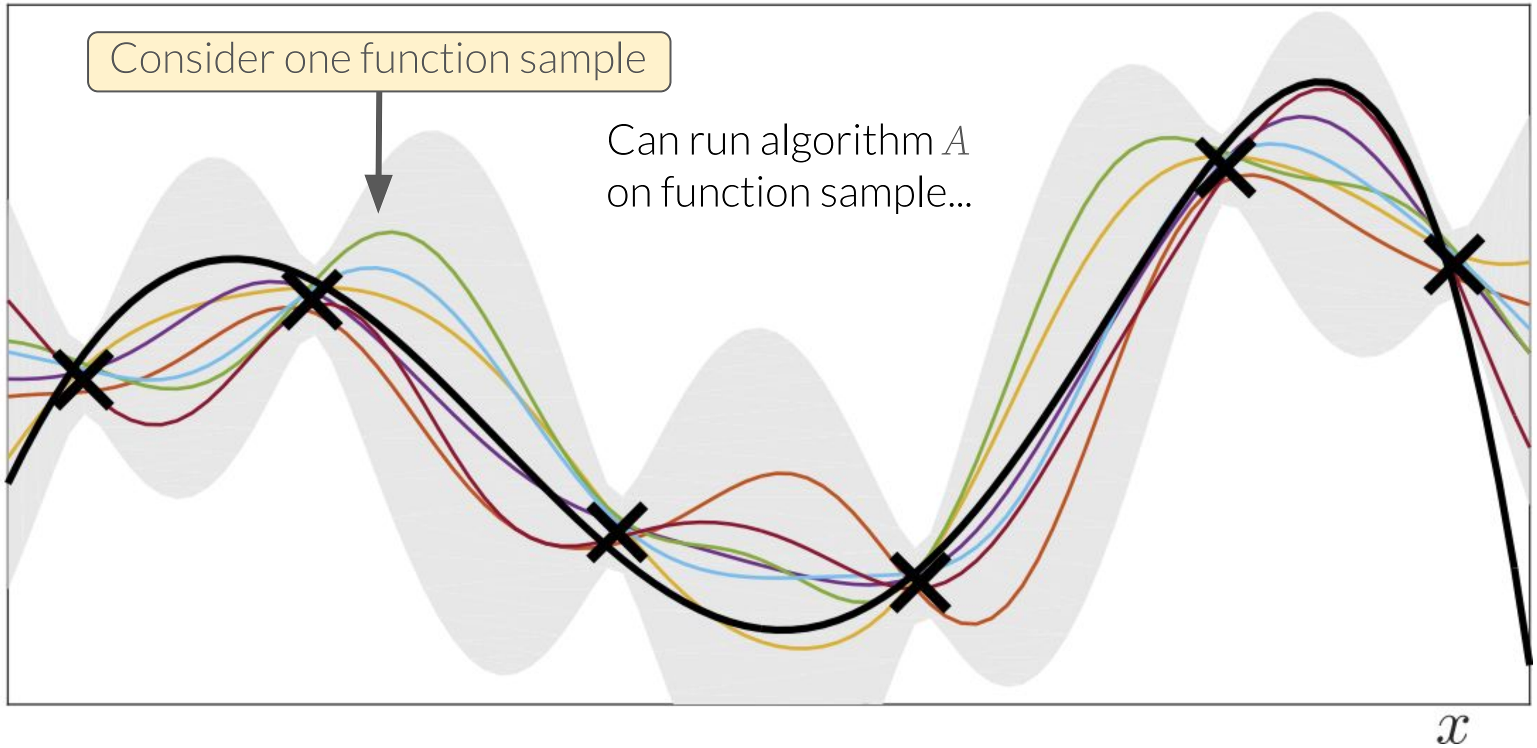

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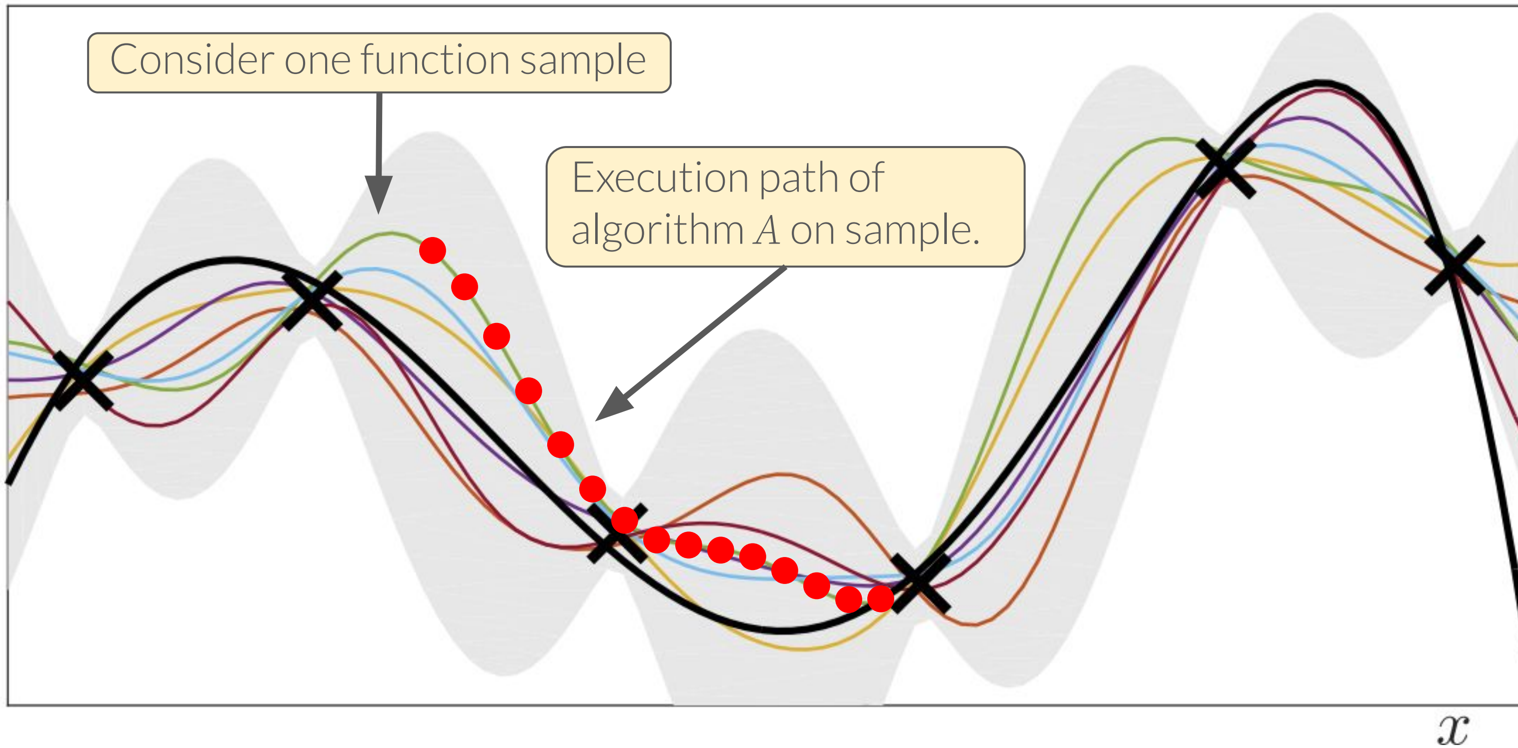

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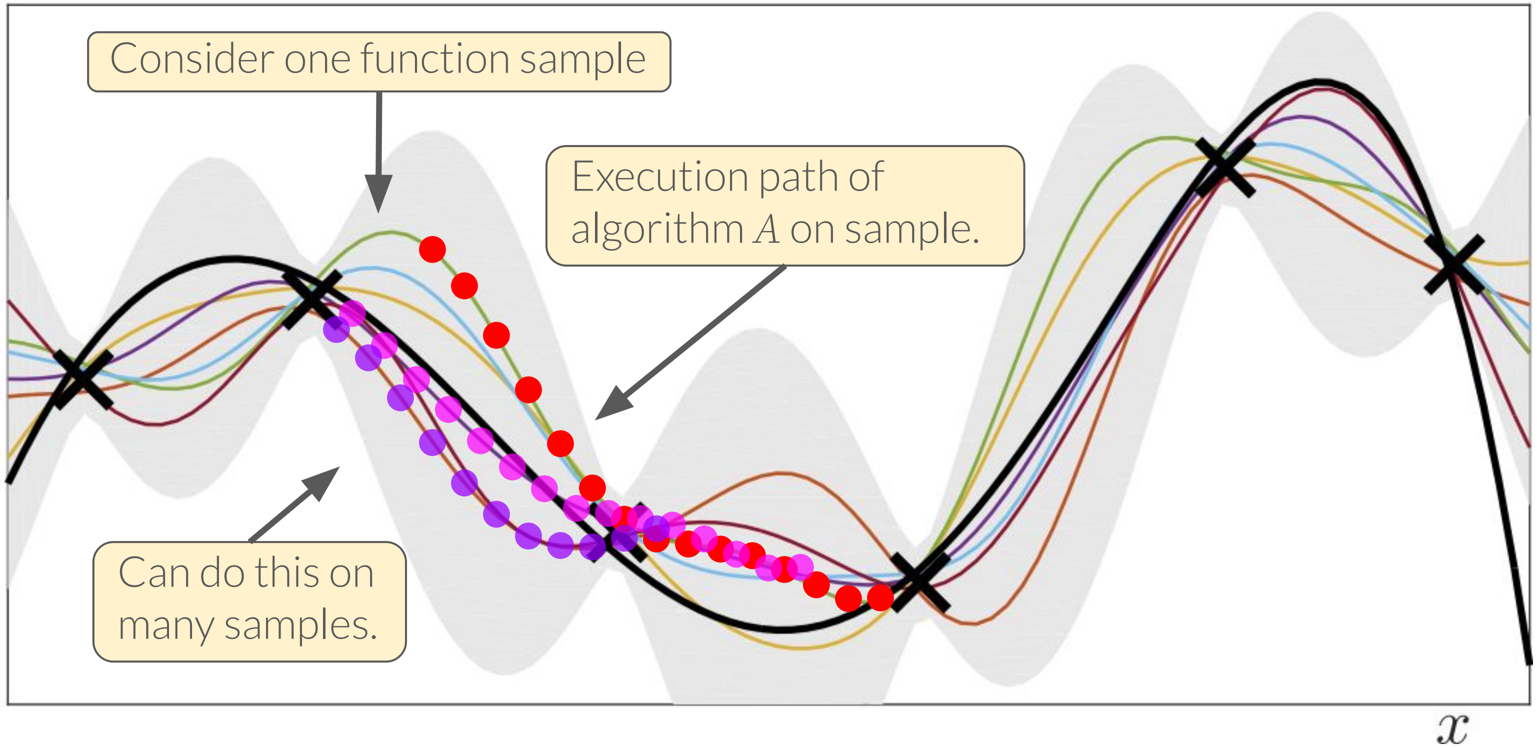

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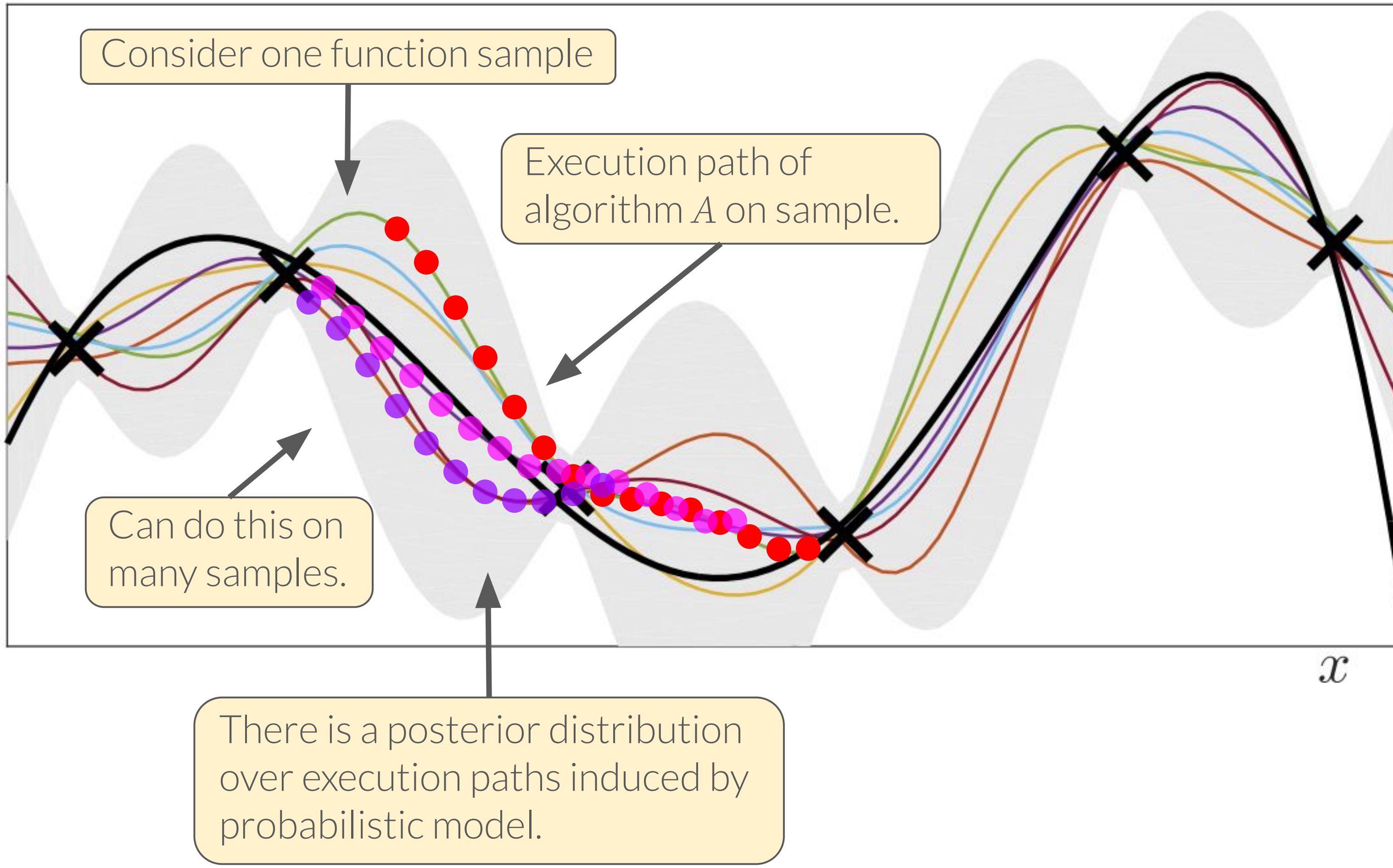

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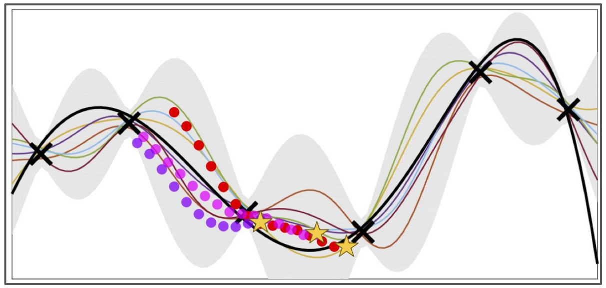

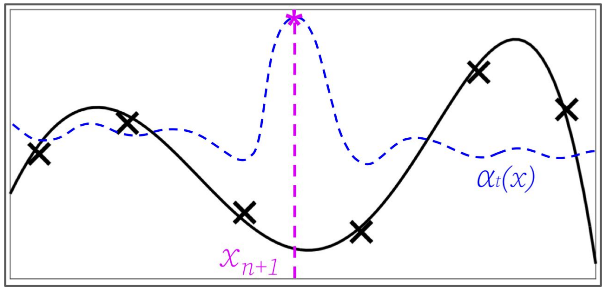

⇒ Similar structure as info-based BO, but replace global opt algorithm with A.

- *Same benefits*: generate samples only once. Then cheaper during iterative acquisition opt.

⇒ Look in paper for math on computing EIG $\alpha_t(x)$ with samples.

Information-based Bayesian algorithm execution

Algorithm 1 InfoBAX

Input: dataset $\mathcal{D}_1$, prior distribution $p(f)$, algorithm $\mathcal{A}$

1: **for** $t = 1, \ldots, T$ **do**

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4: $\quad \mathcal{D}_{t+1} \leftarrow \mathcal{D}_t \cup \{(x_t, y_{x_t})\}$

Output: final dataset $\mathcal{D}_{T+1}$

(1) Run algorithm on posterior function samples.
(2) Optimize $\alpha_t(x)$ using resulting execution paths.

InfoBAX — one-slide summary of the full story

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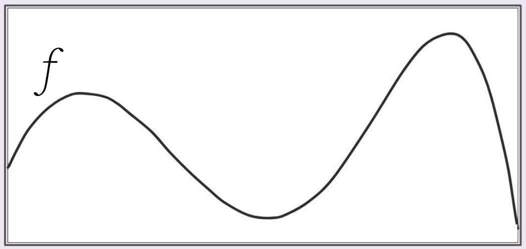
Suppose we have a black-box function f and a ***property of interest***



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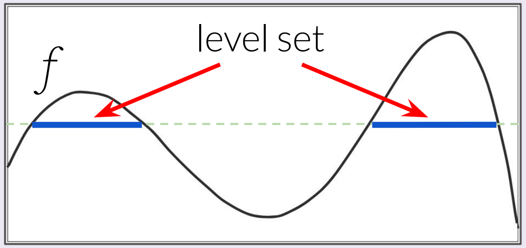

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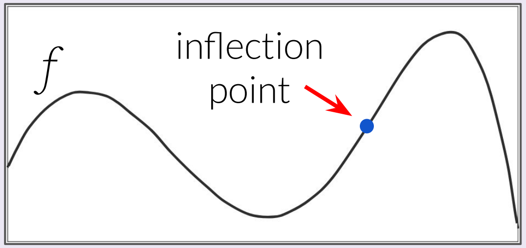

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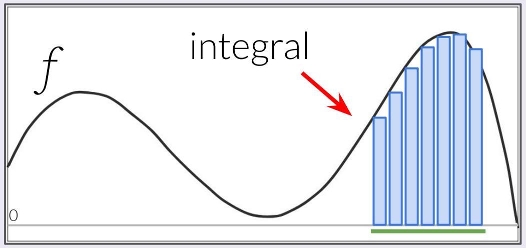

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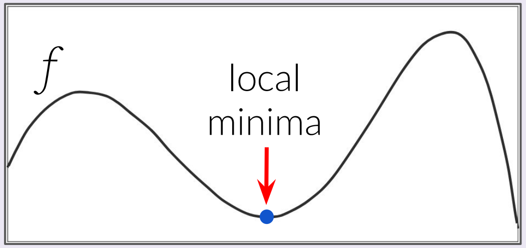

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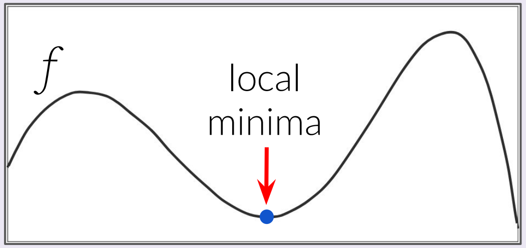
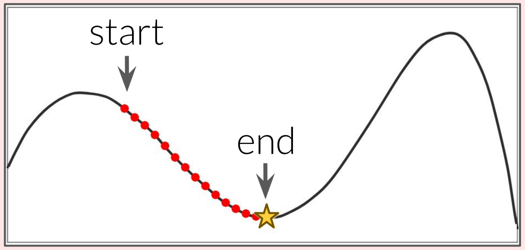


Suppose property is ***computable*** $\Rightarrow$ *there exists an algorithm A (of any budget)*



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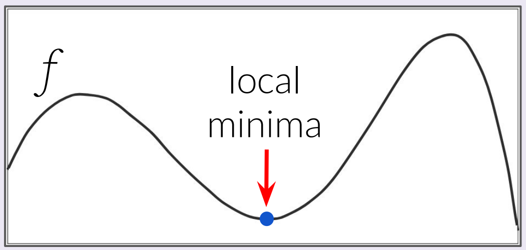

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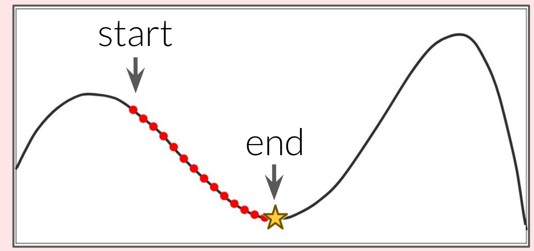

⇒ ***Goal:*** *estimate the property (i.e. output of A) with minimal function queries*

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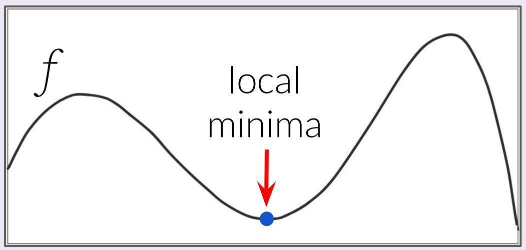

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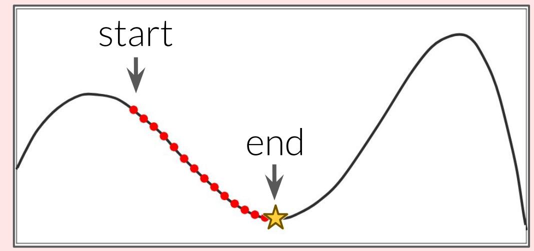


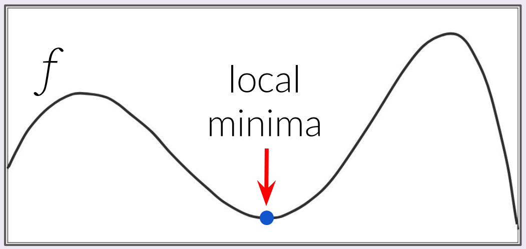
⇒ ***Goal:*** *estimate the property (i.e. output of A) with minimal function queries*

Run ***InfoBAX****, a sequential algorithm*
(similar in structure to BO)

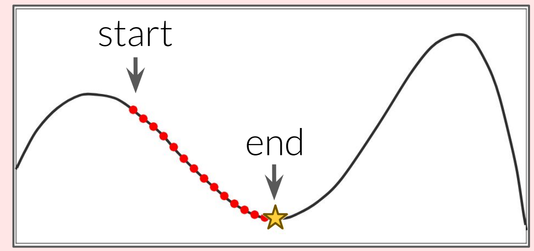
for $t = 1, \ldots, T$ **do**
  $x_t \leftarrow \arg\max_{x \in \mathcal{X}} \alpha_t(x, \mathcal{A})$
  $y_{x_t} \sim f(x_t) + \epsilon$
  $\mathcal{D}_{t+1} \leftarrow \mathcal{D}_t \cup \{(x_t, y_{x_t})\}$

InfoBAX — one-slide summary of the full story

*Suppose we have a black-box function f and a **property of interest***



*Suppose property is **computable** ⇒ there exists an algorithm $\mathcal{A}$ (of any budget)*



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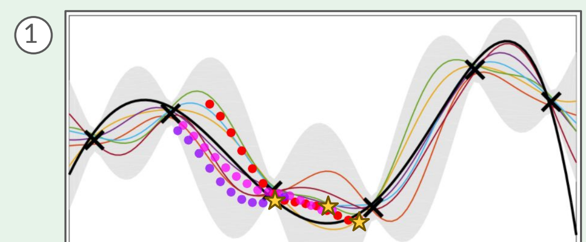
*(at each iteration) To optimize InfoBAX acquisition function: **two stages***



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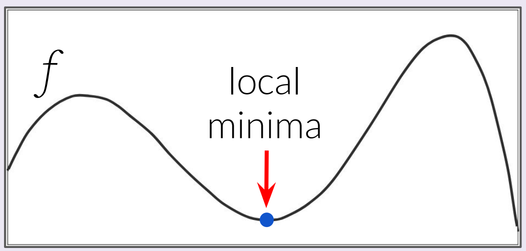

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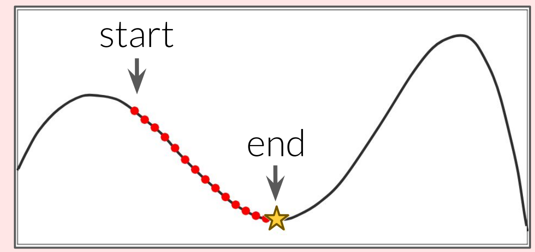

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$$
\begin{array}{l}
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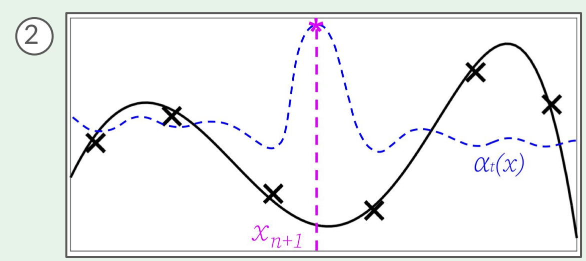

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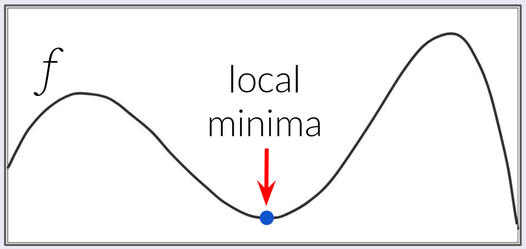

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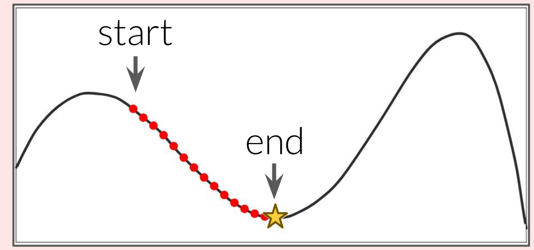

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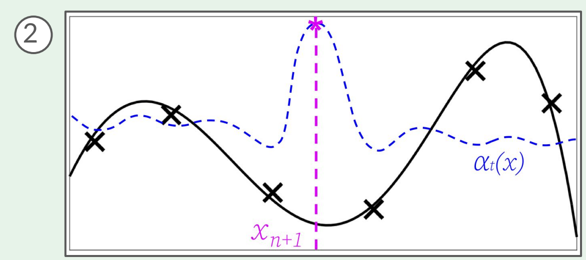


⇒ ***Output:*** *posterior estimate of property (i.e. output of A)*

BAX: Demos and Applications

Applications

We demo BAX to estimate a few different properties of black-box functions
(trying to show the breadth of what we can estimate)

Three applications:

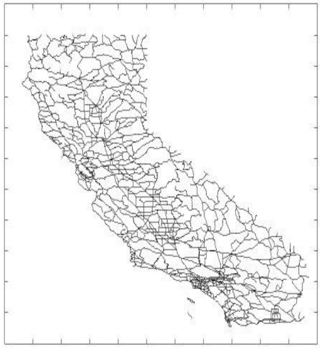
- Estimating shortest paths in graphs ← Black-box function over edges in a network
- Bayesian local optimization ← Optimization variants
- Estimating top-*k* optima ← Optimization variants

Application: *estimating shortest paths in graphs*

Graph traversal/search algorithms can define properties of a black-box function f defined on edge weights in a graph.

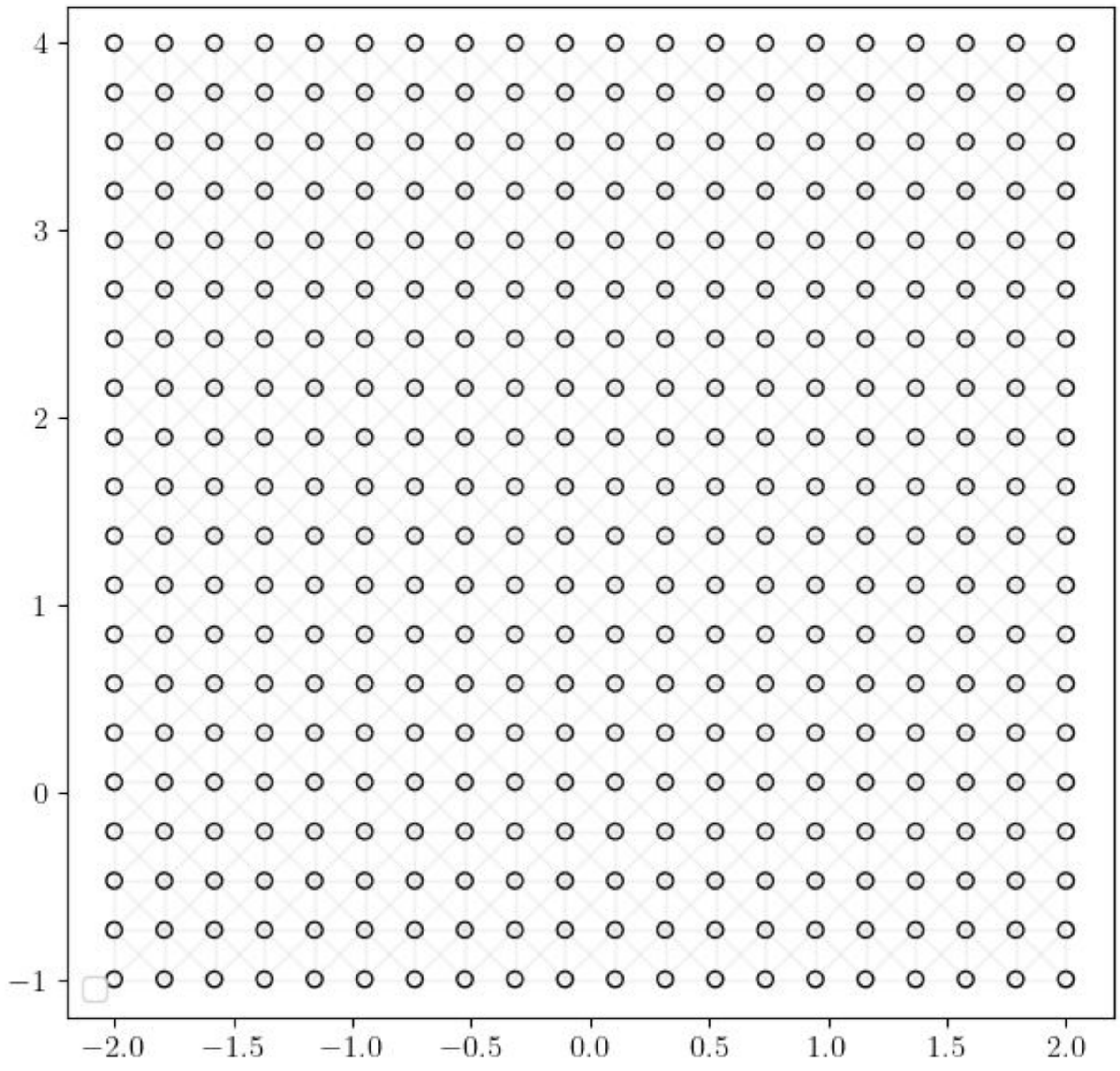
Example: *real-world transportation network*
(e.g. road, railway, shipping, air)

- Suppose we want to find shortest path from location A to location B.
- Shortest path depends on edge weights.
  - e.g. traffic, road conditions, weather, etc.
- It can be ***expensive to query edge weights***
  - e.g. measure traffic/road/weather conditions via satellite.
  - e.g. determine/access shipping costs.
- **Goal**: adaptively query edge weights to estimate shortest path.



California road network.

APPLICATIONS of BAX — *estimating shortest paths in graphs*

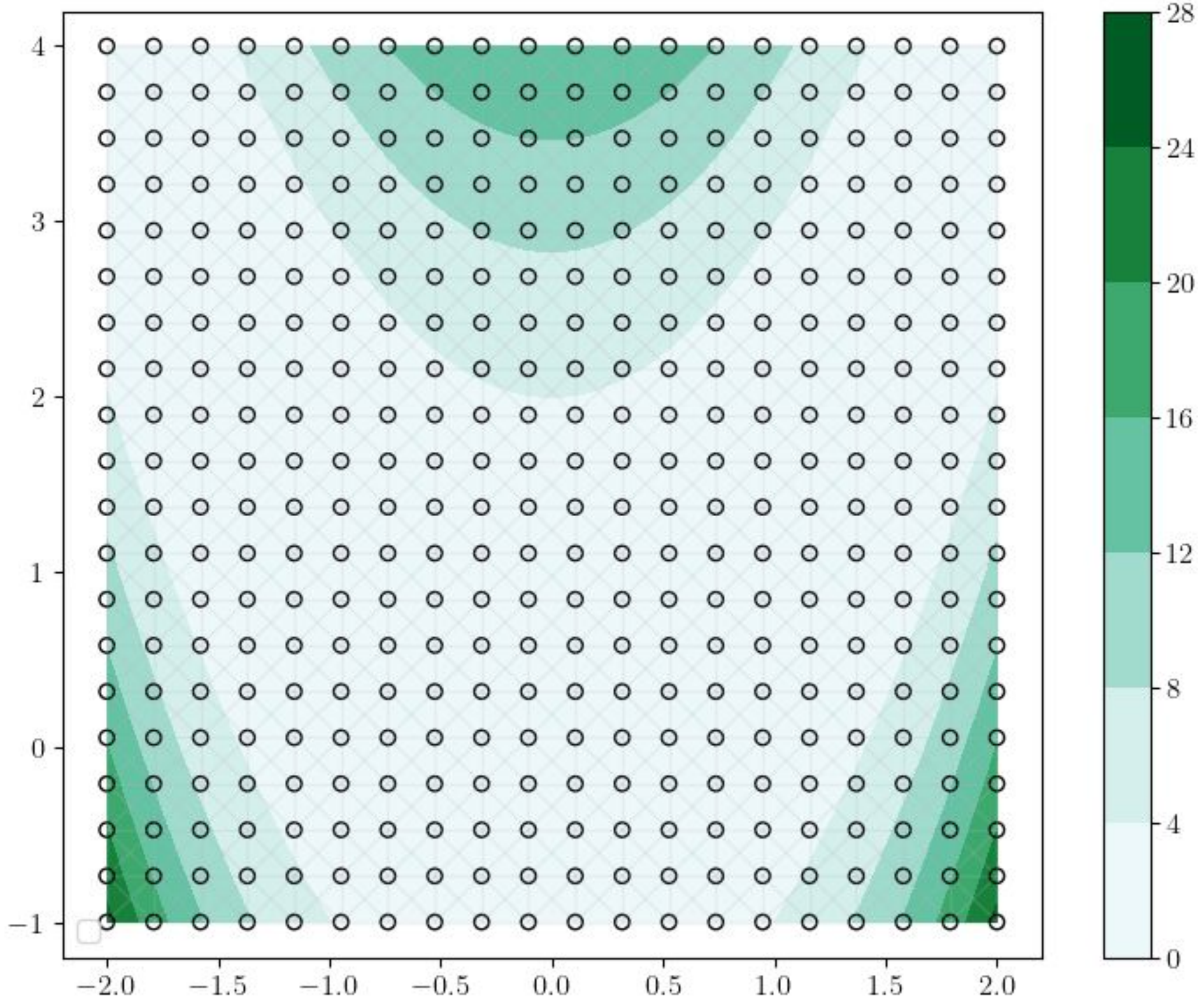


Grid-shaped graph:

- 400 nodes
- 2964 edges

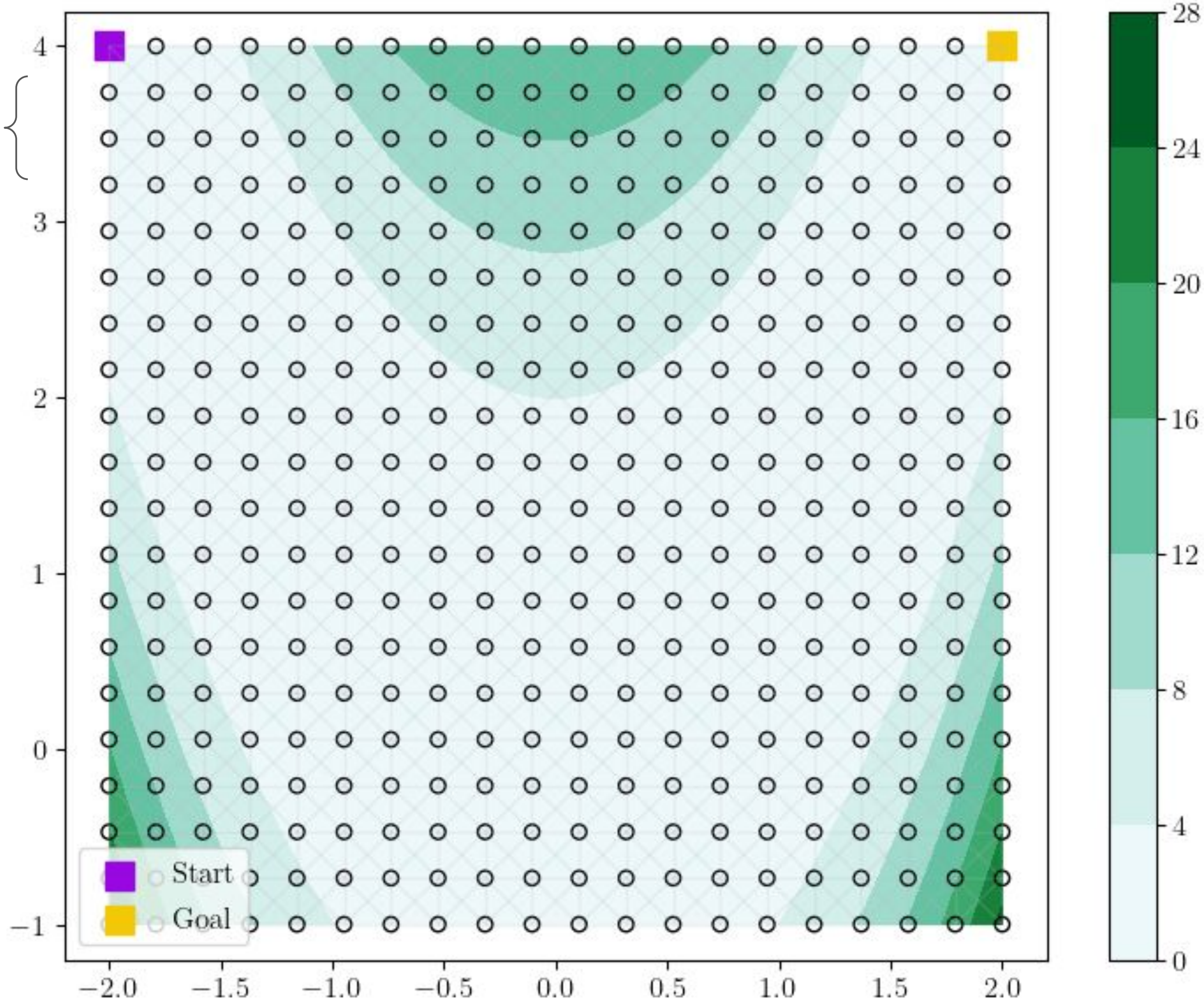
APPLICATIONS of BAX — *estimating shortest paths in graphs*

Edge weights are given by function f (green).



APPLICATIONS of BAX — *estimating shortest paths in graphs*

Want to know shortest path between start and goal.



APPLICATIONS of BAX — *estimating shortest paths in graphs*

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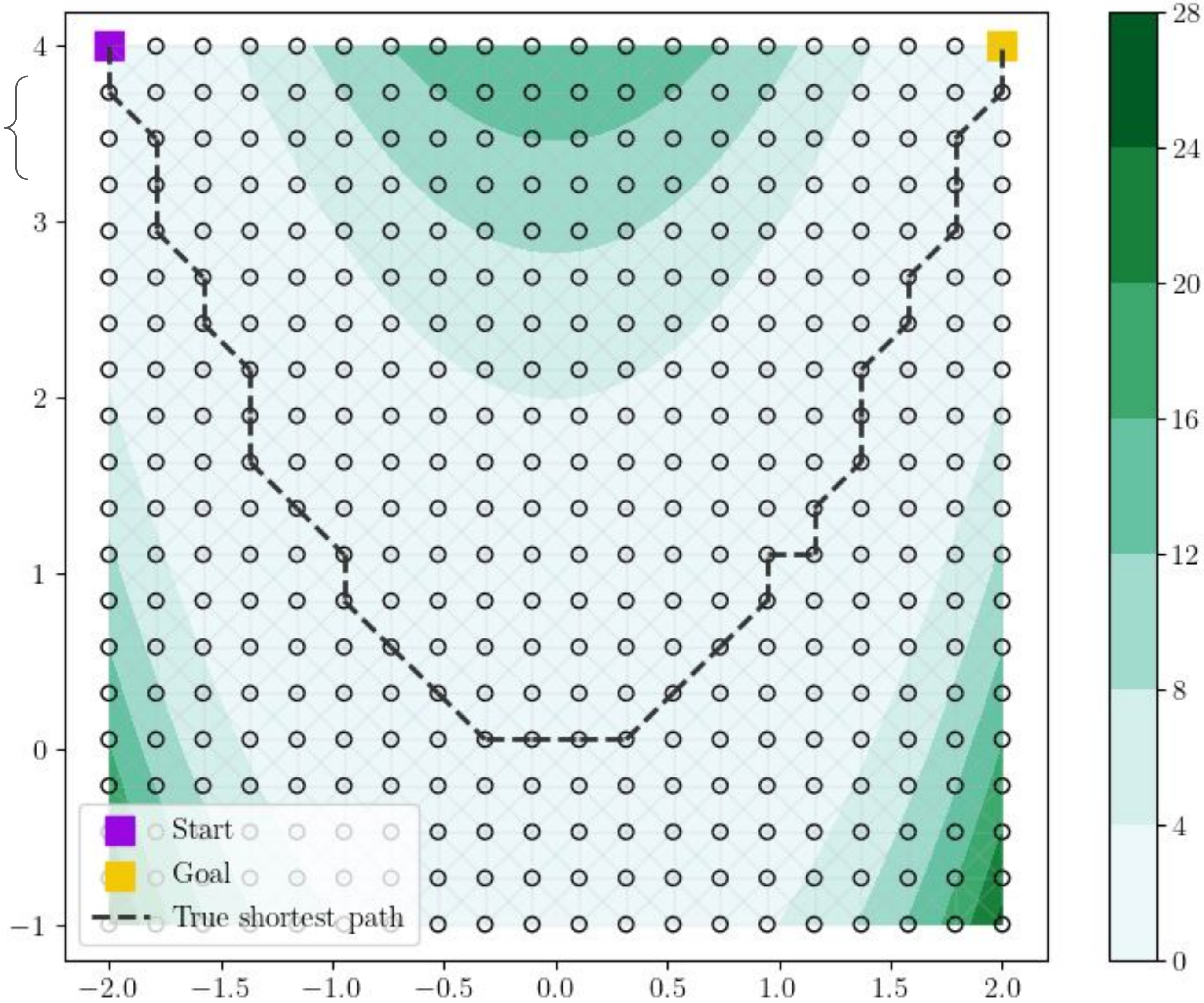

APPLICATIONS of BAX — *estimating shortest paths in graphs*

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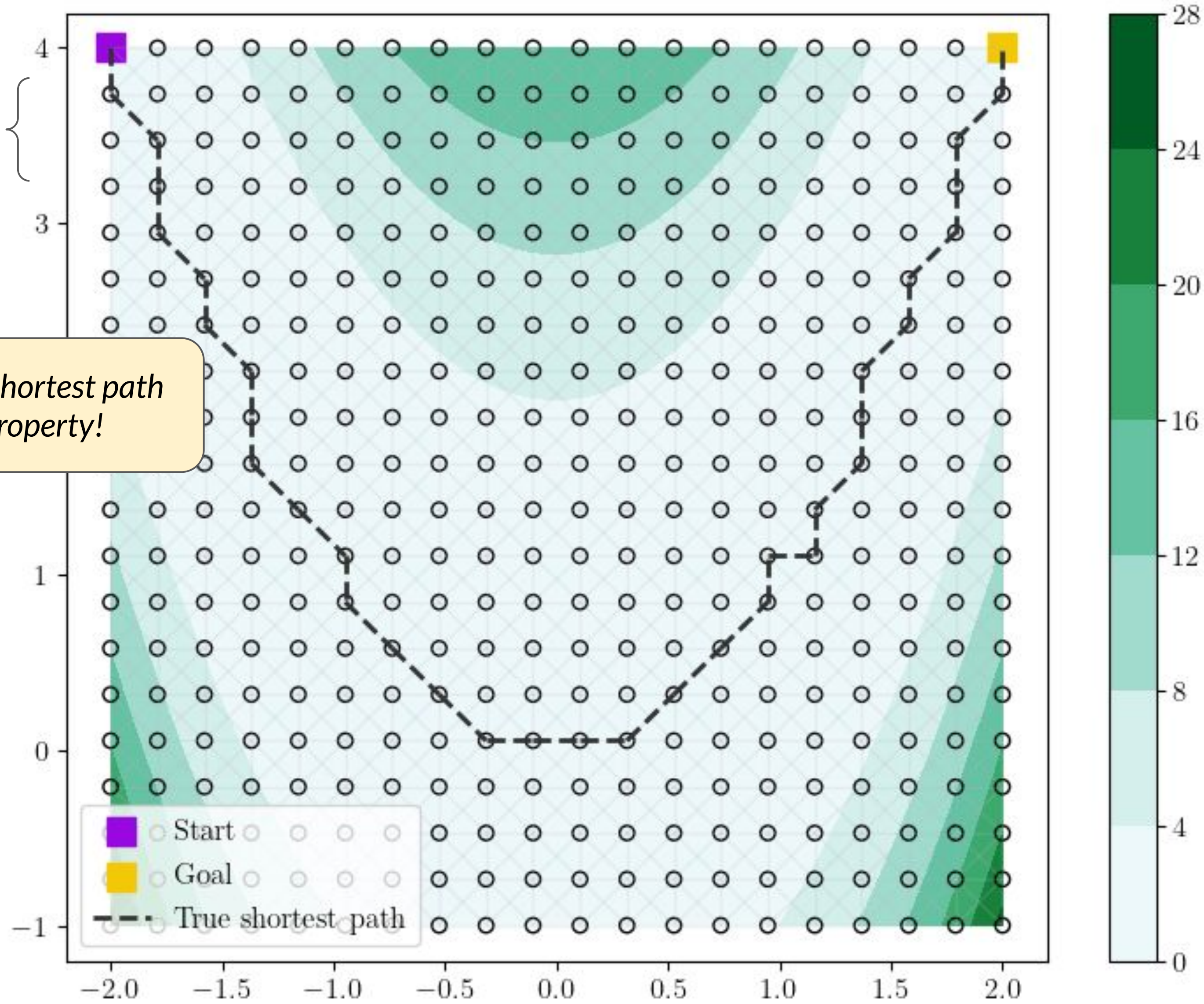
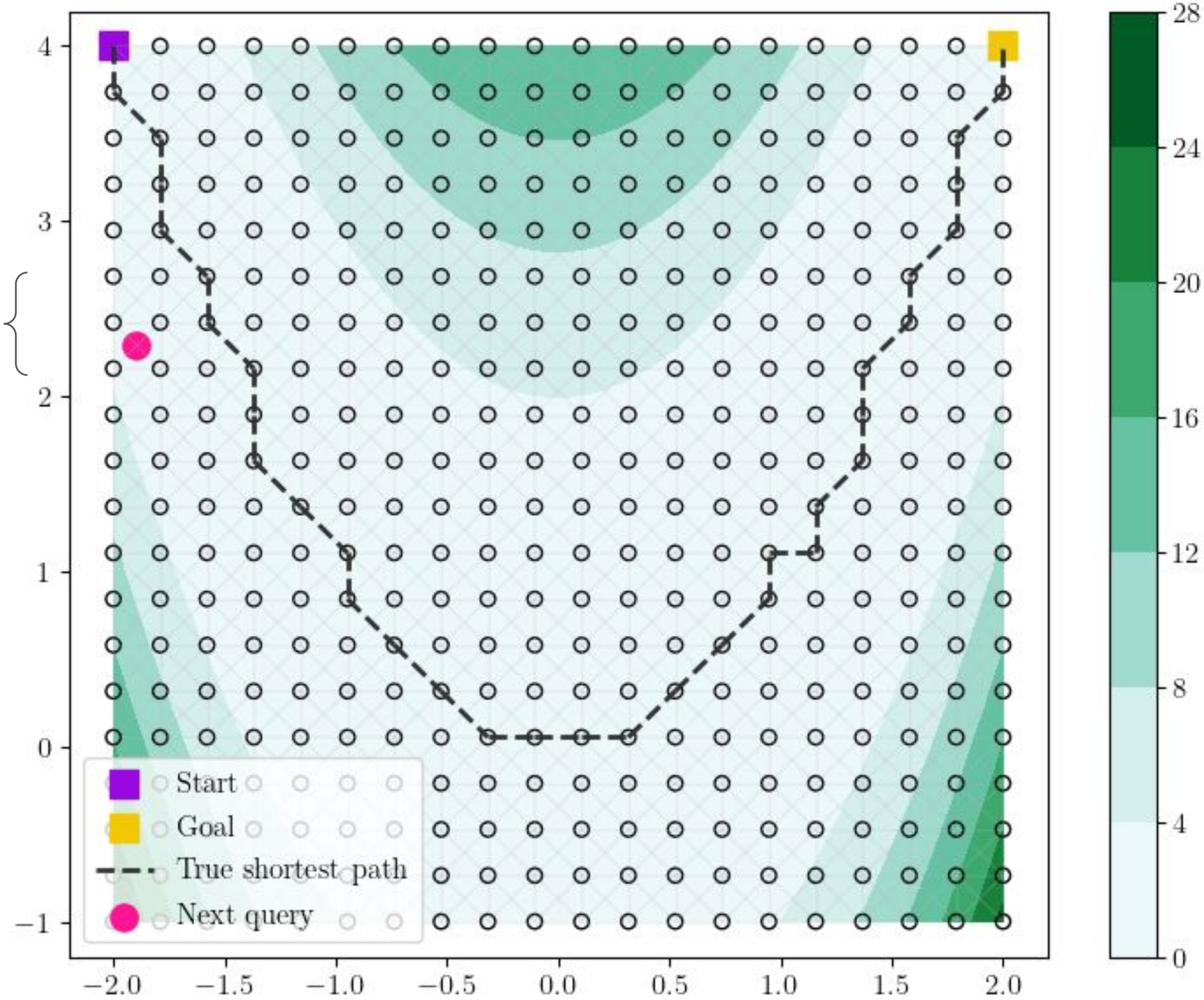


Can view this shortest path as a function property!

APPLICATIONS of BAX — *estimating shortest paths in graphs*

Suppose that accessing (*querying*) edge weights is expensive.

→ e.g. in transportation network examples



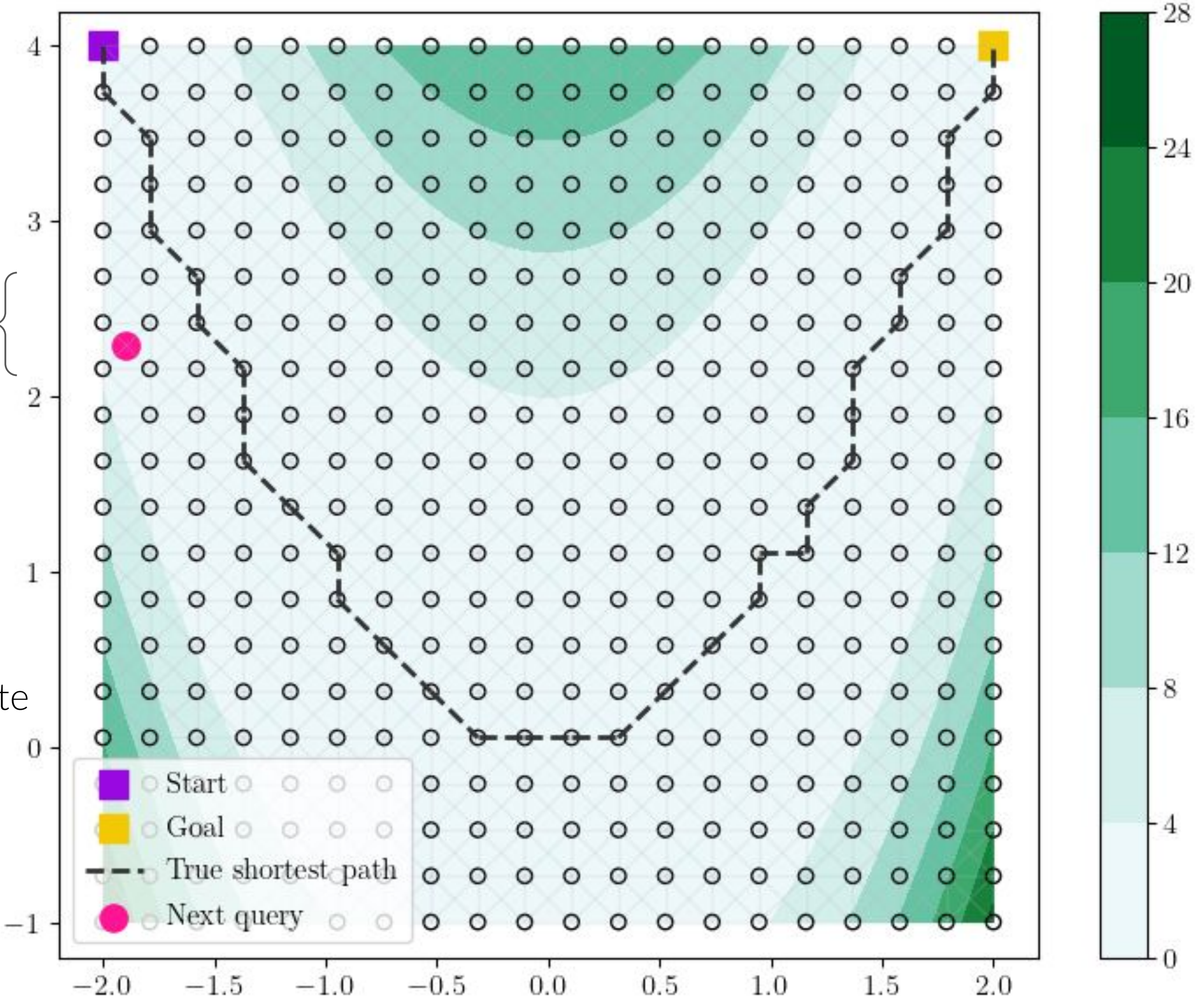
APPLICATIONS of BAX — *estimating shortest paths in graphs*

Suppose that accessing (*querying*) edge weights is expensive.

→ e.g. in transportation network examples

How to estimate shortest path?

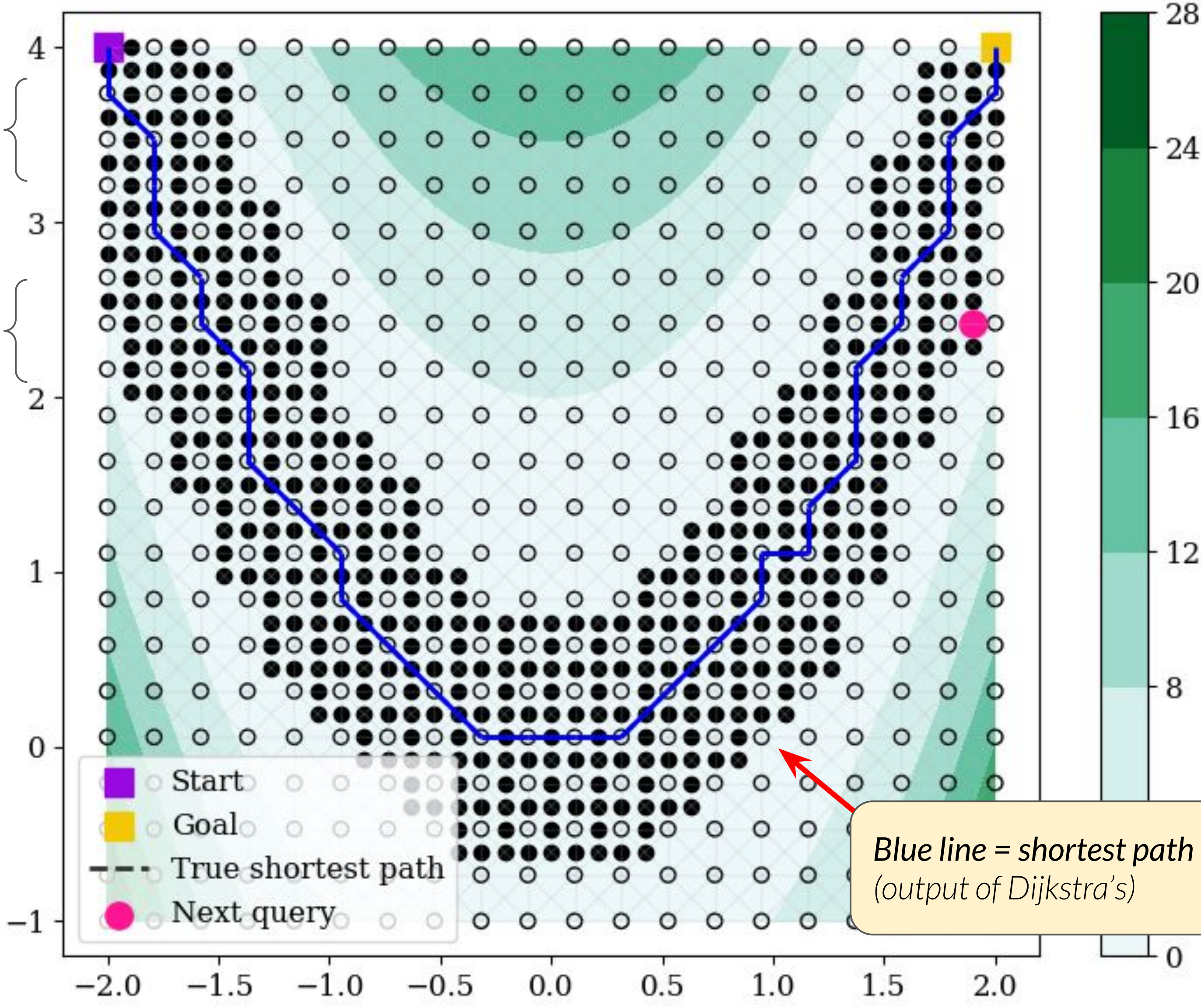
One strategy: use *Dijkstra's algorithm*



APPLICATIONS of BAX — *estimating shortest paths in graphs*

One strategy: use *Dijkstra's algorithm*

Exactly computes the shortest path



Blue line = shortest path
(output of Dijkstra's)

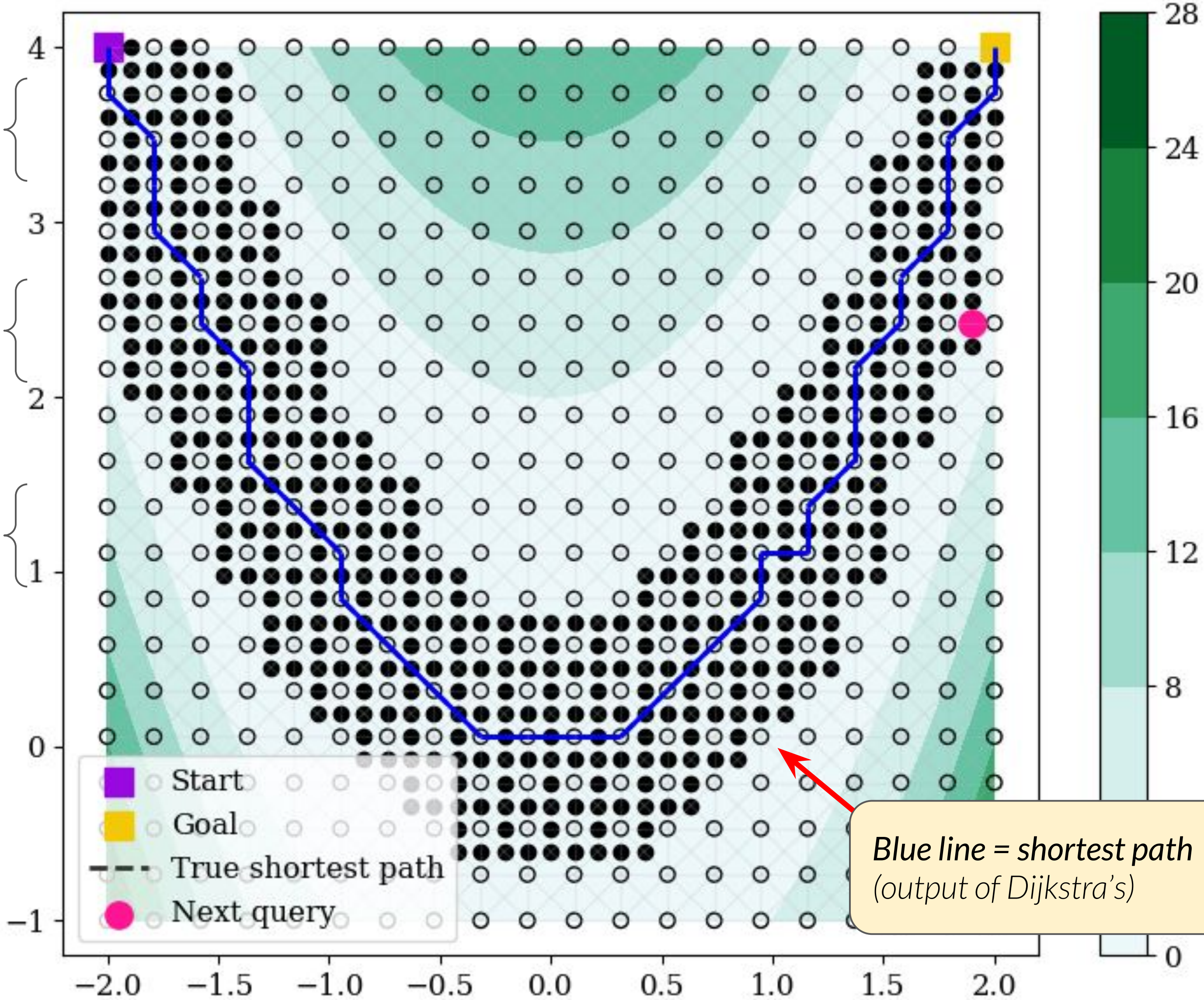
APPLICATIONS of BAX — *estimating shortest paths in graphs*

One strategy: use *Dijkstra's algorithm*

Exactly computes the shortest path

However… requires over 430 queries!

Can try a different strategy…



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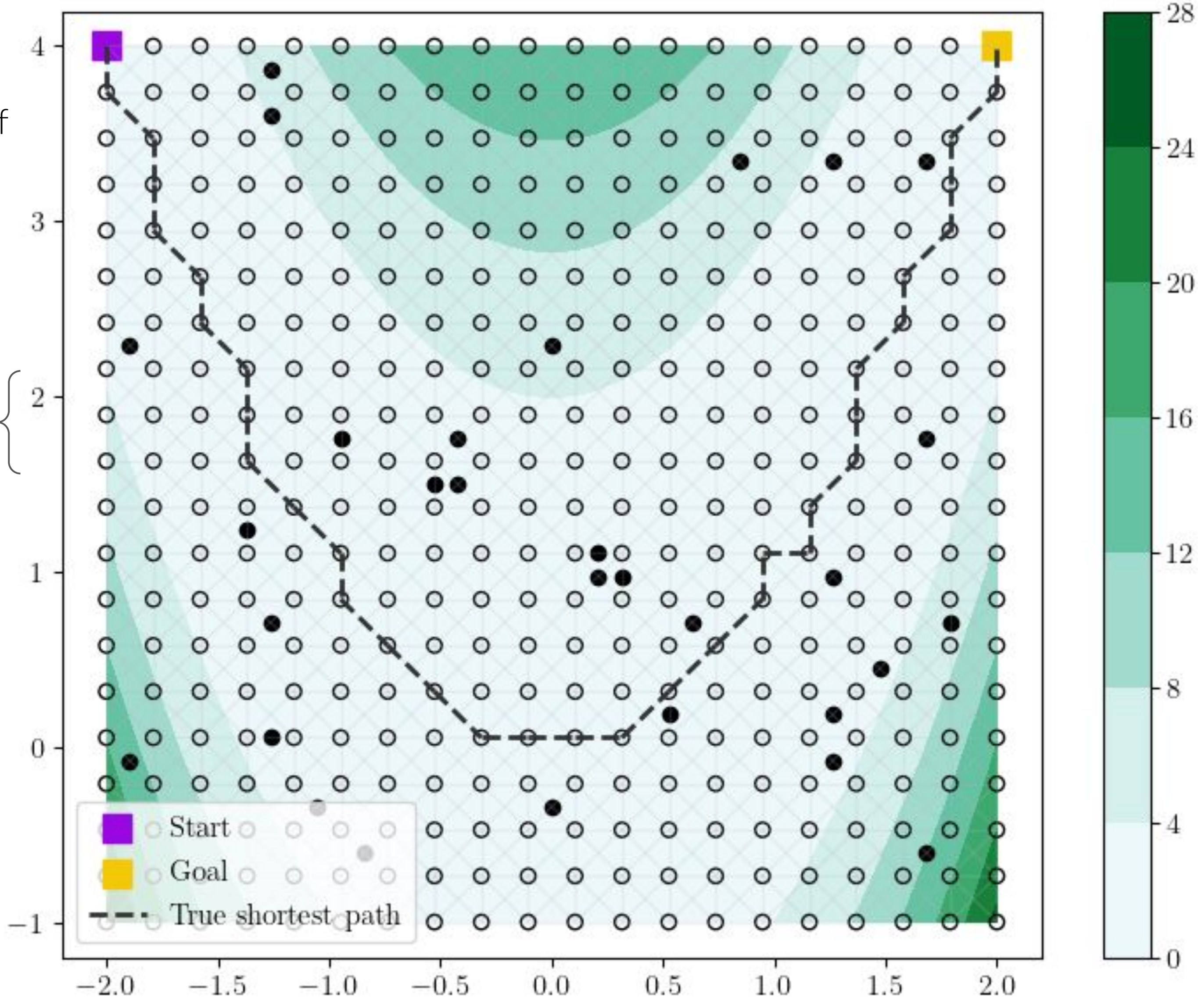
APPLICATIONS of BAX — *estimating shortest paths in graphs*

Suppose we take small set of edge weight queries
(e.g. 30 unif-random)

Could try to infer shortest path from these



APPLICATIONS of BAX — *estimating shortest paths in graphs*

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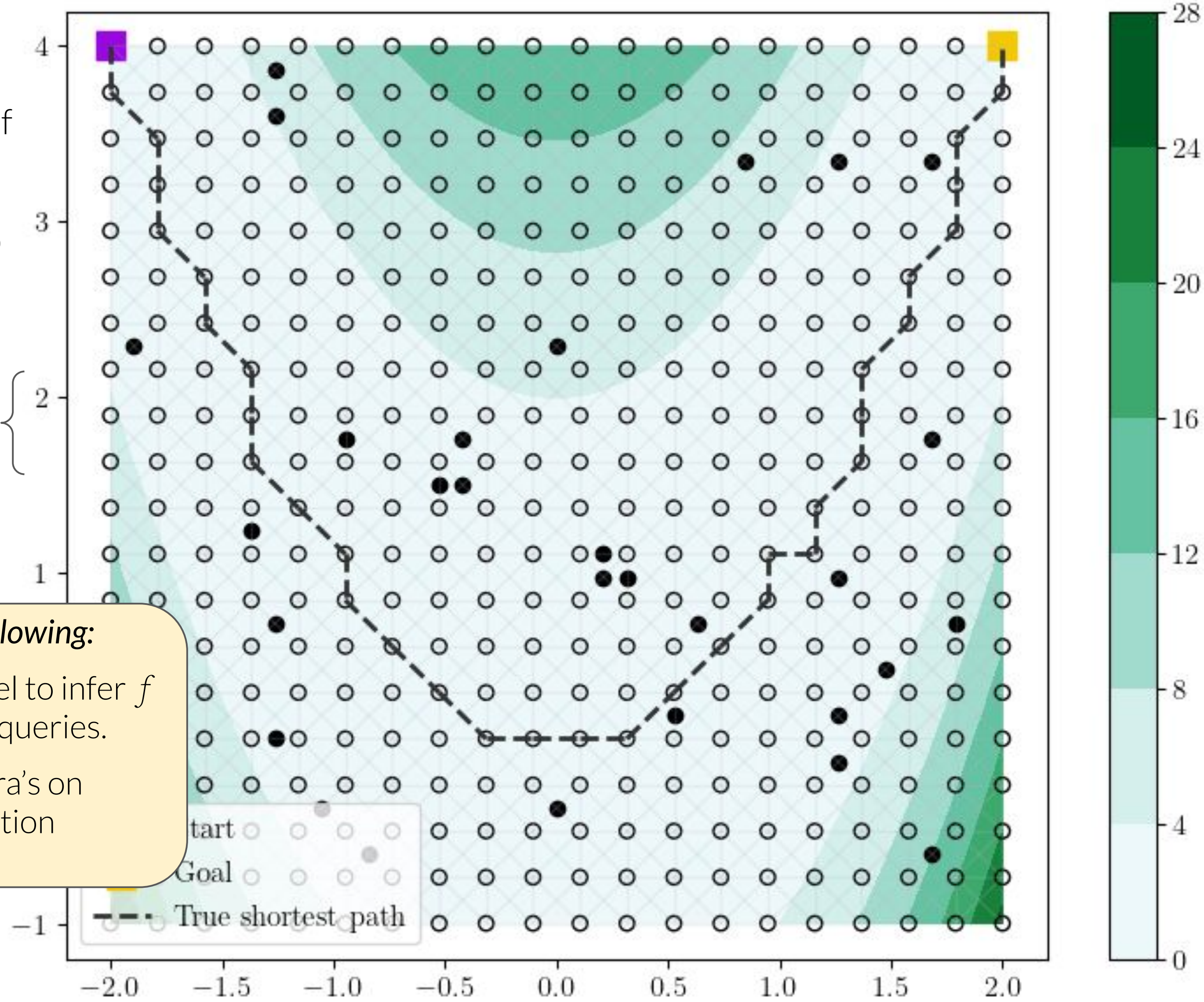


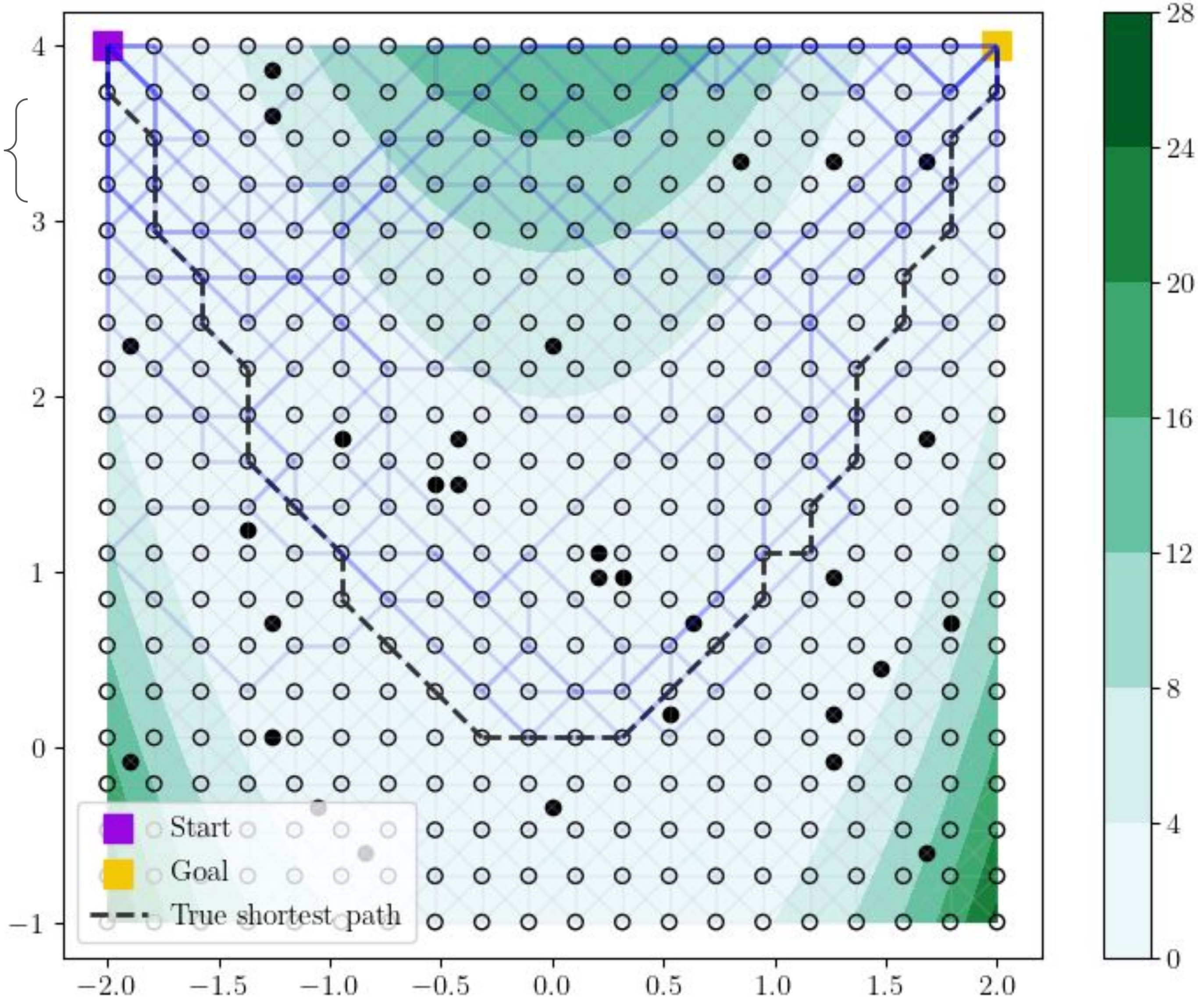
We'll do the following:

(1) Use a model to infer f (e.g. GP), given queries.

(2) Run Dijkstra's on posterior function samples.

APPLICATIONS of BAX — *estimating shortest paths in graphs*

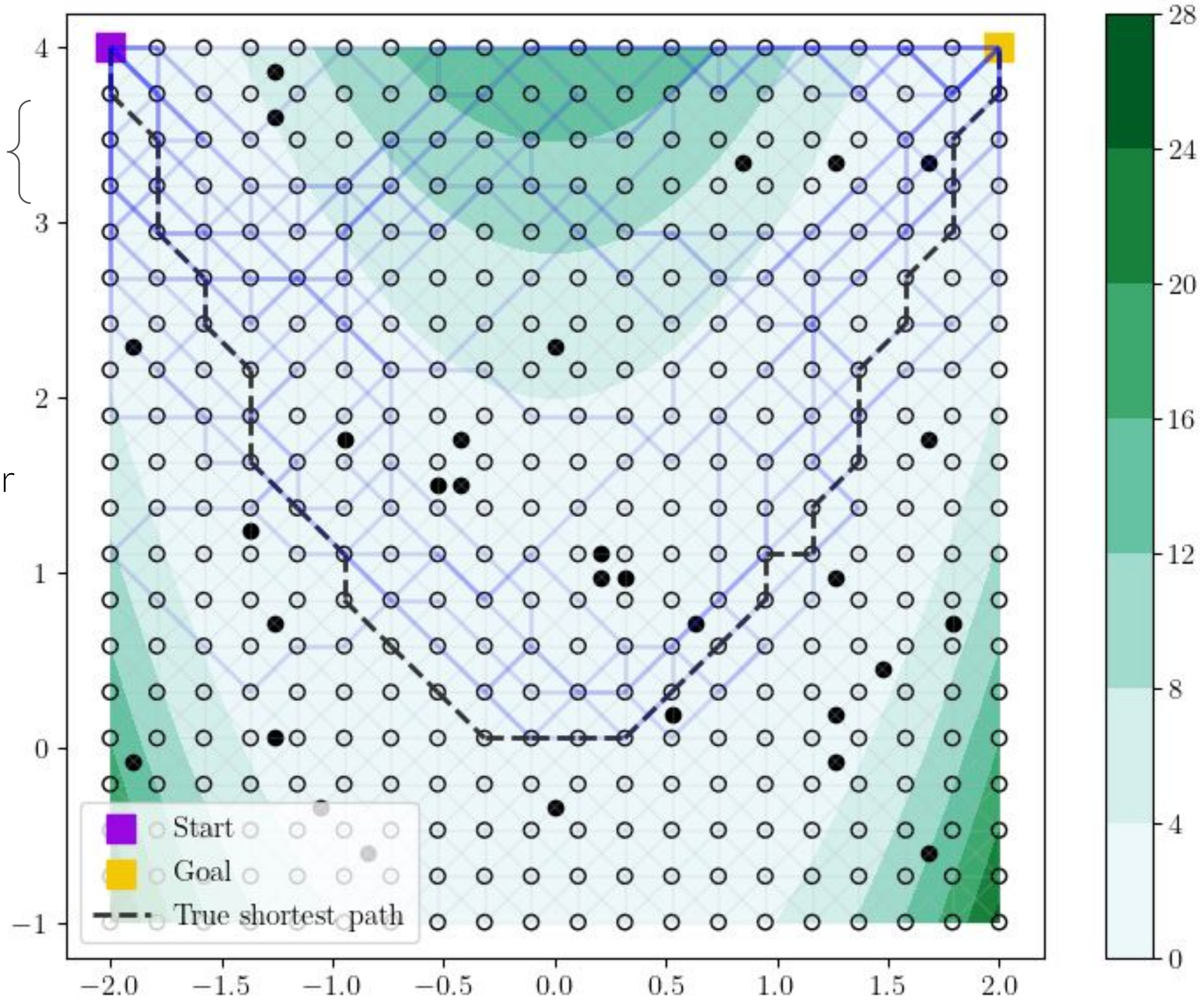
Posterior samples of shortest path (output of Dijkstra's) via GP model



APPLICATIONS of BAX — *estimating shortest paths in graphs*

Posterior samples of shortest path (output of Dijkstra's) via GP model

Estimate after 100 queries?



APPLICATIONS of BAX — *estimating shortest paths in graphs*

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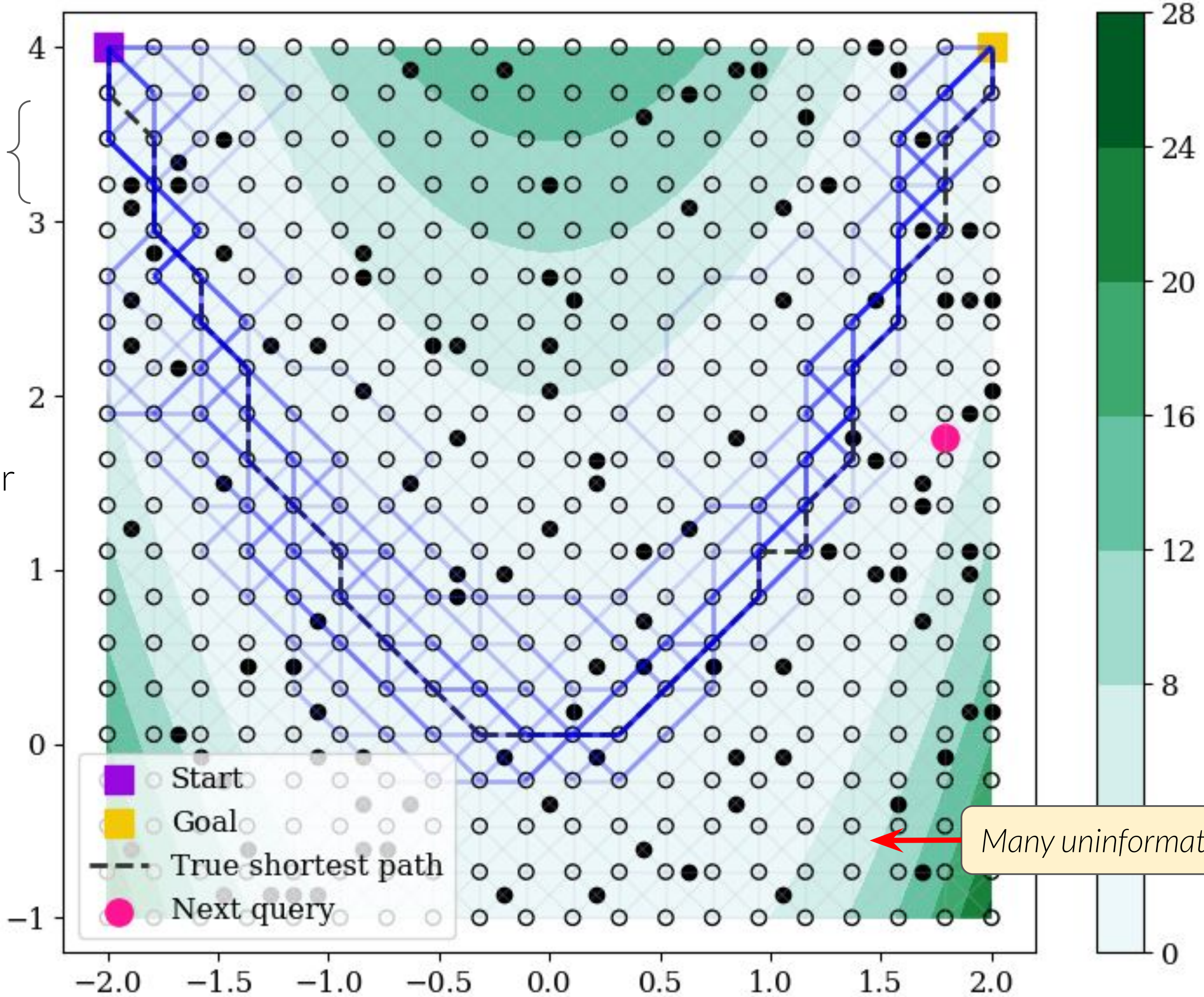
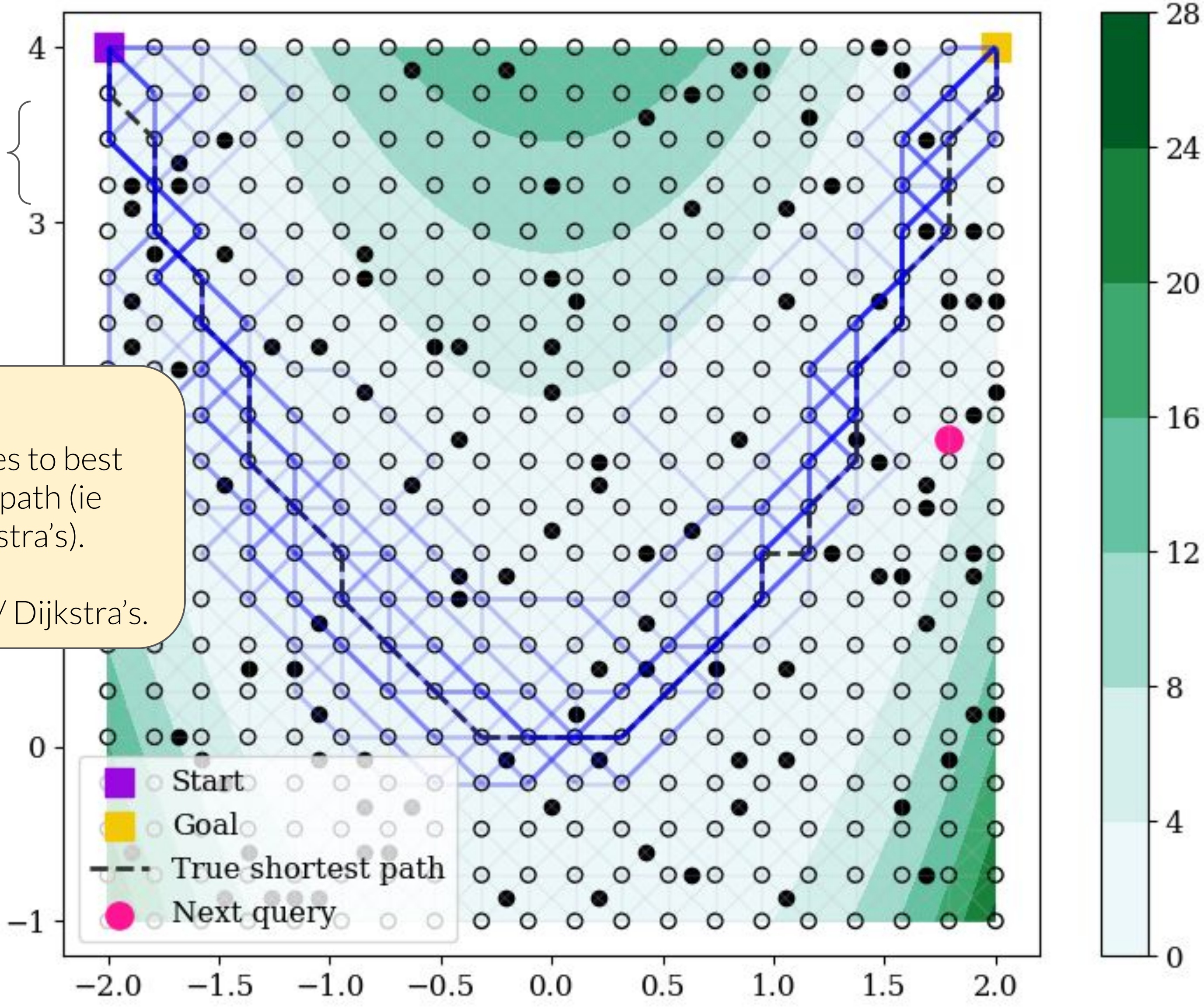


APPLICATIONS of BAX — *estimating shortest paths in graphs*

Posterior samples of shortest path (output of Dijkstra's) via GP model



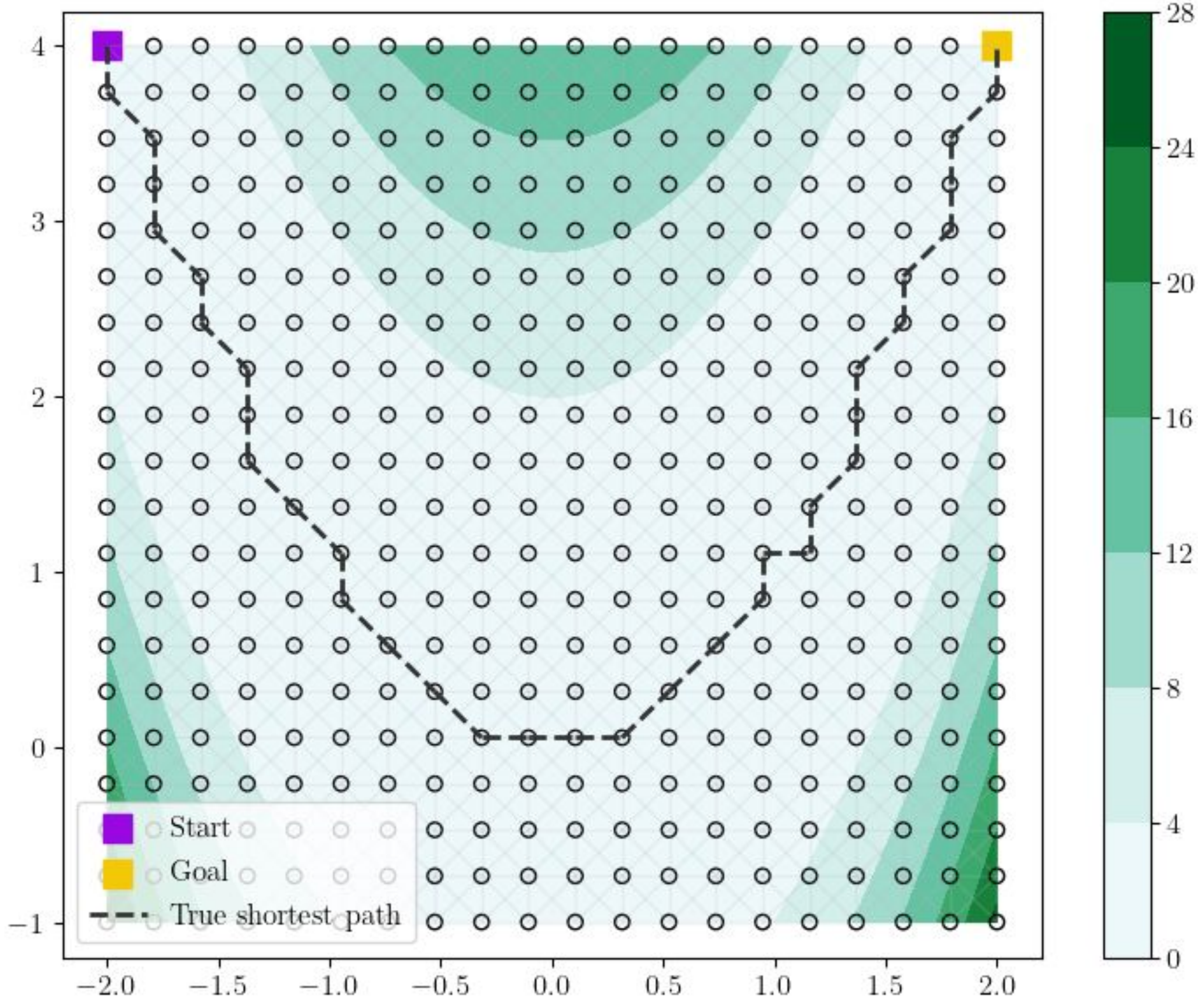
Goal:

Choose queries to best infer shortest path (ie output of Dijkstra's).

⇒ *InfoBAX* w/ Dijkstra's.

APPLICATIONS of BAX — *estimating shortest paths in graphs*

InfoBAX in action ⟶



APPLICATIONS of BAX — *estimating shortest paths in graphs*

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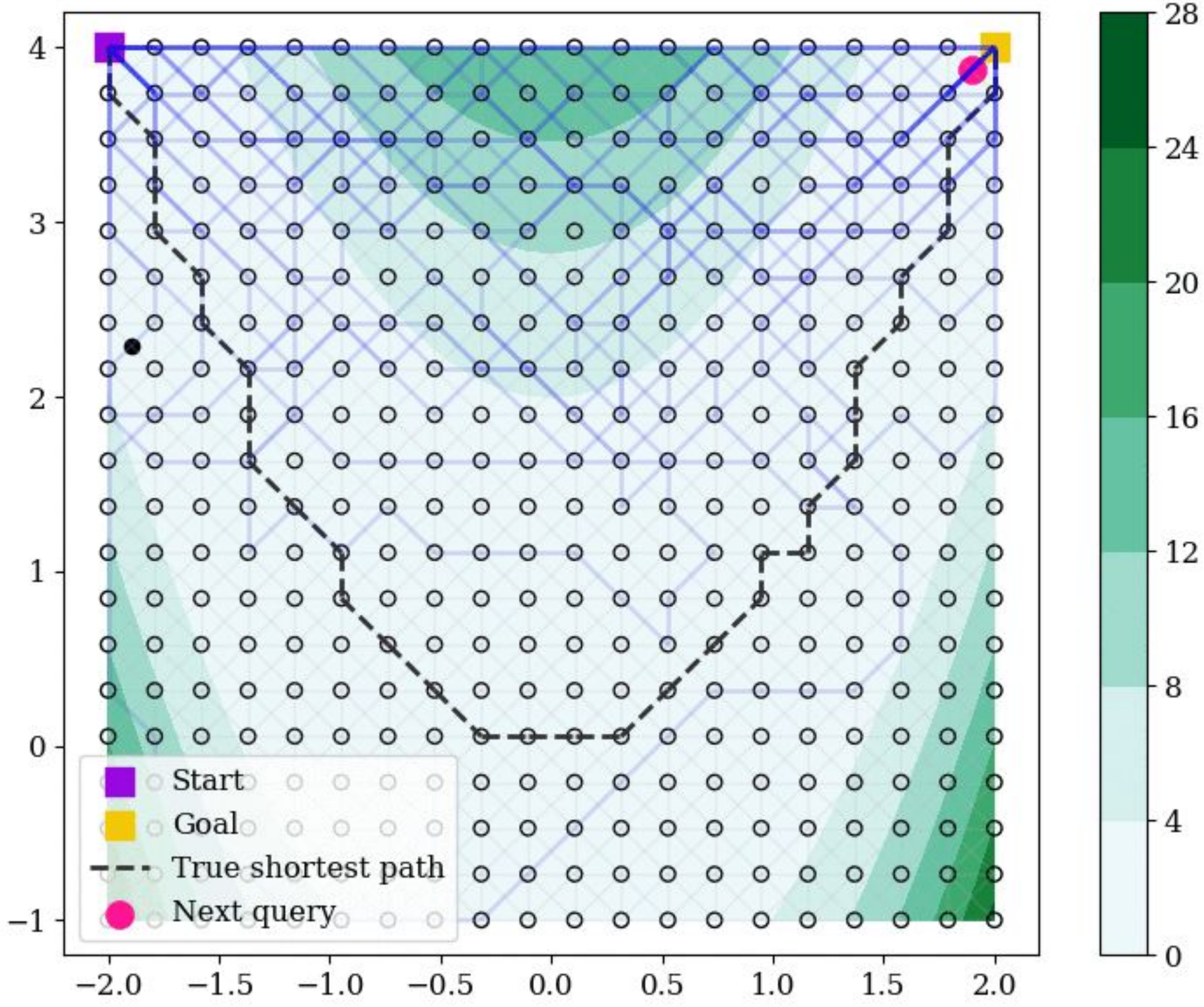
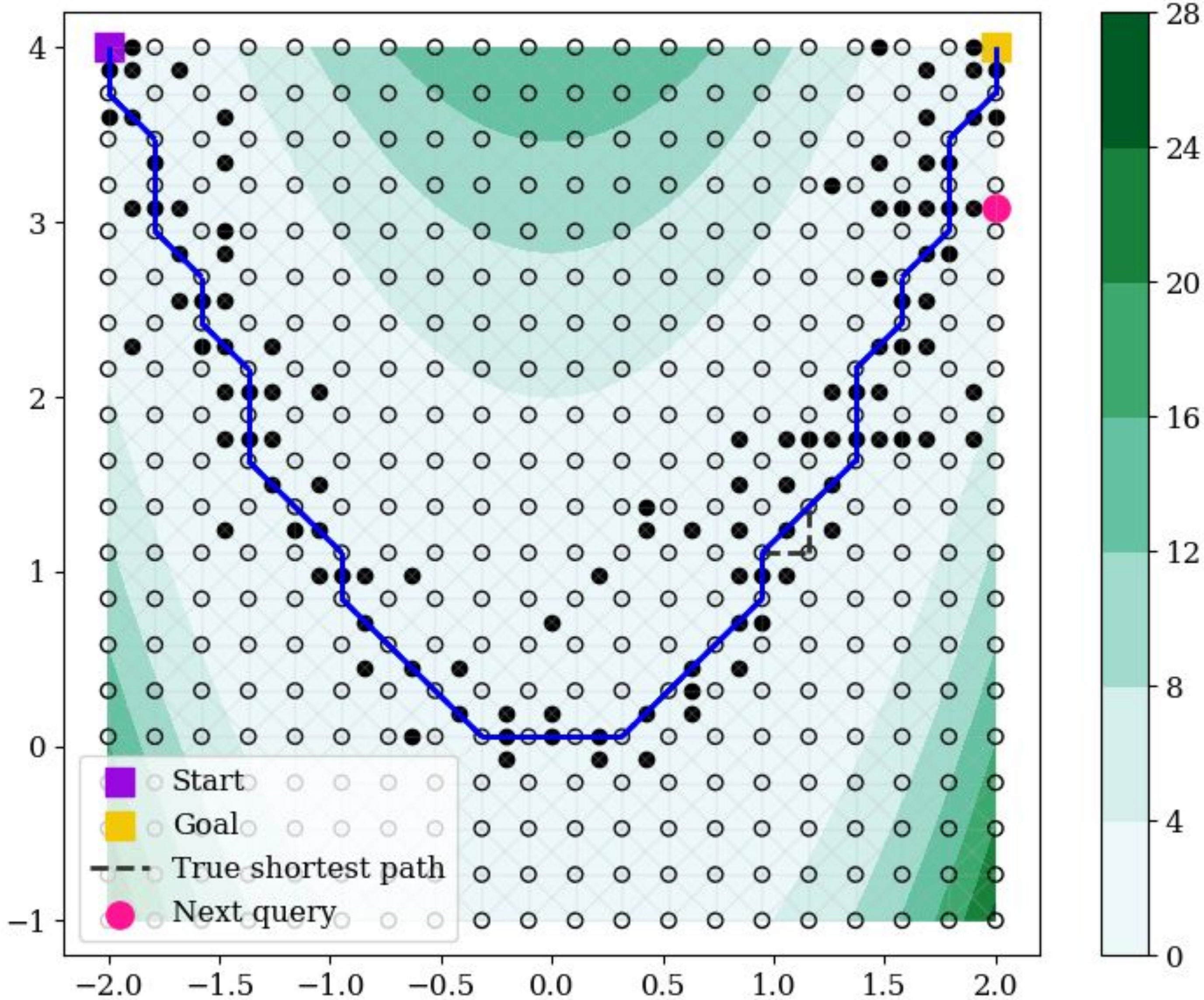


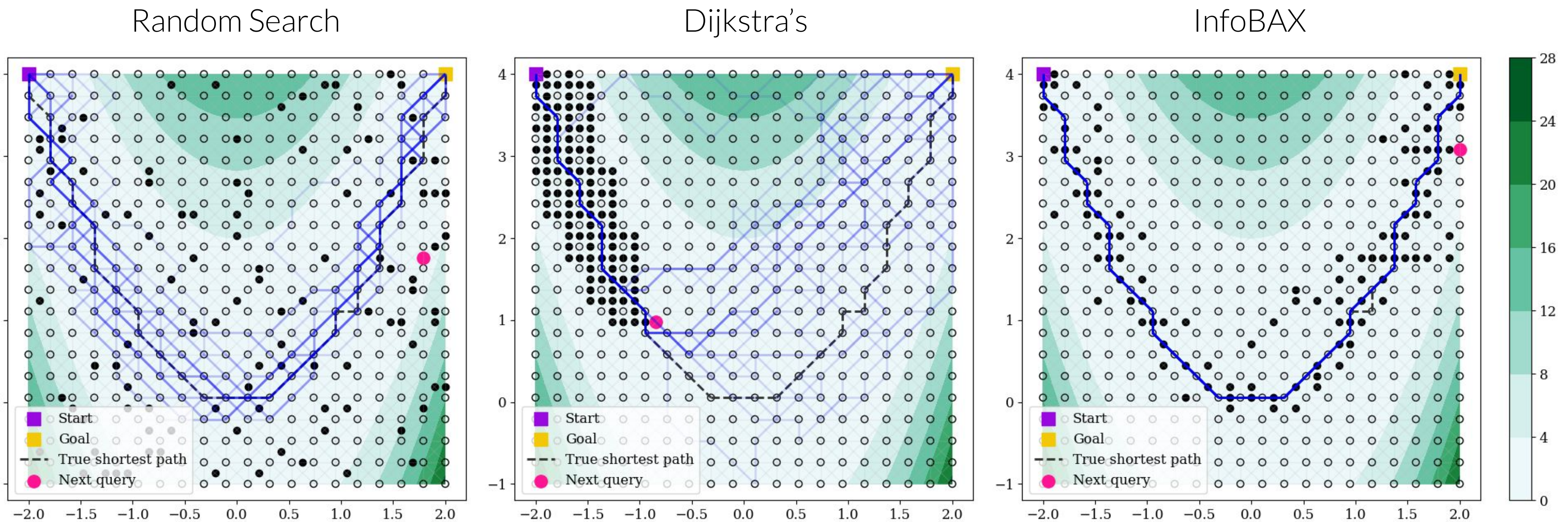
InfoBAX in action ⟶

After 100 queries.



APPLICATIONS of BAX — *estimating shortest paths in graphs*

Comparison after **100 queries**:



Application: *Bayesian local optimization*

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BO (typically) aims to estimate global optima.

However, many *local optimization* algorithms only aim to find a local optima (nearby some initial point)

- e.g. gradient descent, evolutionary algorithms, nelder-mead/simplex, etc.

Local opt can be very effective for certain settings (e.g. high dimensions), but can require large numbers of queries.

- Sometimes many redundant queries.
- Not effective if each query is very expensive.

We can use the local opt algorithms in *InfoBAX* procedure.

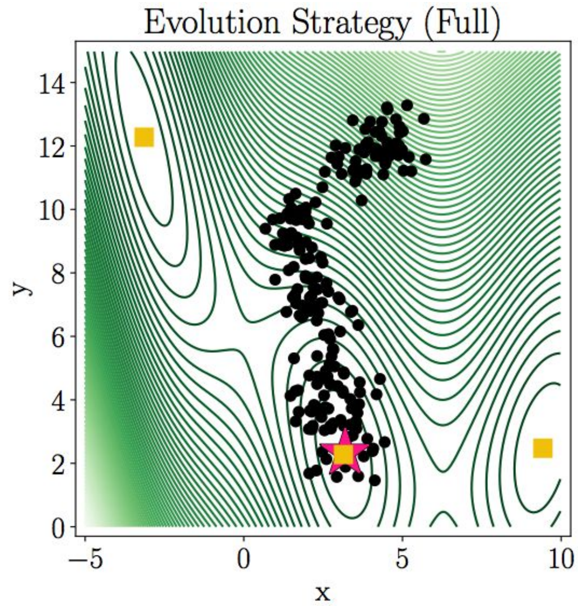
- ⇒ Yields local variants of BO parameterized by a local opt algorithm.

Overall intuition — view optimization as:

- Trying to estimate the output of a local opt algo, given limited budget of queries.

APPLICATIONS of BAX — *Bayesian local optimization*

After *208* queries



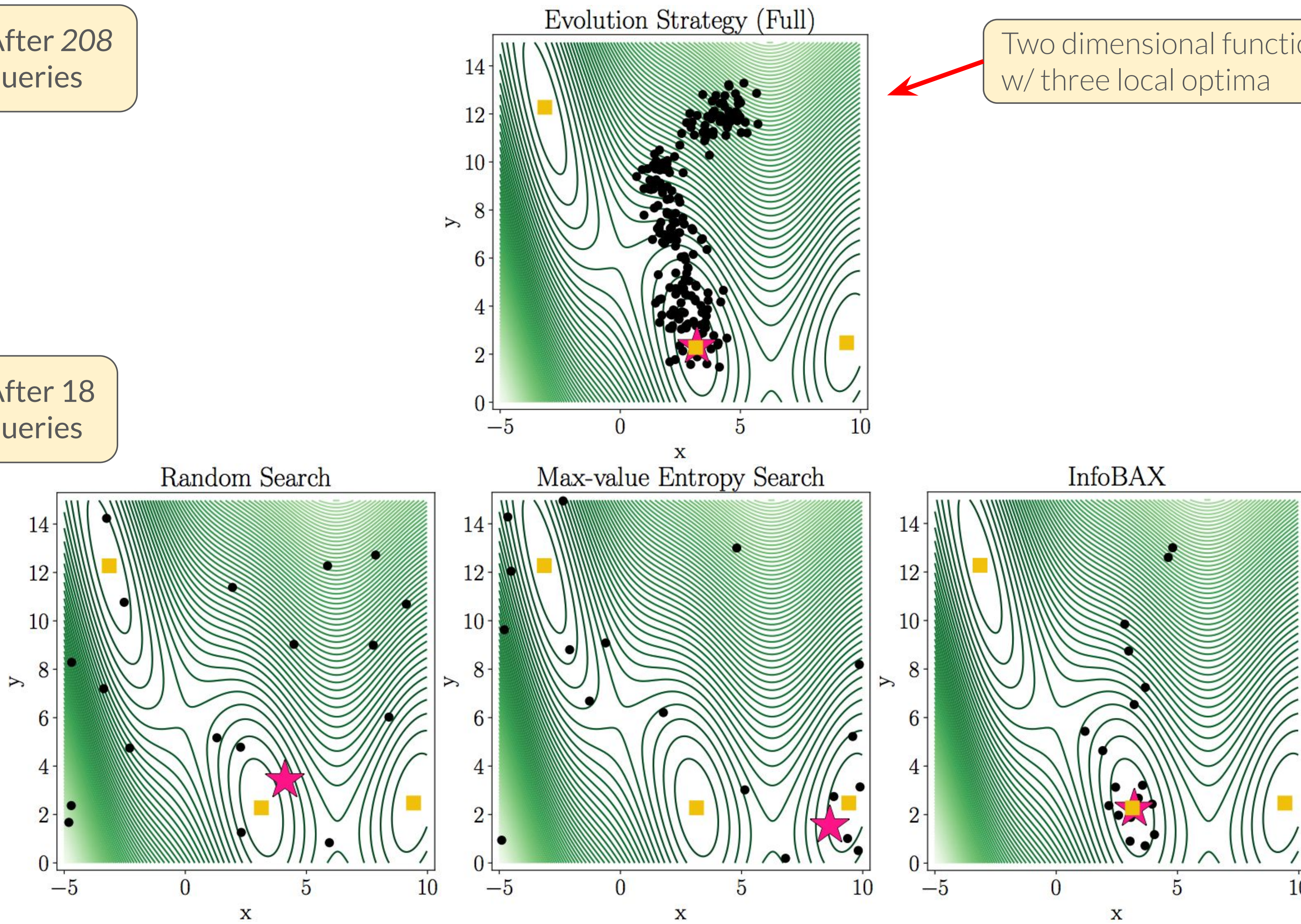
Two dimensional function, w/ three local optima

APPLICATIONS of BAX — *Bayesian local optimization*

After 208 queries

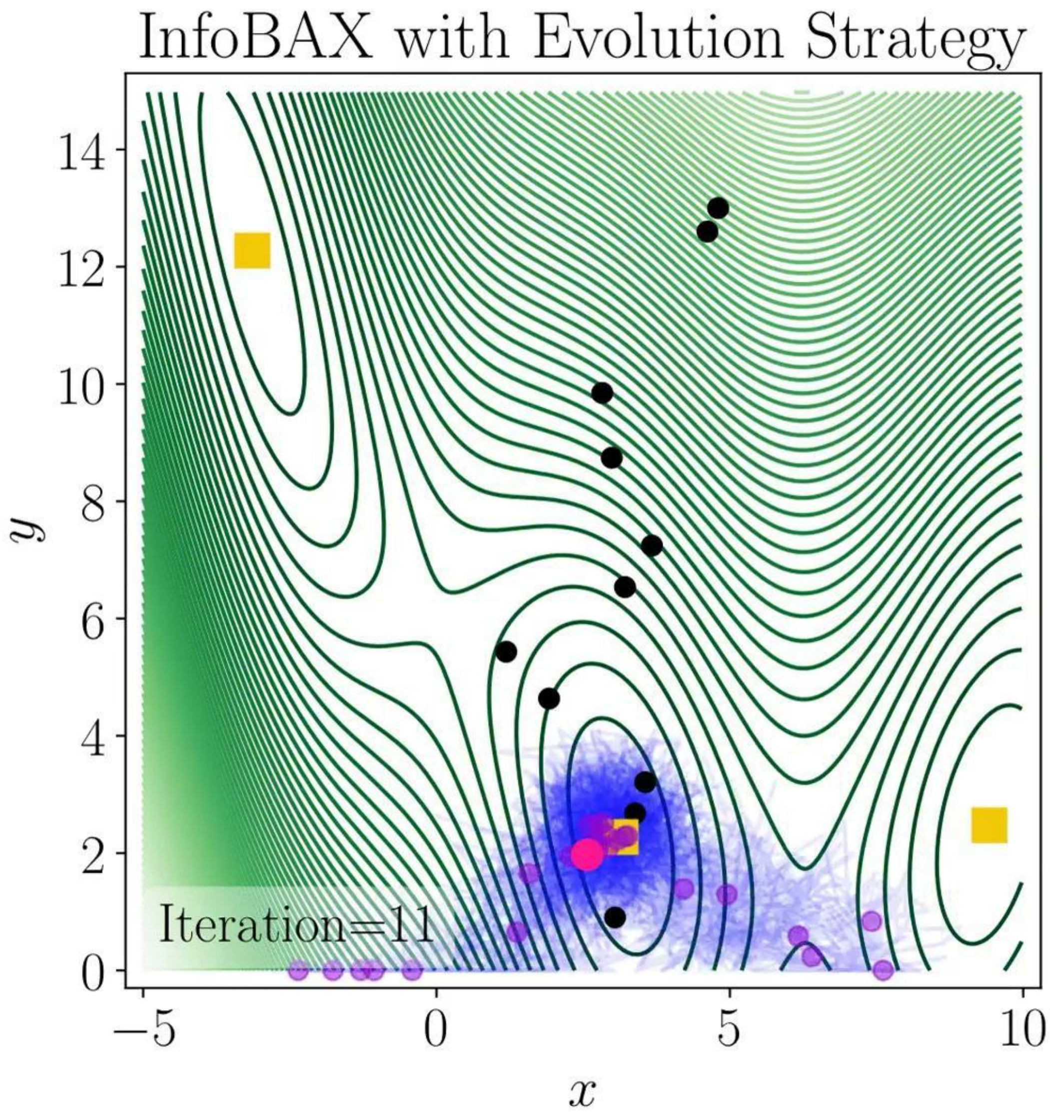
Two dimensional function, w/ three local optima

After 18 queries



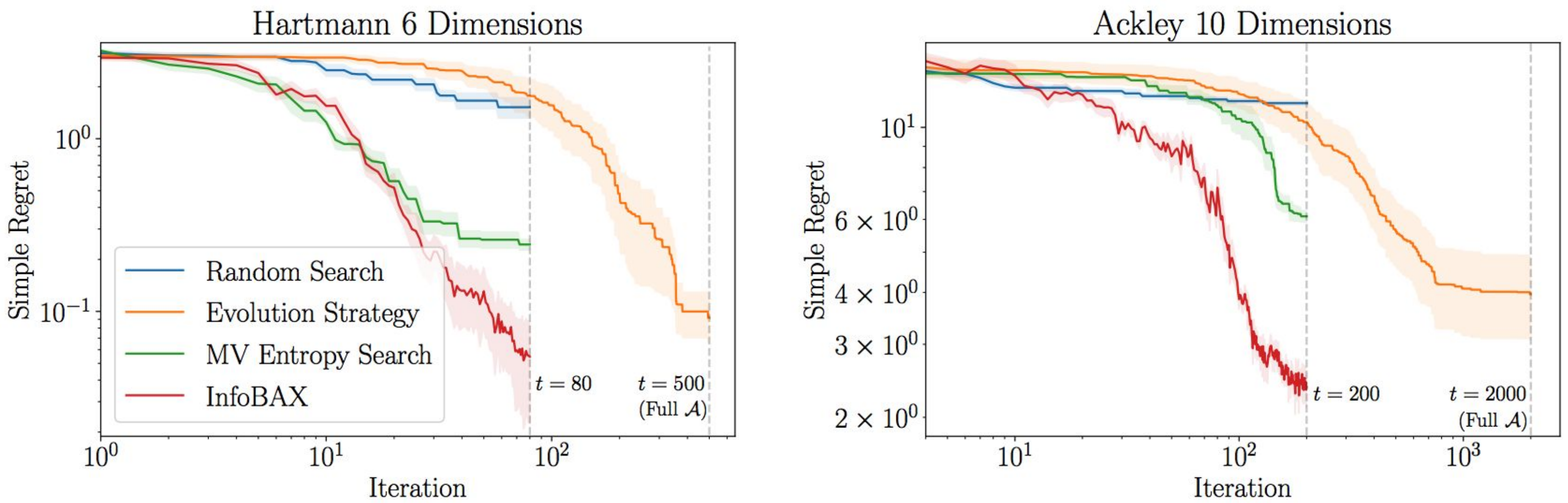
APPLICATIONS of BAX — *estimating shortest paths in graphs*

InfoBAX in action →



APPLICATIONS of BAX — *Bayesian local optimization*

InfoBAX matches performance of Evolution Strategy, using ***<10%*** of the queries.



***Future steps*:** try this out with a variety of local optimizers.

Application: *top-k estimation*

Suppose we have a large set of items.

- E.g. set of 500 catalyst materials / bulks.

Each item has a value under an expensive black-box function f.

- E.g. each catalyst bulk has an *activity level*, which is expensive to measure (simulate).

Suppose we want to determine the ***top-k*** items in the set.

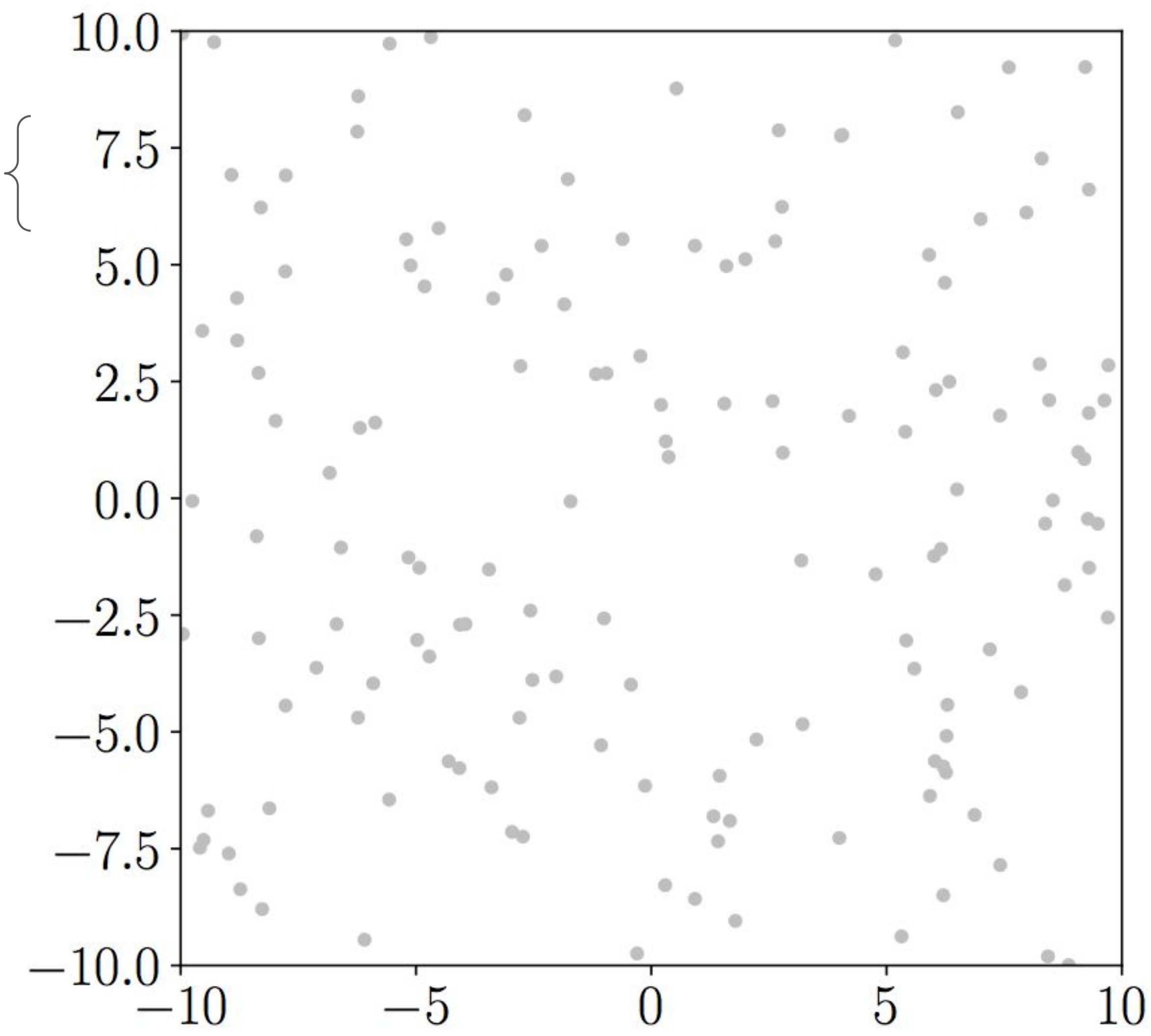
- E.g. the *top-10* catalysts, with highest activity ⇒ for experimental evaluation.
- (These ***top-k*** might then be filtered further based on additional tests)

⇒ distinct from both global optimization ($k=1$) and level set estimation.

Visualizing this…

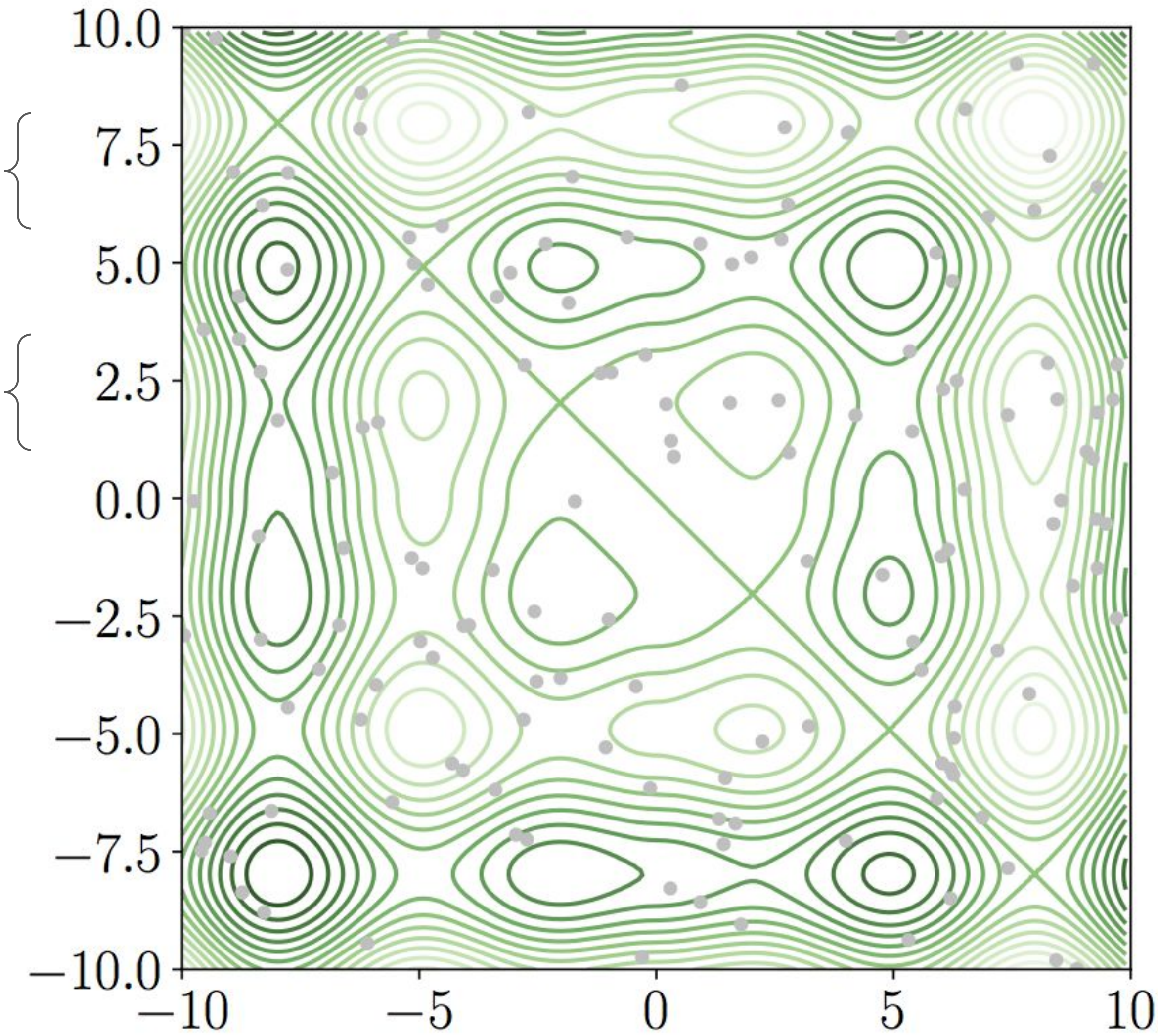
APPLICATIONS of BAX — *top-k estimation*

250 items



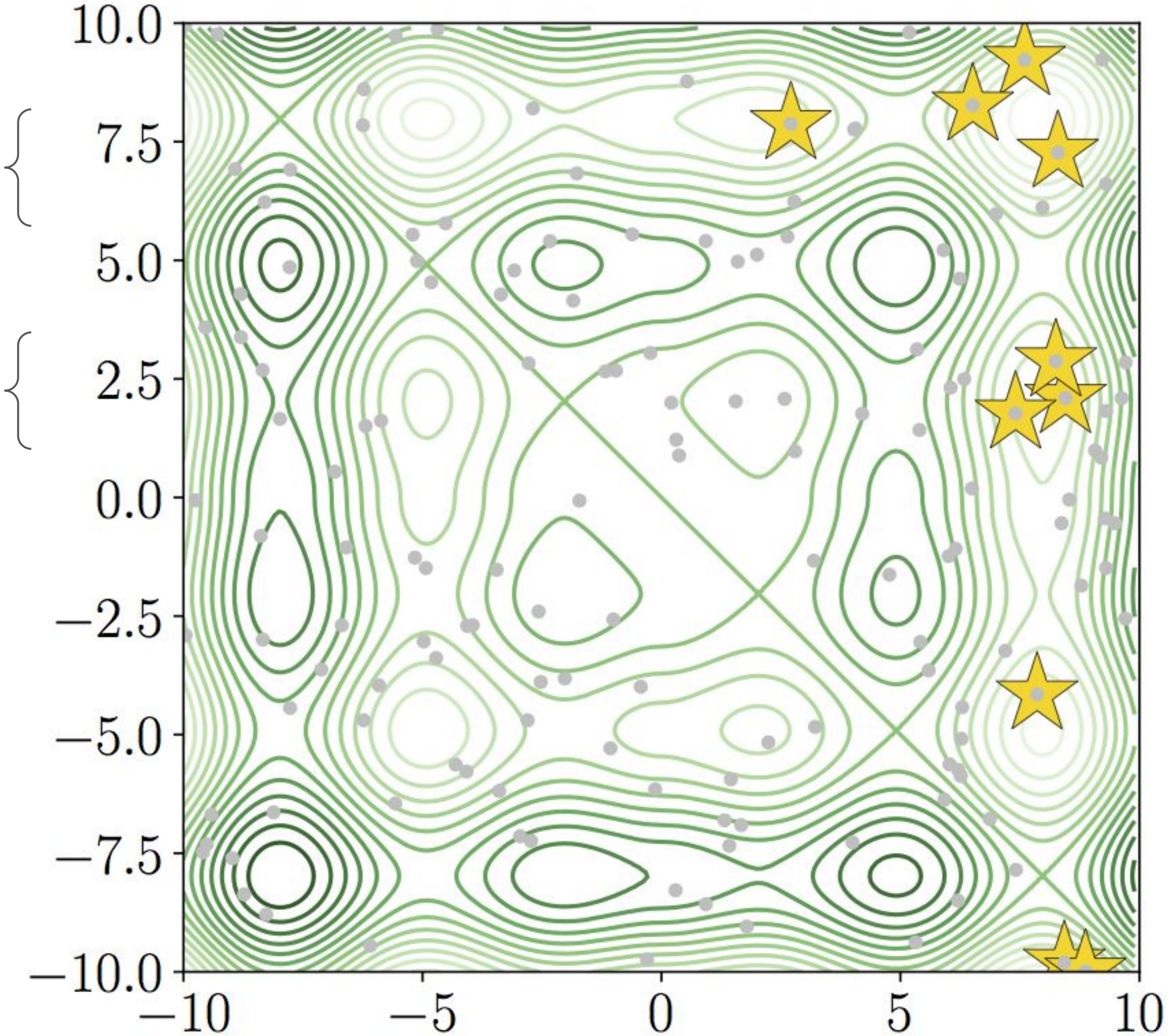
250 items

Black-box function f (green).



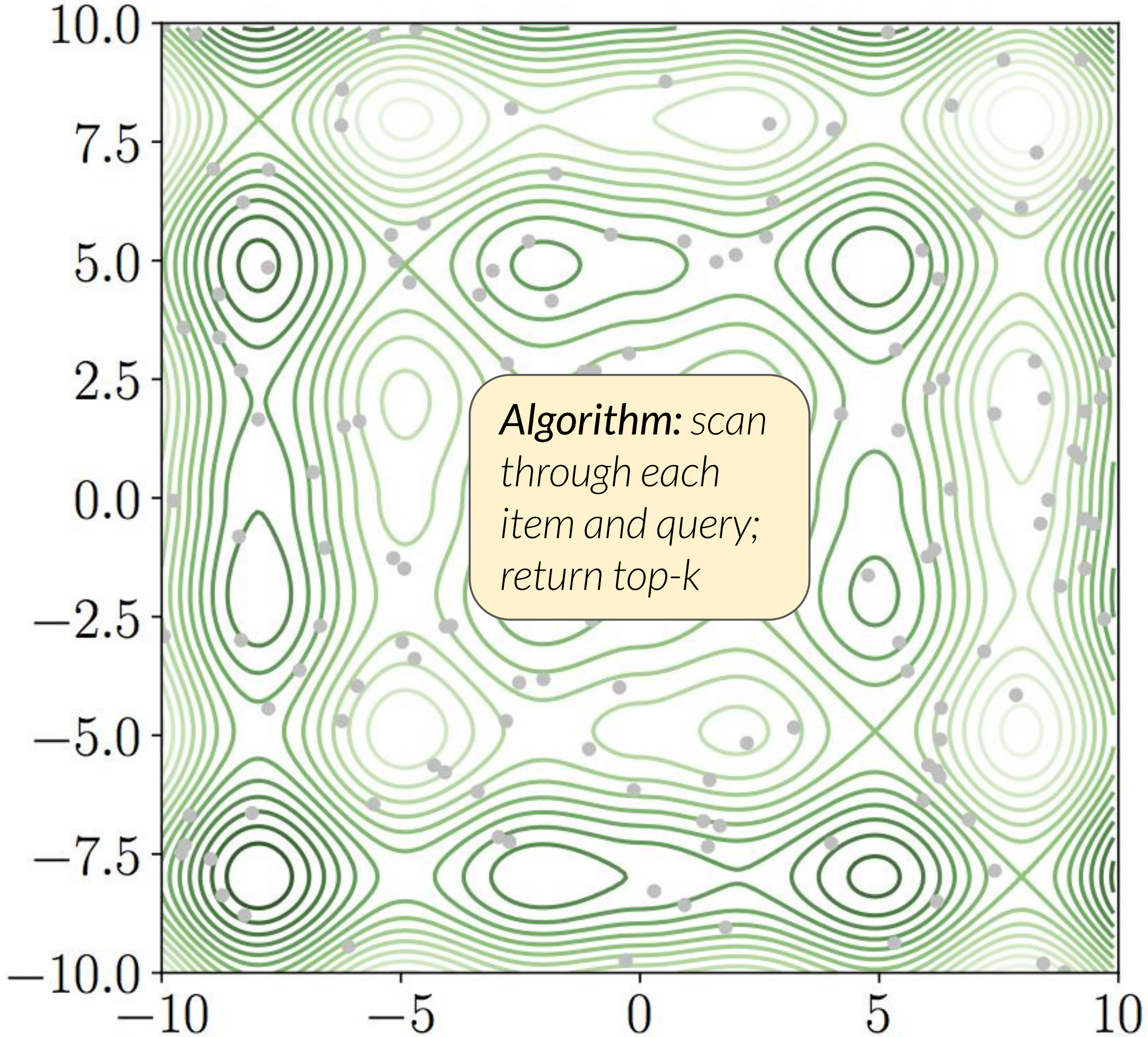
250 items

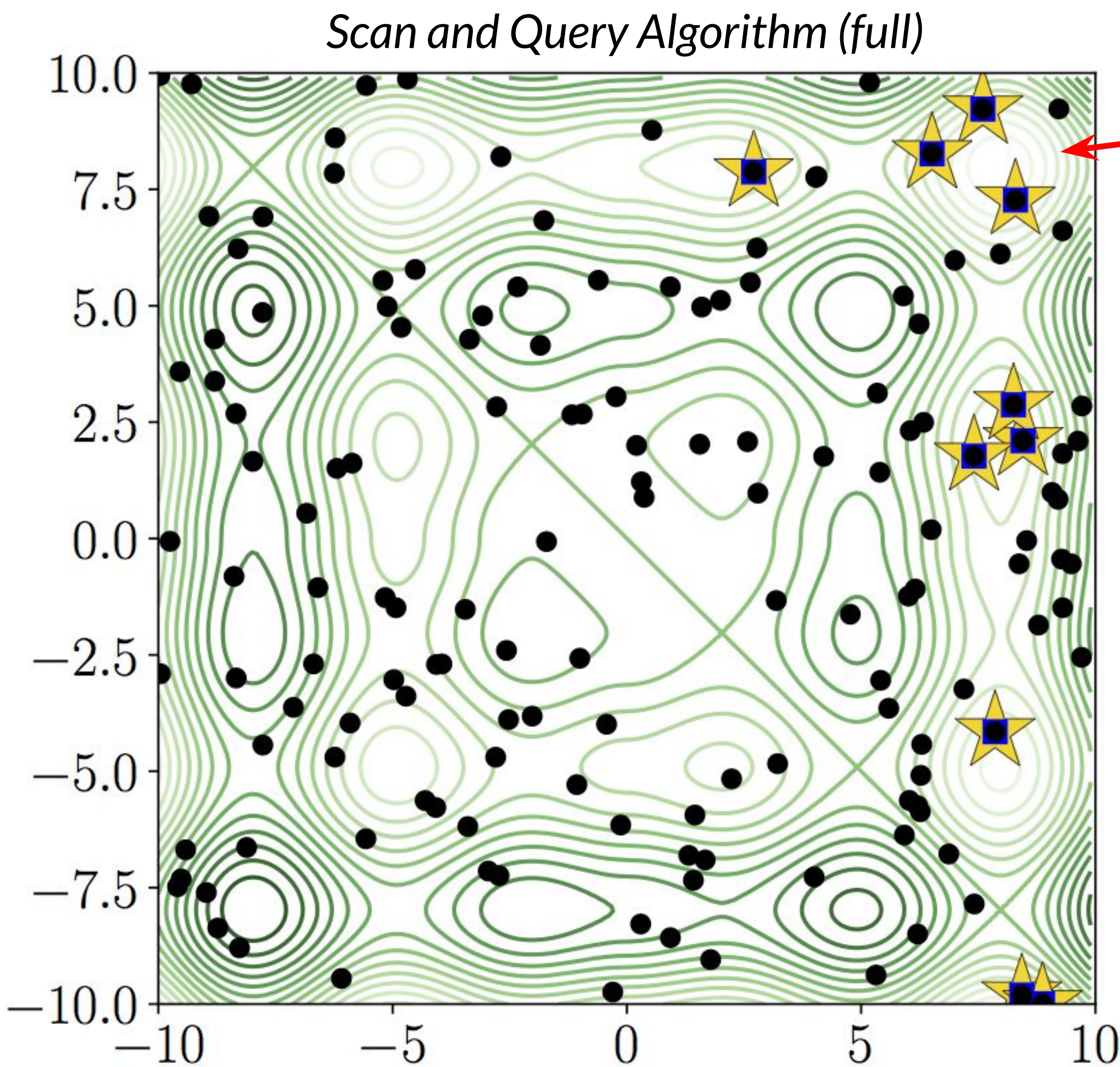
Black-box function f (green).



Stars denote *top-10* items

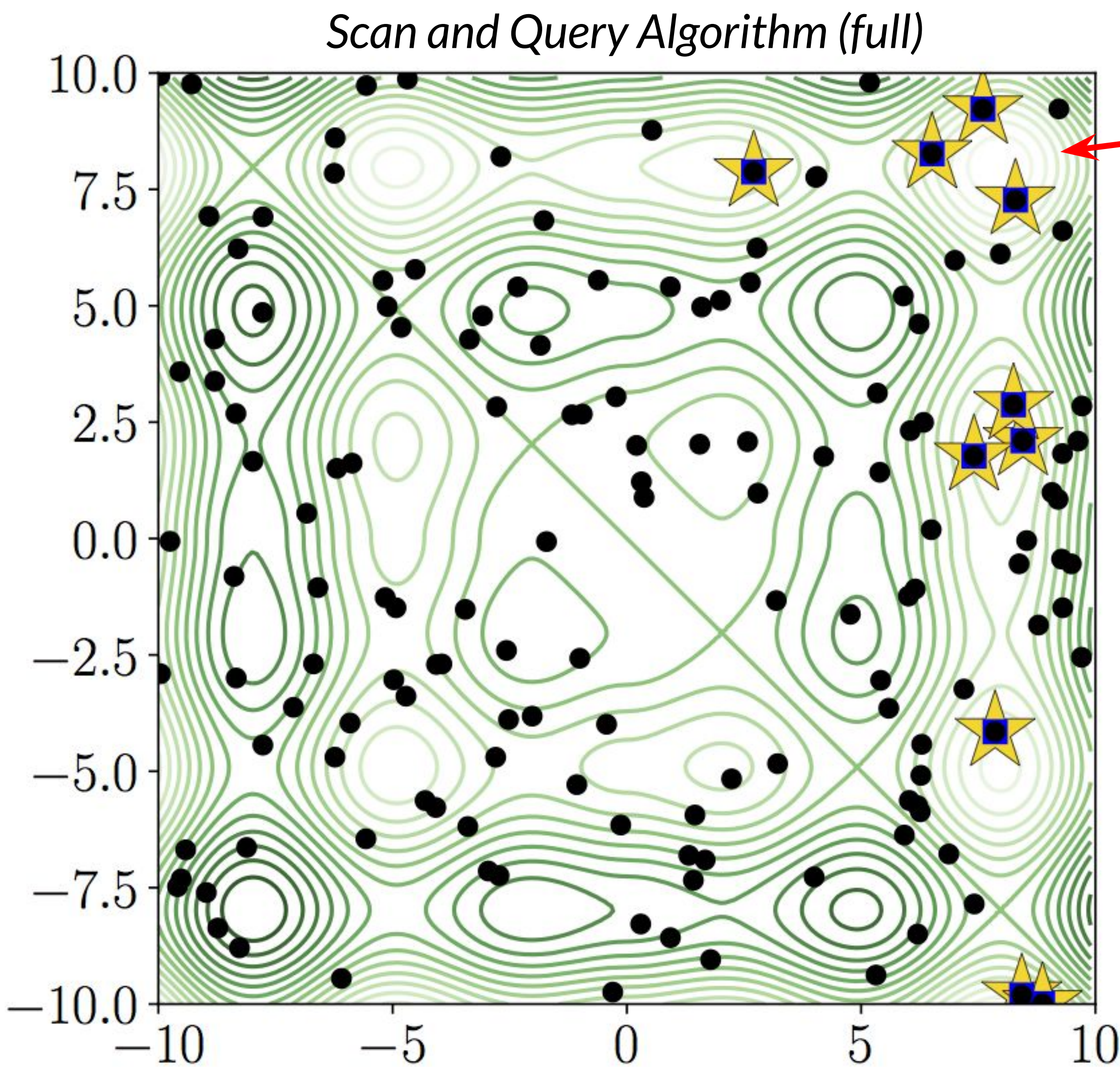
APPLICATIONS of BAX — *top-k estimation*





Algorithm yields perfect estimate

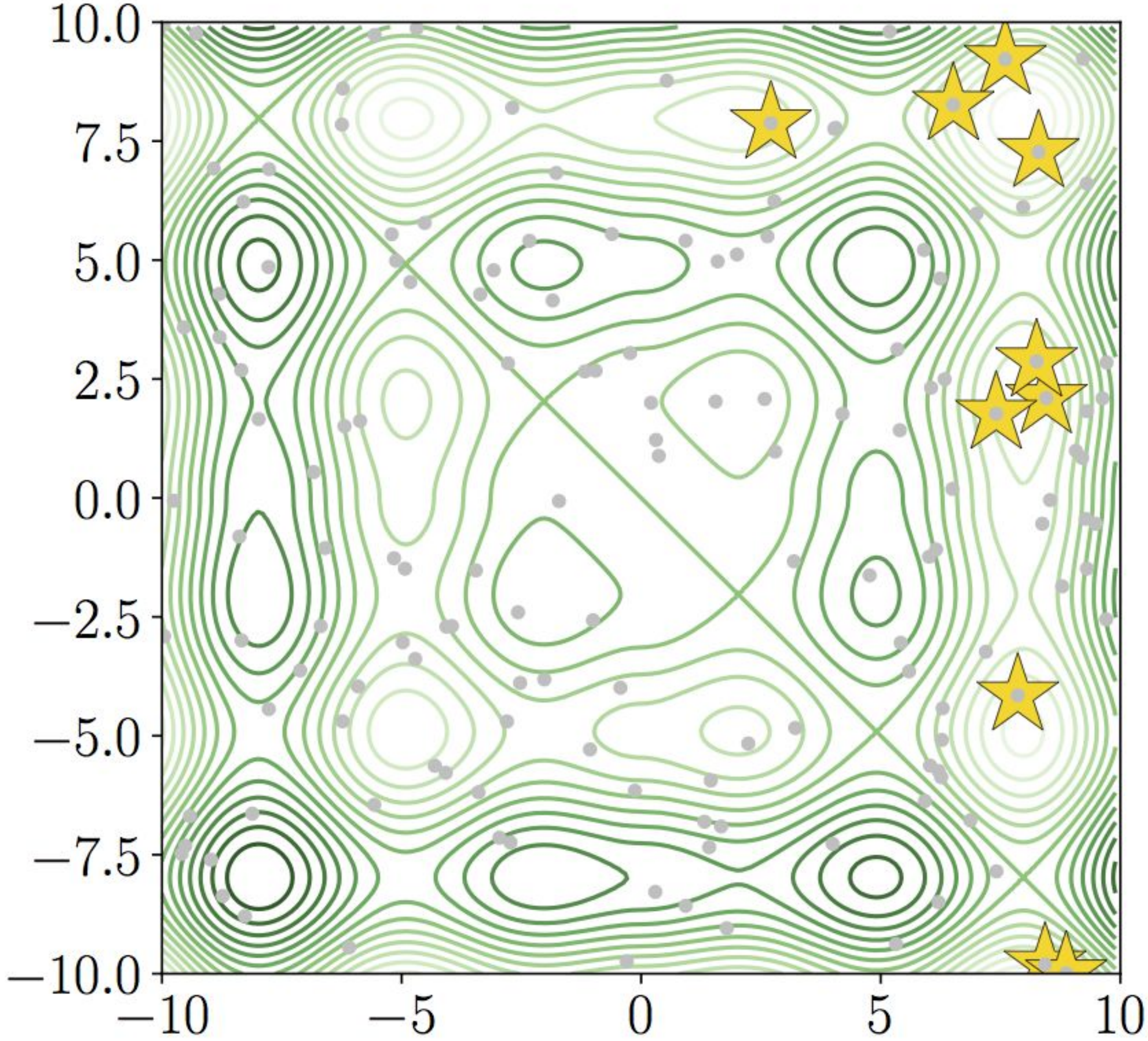
APPLICATIONS of BAX — *top-k estimation*



Algorithm yields perfect estimate

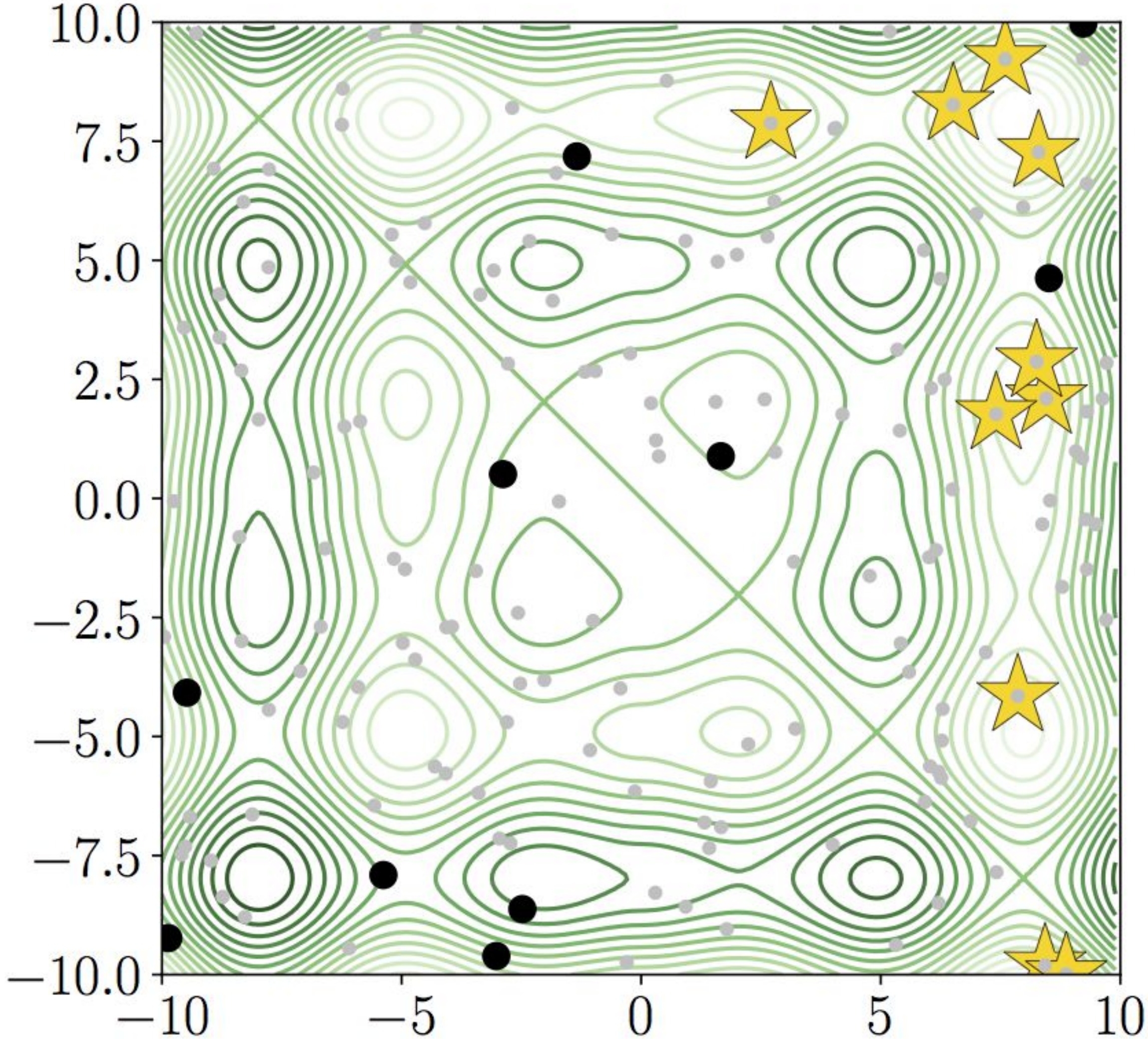
However: *uses 250 queries*

APPLICATIONS of BAX — *top-k estimation*



New strategy:
Make a few queries and infer top-10 items

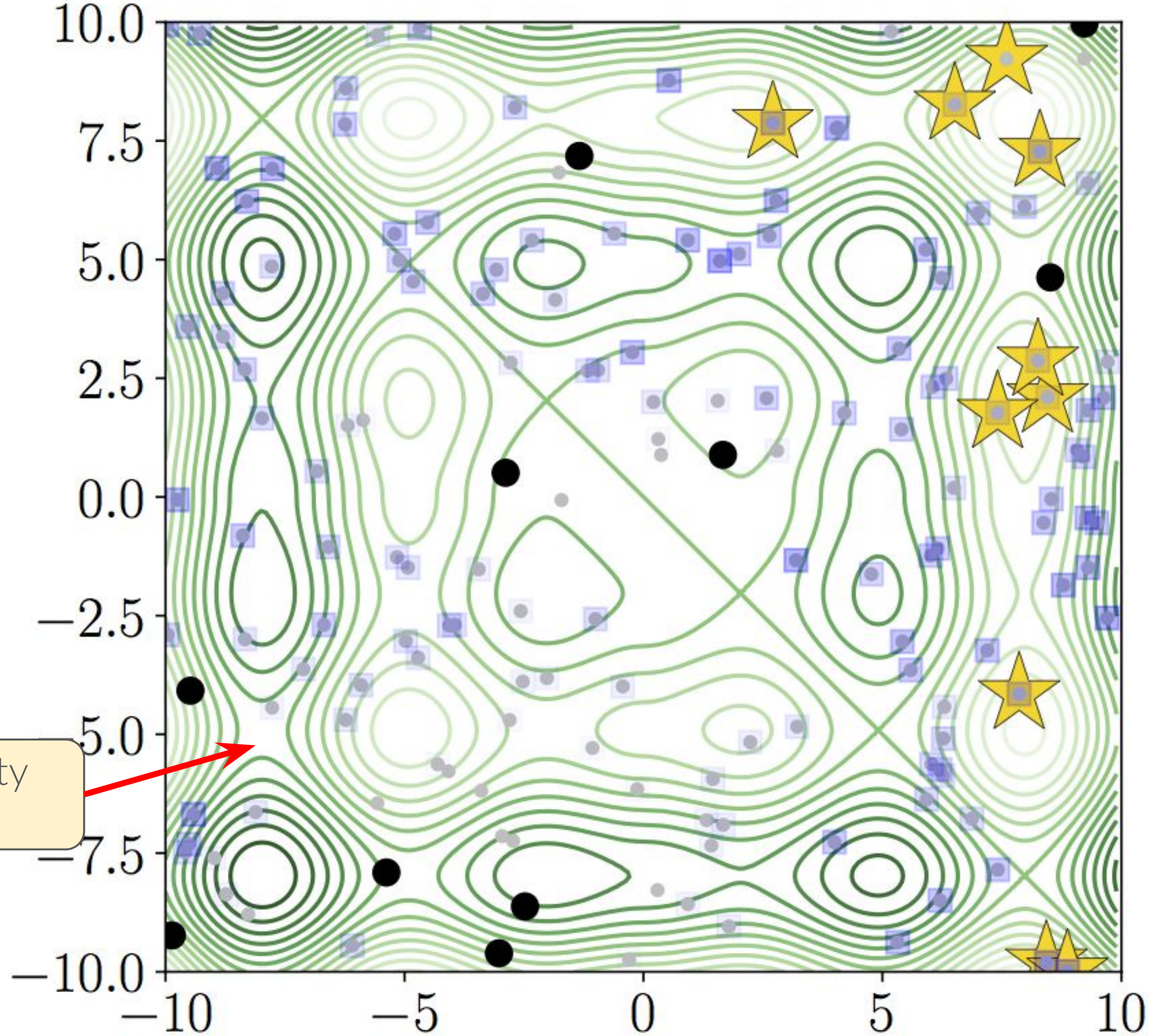
APPLICATIONS of BAX — *top-k estimation*



New strategy:
Make a few queries and infer top-10 items

10 queries (black dots)

APPLICATIONS of BAX — *top-k estimation*



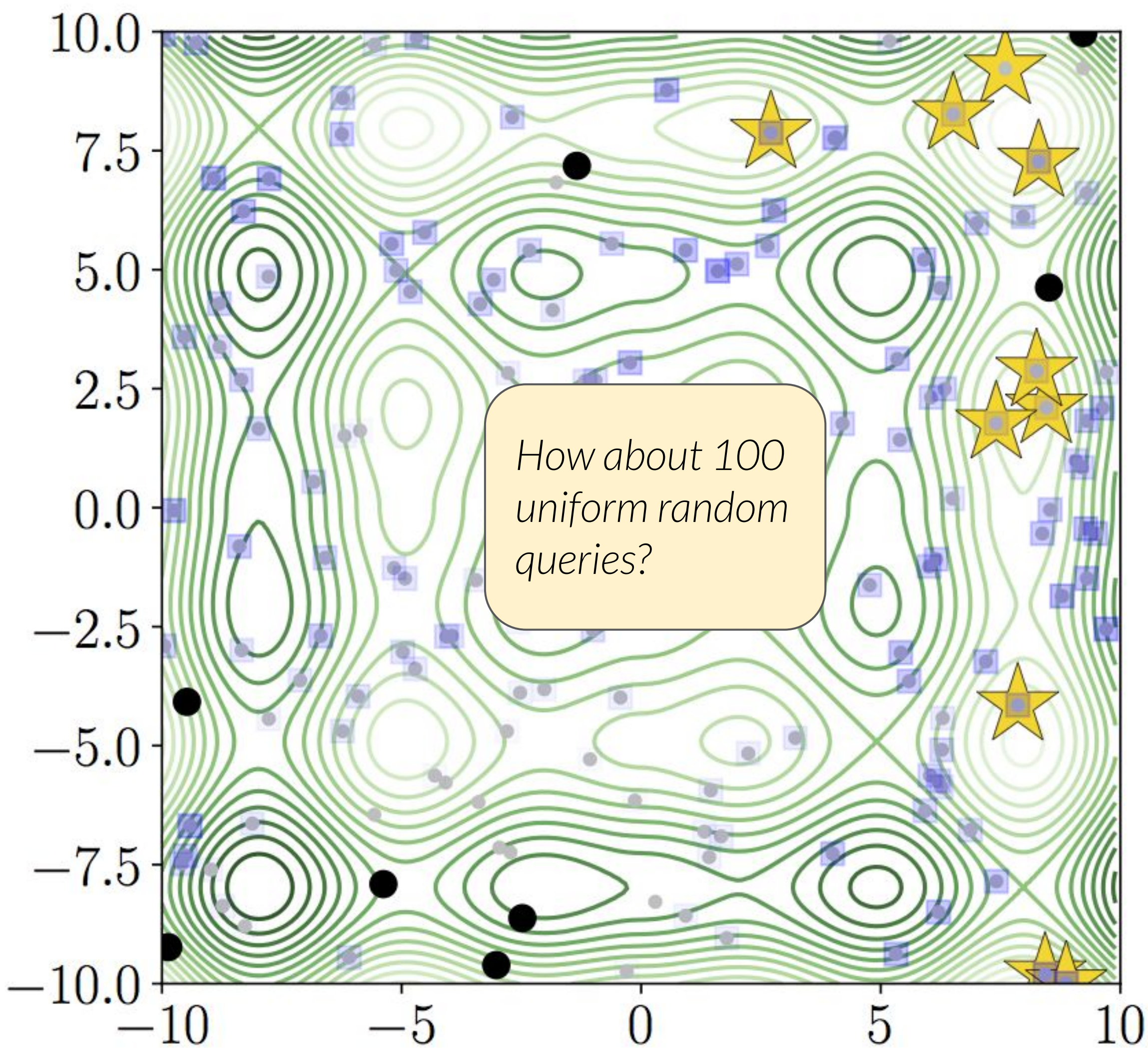
New strategy:
Make a few queries and infer top-10 items

Posterior samples of *top-10* items (blue squares)

10 queries (black dots)

Estimate is pretty bad

APPLICATIONS of BAX — *top-k estimation*



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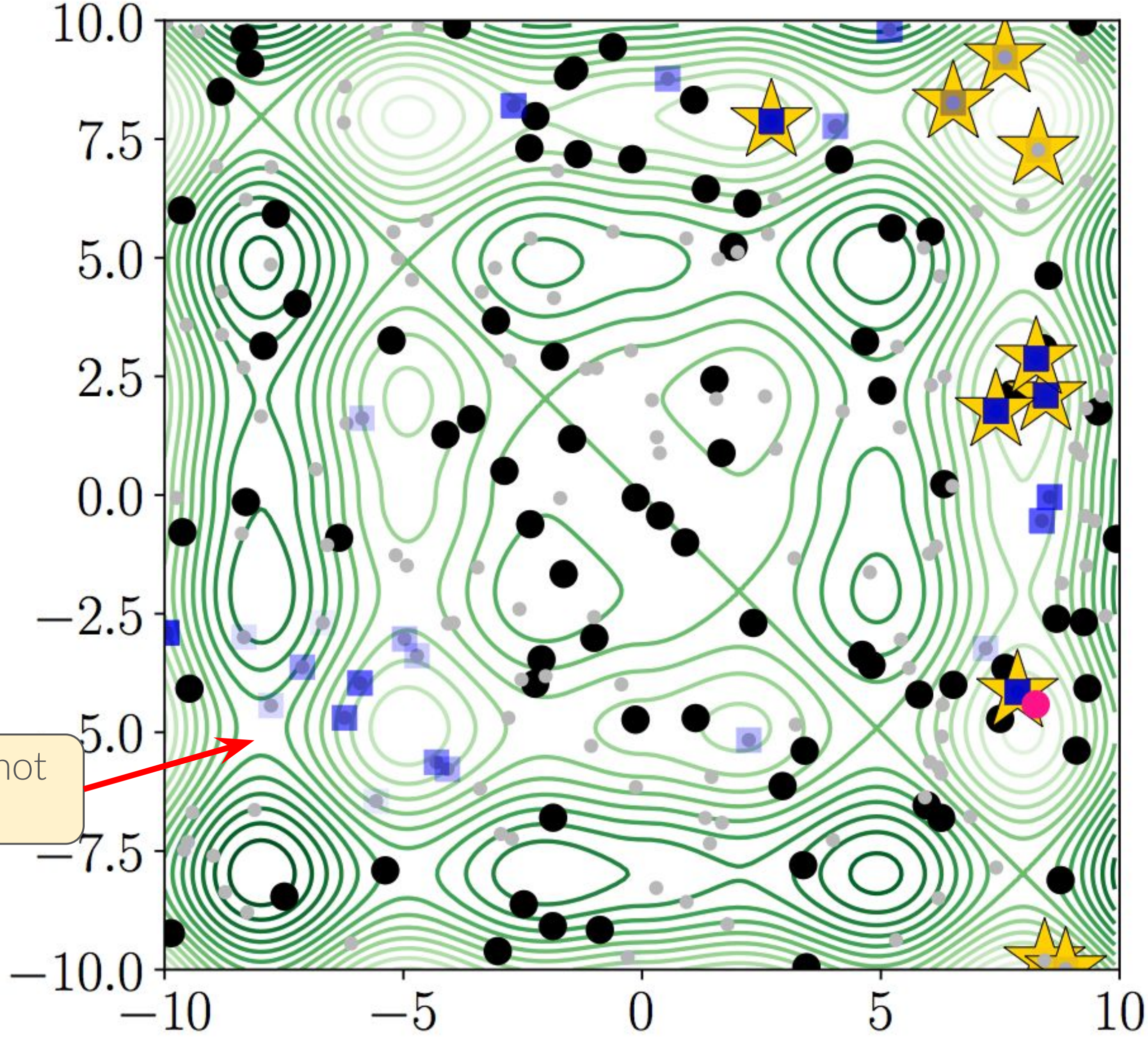

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Estimate is still not great

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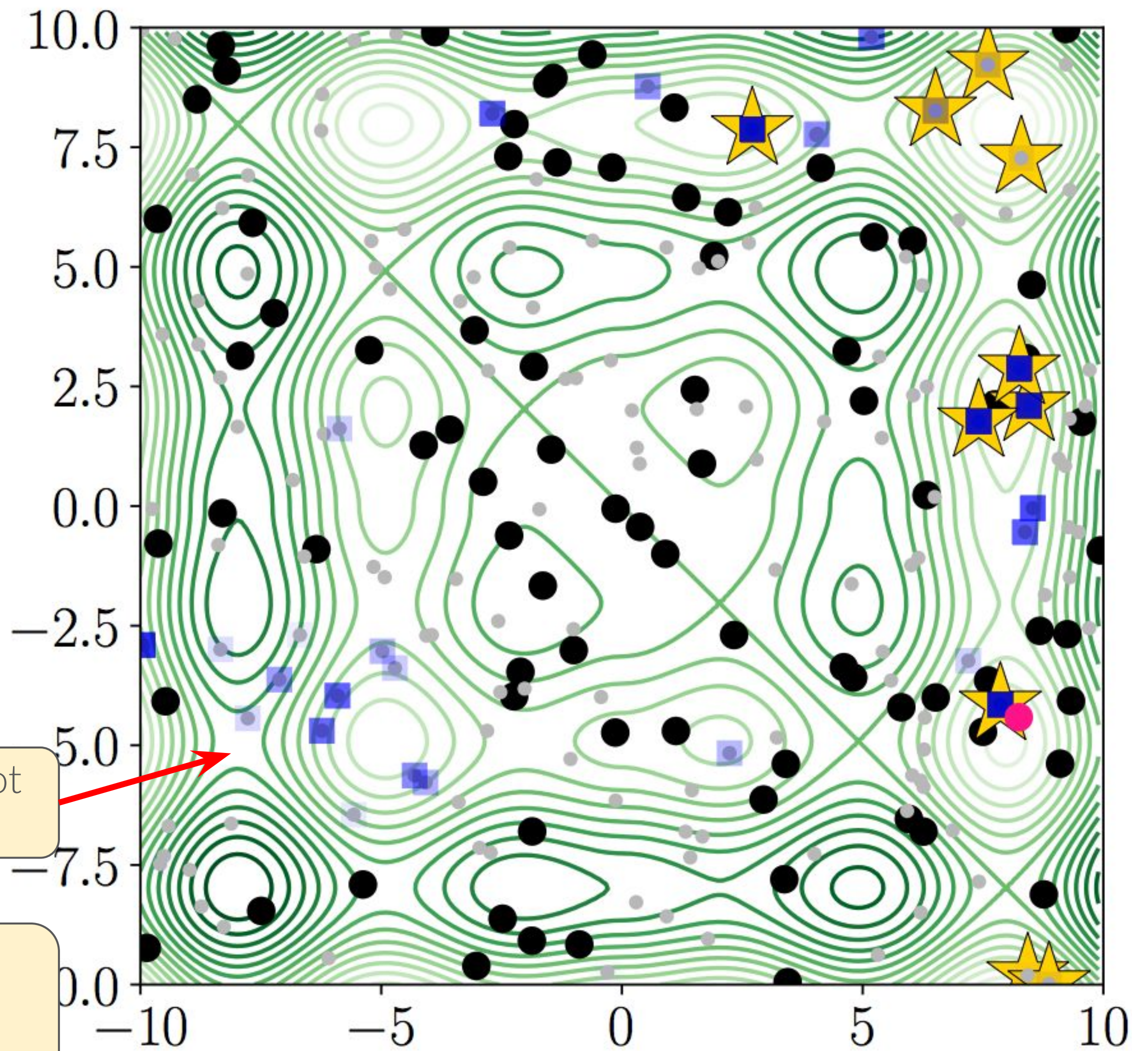


New strategy:
Make a few queries and infer top-10 items

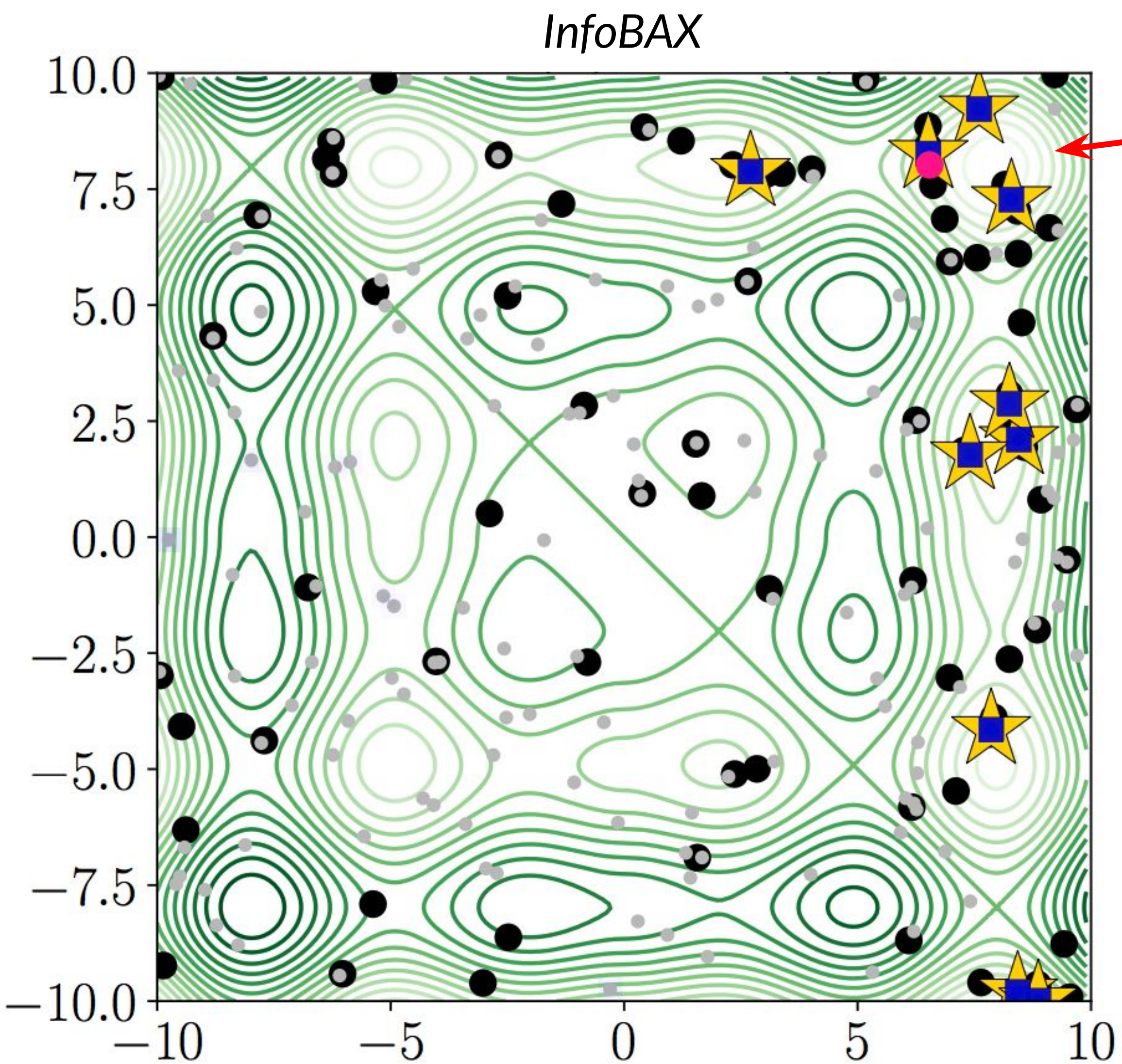
Posterior samples of *top-10* items (blue squares)

100 queries (black dots)

Estimate is still not great

Try ***InfoBAX*** *with "scan and query" algorithm*

APPLICATIONS of BAX — *top-k estimation*



Good estimate in <*100* queries

InfoBAX explores the space but samples densely around high-value items.

UNCERTAINTY MODELS

Final topic: software tools for uncertainty models

The BAX/BO procedures discussed all use *predictive uncertainty models*.

"A model of the conditional distribution over output y given an input x"

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> *"A model of the conditional distribution over output y given an input x"*

⇒ in BAX we focus on GP models, but we may wish to run similar procedures on a variety of probabilistic models (*and to know if our models are good)*

Final topic: software tools for uncertainty models

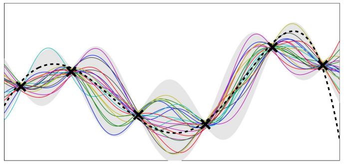
The BAX/BO procedures discussed all use *predictive uncertainty models*.

"A model of the conditional distribution over output y given an input x"

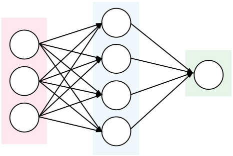
⇒ in BAX we focus on GP models, but we may wish to run similar procedures on a variety of probabilistic models (*and to know if our models are good)*

Types of uncertainty models:

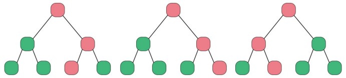
"Classic" Bayesian models: GPs, various (non)lin/hier/add or other Bayesian models



Neural models: probabilistic neural networks, BNN, neural processes, deep generative models



Also: ensembles, quantile regression, conformal prediction, etc.



ASSESSING UNCERTAINTY

How can we assess quality of predictive uncertainty?

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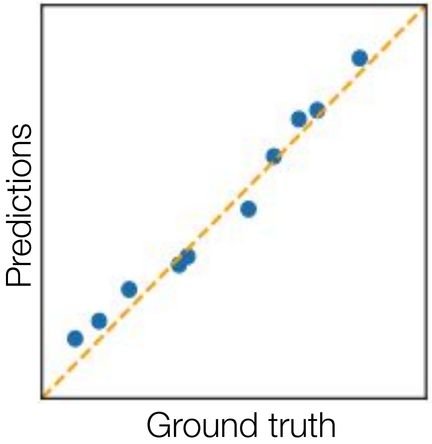
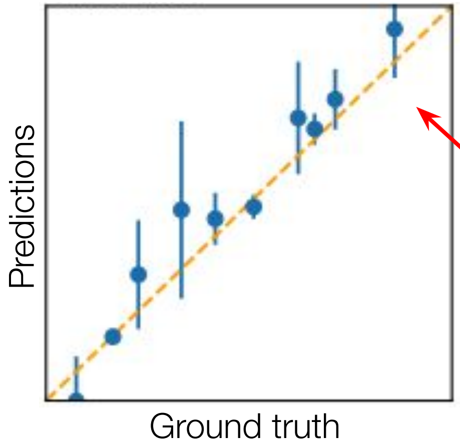
We can visualize point-predictions and predictive uncertainties on a given test set.

For each test point, plot ***predictions*** *vs.* ***ground truth values****:*

Point prediction model



Predictive uncertainty model



Uncertainty for point prediction: *interval, parametric distribution, samples, etc.*

ASSESSING UNCERTAINTY

How can we empirically assess predictive uncertainty?

Three important criteria are...

ASSESSING UNCERTAINTY

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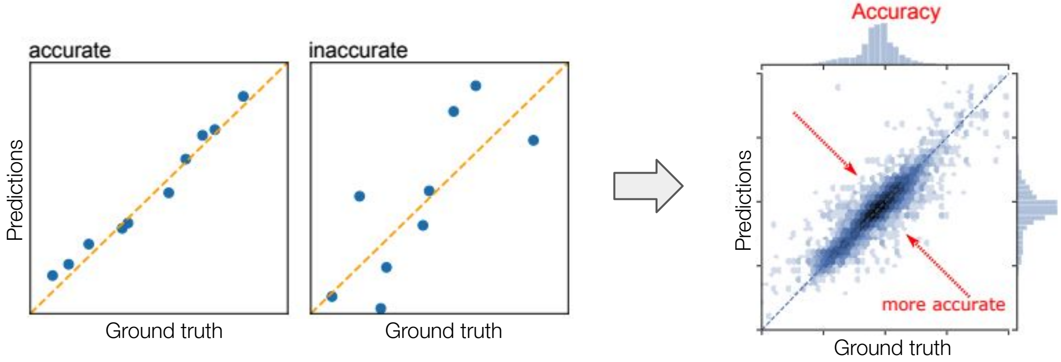
Three important criteria are...

Accuracy:

"How good is mean prediction? (agnostic to uncertainty)"



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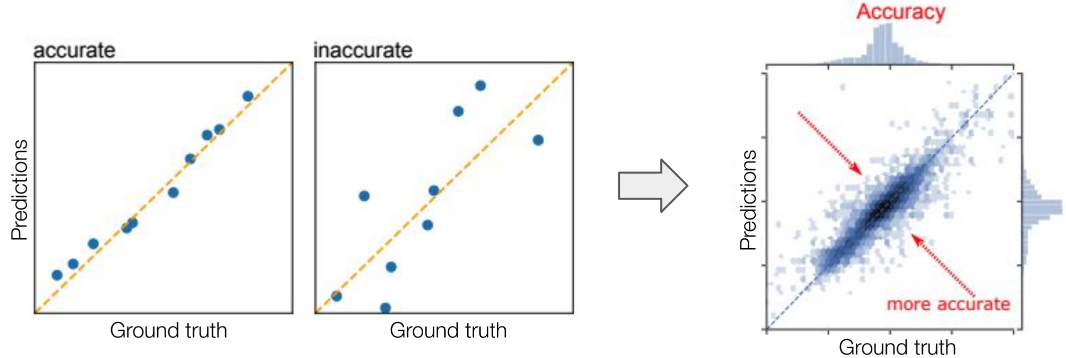
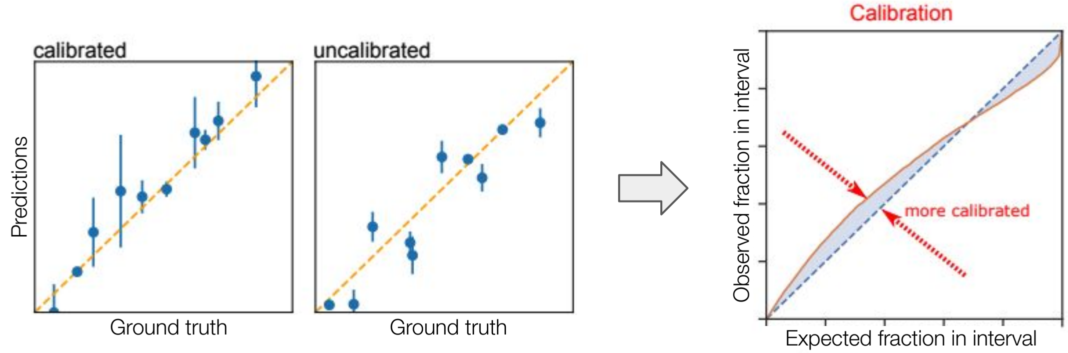


Calibration:

"Is predictive uncertainty distribution under/over confident? (ignoring prediction accuracy)"



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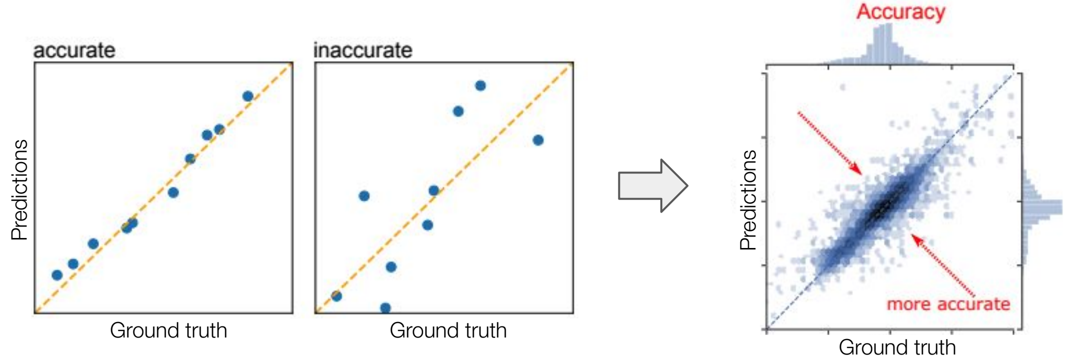

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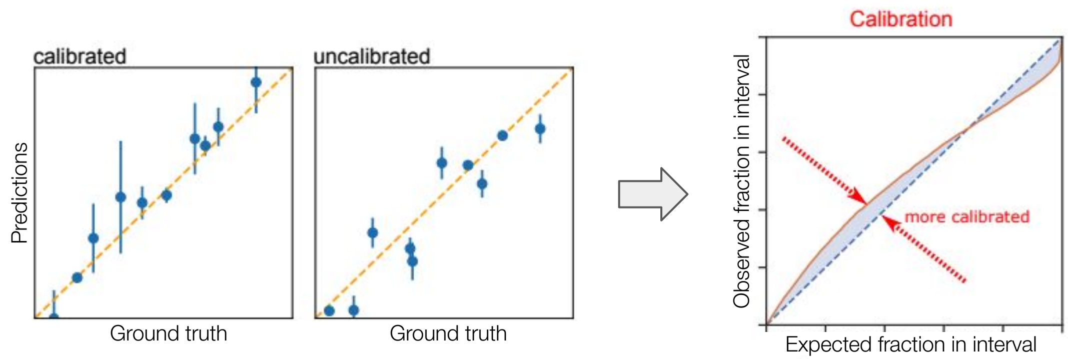
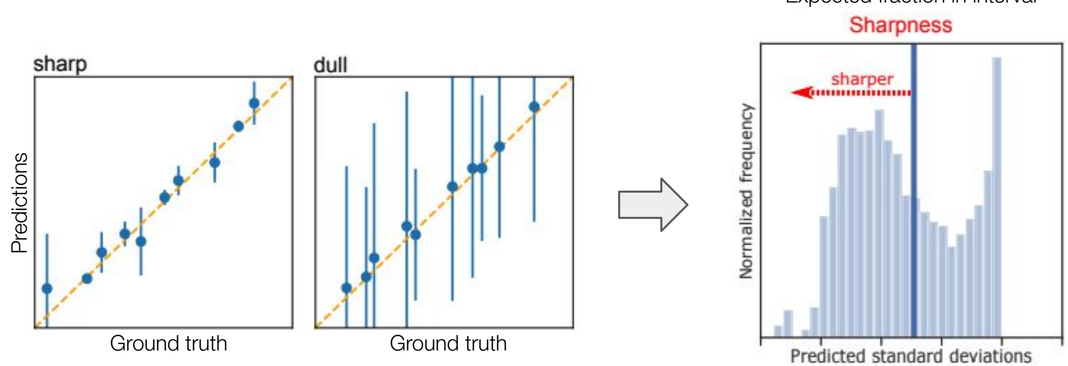


Sharpness:

"On average, how confident are the predictions? (ignoring both of the above)"



Metrics for calibration

Suppose for each test point, our predictive uncertainty model returns a (1-α)-interval (e.g. 95% interval) of the predictive distribution.

Well-calibrated ⇒ *"the (1-α)-interval covers the true value (1-α)-proportion of the time, for all α"*

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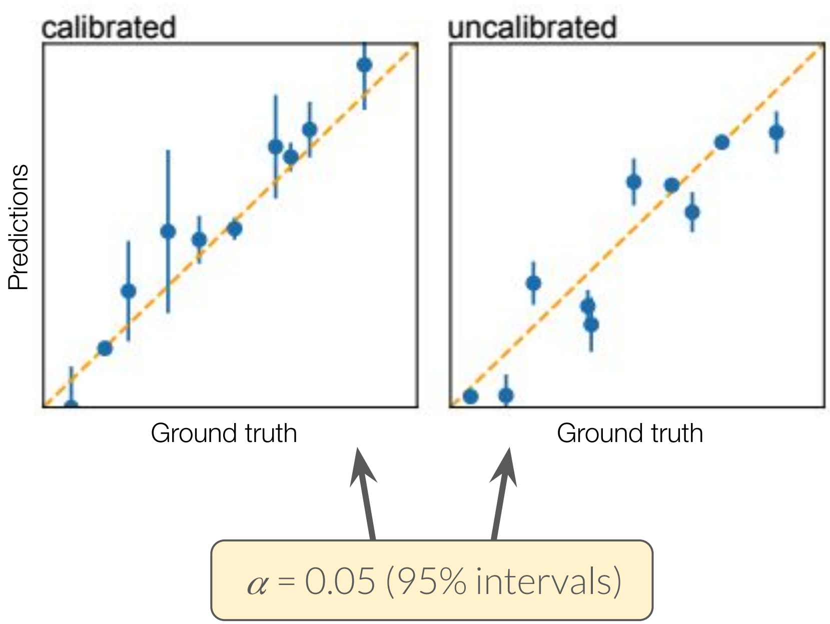

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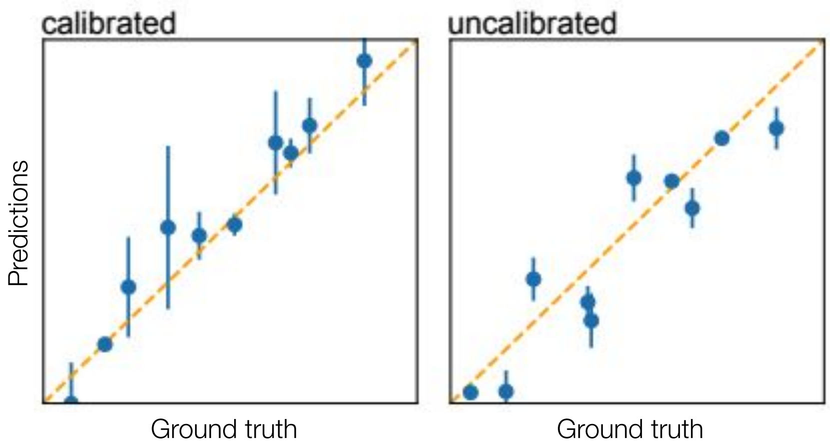
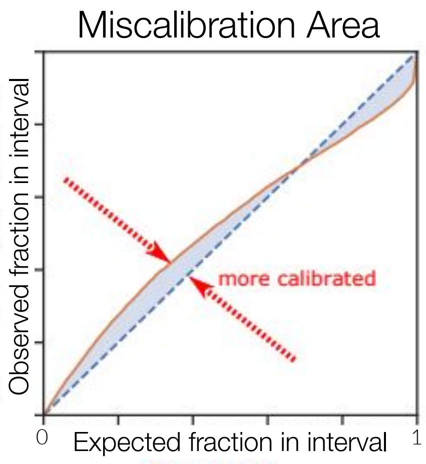




Can scan from α=0 to α=1, and compute:

(1) expected fraction of true values contained in interval

(2) observed fraction of true values contained in interval

Uncertainty Toolbox

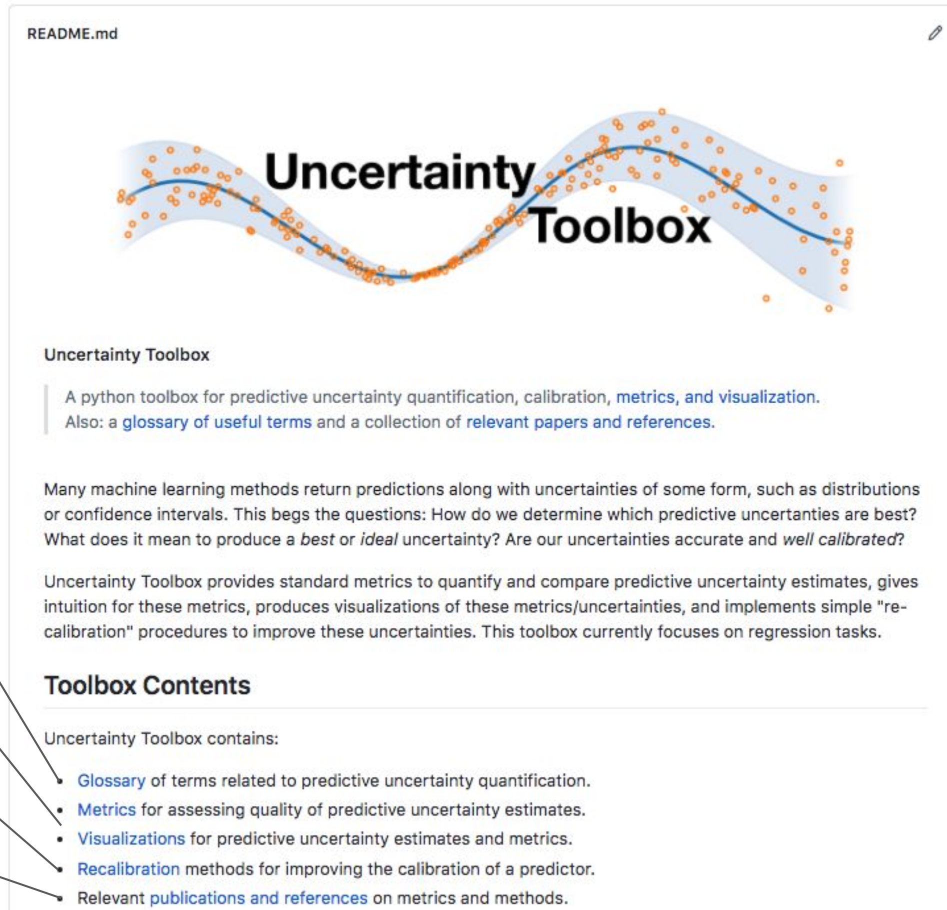
- To help assess uncertainty quantification methods, we released Uncertainty Toolbox.
- "A python toolbox for predictive uncertainty quantification, calibration, metrics, and visualization" → github.com/uncertainty-toolbox/uncertainty-toolbox

Glossary

Metrics / Viz

Recalibration

Relevant Papers


README.md

Uncertainty Toolbox

Uncertainty Toolbox

> A python toolbox for predictive uncertainty quantification, calibration, metrics, and visualization.
> Also: a glossary of useful terms and a collection of relevant papers and references.

Many machine learning methods return predictions along with uncertainties of some form, such as distributions or confidence intervals. This begs the questions: How do we determine which predictive uncertanties are best? What does it mean to produce a *best* or *ideal* uncertainty? Are our uncertainties accurate and *well calibrated*?

Uncertainty Toolbox provides standard metrics to quantify and compare predictive uncertainty estimates, gives intuition for these metrics, produces visualizations of these metrics/uncertainties, and implements simple "re-calibration" procedures to improve these uncertainties. This toolbox currently focuses on regression tasks.

Toolbox Contents

Uncertainty Toolbox contains:

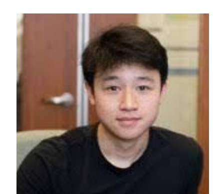
- Glossary of terms related to predictive uncertainty quantification.
- Metrics for assessing quality of predictive uncertainty estimates.
- Visualizations for predictive uncertainty estimates and metrics.
- Recalibration methods for improving the calibration of a predictor.
- Relevant publications and references on metrics and methods.

Collaborators


Kevin Tran


Young Chung


Ian Char


Han Guo

CONCLUSION

In summary…

We extend Bayesian optimization from targeting *global optima* to targeting *other function properties defined by algorithms*.

⇒ Introduce the task of **BAX**,
and the information-based procedure ***InfoBAX***

BAX Paper: *arxiv.org/abs/2104.09460*

Uncertainty Toolbox: *github.com/uncertainty-toolbox/uncertainty-toolbox*

Thanks for listening!

ACQUISITION FUNCTION DETAILS

ACQUISITION FUNCTION DETAILS

InfoBAX expected info gain (EIG) acquisition function

"Expected decrease in entropy on the ***algorithm output****, if we were to query f at x."*

$$\mathrm{EIG}_t(x) = H[p(O_{\mathcal{A}} \mid \mathcal{D}_t)] - \mathbb{E}_{p(y_x \mid \mathcal{D}_t)}[H[p(O_{\mathcal{A}} \mid \mathcal{D}_t \cup \{(x, y_x)\})]]$$

- entropy of posterior distribution over algorithm output
- minus
- expected entropy of posterior distribution over algorithm output, *... if we were to make a query at x*

ACQUISITION FUNCTION DETAILS

InfoBAX expected info gain (EIG) acquisition function

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entropy of posterior distribution over algorithm output

minus

expected entropy of posterior distribution over algorithm output, *... if we were to make a query at x*

Can consider the following related objective...

ACQUISITION FUNCTION DETAILS

Related objective: EIG on execution path

"Expected decrease in entropy on the ***execution path****, if we were to query f at x."*

$$\mathrm{EIG}_t^e(x) = \mathrm{H}\left[e_\mathcal{A} \mid \mathcal{D}_t\right] - \mathbb{E}_{p(y_x|\mathcal{D}_t)}\left[\mathrm{H}\left[e_\mathcal{A} \mid D_t \cup \{(x, y_x)\}\right]\right]$$

ACQUISITION FUNCTION DETAILS

Related objective: EIG on execution path

*"Expected decrease in entropy on the **execution path**, if we were to query f at x."*

$$\mathrm{EIG}_t^e(x) = \mathrm{H}\left[e_{\mathcal{A}} \mid \mathcal{D}_t\right] - \mathbb{E}_{p(y_x \mid \mathcal{D}_t)}\left[\mathrm{H}\left[e_{\mathcal{A}} \mid D_t \cup \{(x, y_x)\}\right]\right]$$

entropy of posterior distribution over **execution path**

minus

expected entropy of posterior distribution over **execution path**, *… if we were to make a query at x*

Related objective: EIG on execution path

*"Expected decrease in entropy on the **execution path**, if we were to query f at x."*

$$\mathrm{EIG}_t^e(x) = \mathrm{H}\left[e_{\mathcal{A}} \mid \mathcal{D}_t\right] - \mathbb{E}_{p(y_x \mid \mathcal{D}_t)}\left[\mathrm{H}\left[e_{\mathcal{A}} \mid D_t \cup \{(x, y_x)\}\right]\right]$$

entropy of posterior distribution over **execution path**

minus

expected entropy of posterior distribution over **execution path**, *... if we were to make a query at x*

If we know function value at each point in execution path ⇒ we know property.

However: this acquisition function may be effective, but *suboptimal in general*.

(Parts of execution path may not be very important for final output)

(E.g. consider case where subsequence in execution path has no influence on later steps/output)

ACQUISITION FUNCTION DETAILS

Related objective: EIG on execution path

We can efficiently estimate this via following trick:

$$\text{EIG}_t^e(x) = \text{H}\left[e_{\mathcal{A}} \mid \mathcal{D}_t\right] - \mathbb{E}_{p(y_x|\mathcal{D}_t)}\left[\text{H}\left[e_{\mathcal{A}} \mid D_t \cup \{(x, y_x)\}\right]\right]$$

ACQUISITION FUNCTION DETAILS

Related objective: EIG on execution path

We can efficiently estimate this via following trick:

$$\mathrm{EIG}_t^e(x) = \mathrm{H}\left[e_{\mathcal{A}} \mid \mathcal{D}_t\right] - \mathbb{E}_{p(y_x \mid \mathcal{D}_t)}\left[\mathrm{H}\left[e_{\mathcal{A}} \mid D_t \cup \{(x, y_x)\}\right]\right]$$

$$= \mathrm{H}\left[y_x \mid \mathcal{D}_t\right] - \mathbb{E}_{p(e_{\mathcal{A}} \mid \mathcal{D}_t)}\left[\mathrm{H}\left[y_x \mid \mathcal{D}_t, e_{\mathcal{A}}\right]\right]$$

entropy of posterior predictive at x.

minus

expected entropy of posterior predictive **given execution path**, *… if we were to make a query at* x

ACQUISITION FUNCTION DETAILS

Related objective: EIG on execution path

We can efficiently estimate this via following trick:

$$\mathrm{EIG}_t^e(x) = \mathrm{H}\left[e_{\mathcal{A}} \mid \mathcal{D}_t\right] - \mathbb{E}_{p(y_x \mid \mathcal{D}_t)}\left[\mathrm{H}\left[e_{\mathcal{A}} \mid D_t \cup \{(x, y_x)\}\right]\right]$$

$$= \mathrm{H}\left[y_x \mid \mathcal{D}_t\right] - \mathbb{E}_{p(e_{\mathcal{A}} \mid \mathcal{D}_t)}\left[\mathrm{H}\left[y_x \mid \mathcal{D}_t, e_{\mathcal{A}}\right]\right]$$

entropy of posterior predictive at x.

minus

expected entropy of posterior predictive **given execution path**,
... if we were to make a query at x

And note that

$$p\left(y_x \mid \mathcal{D}_t, \tilde{e}_{\mathcal{A}}\right) = p\left(y_x \,\middle|\, \mathcal{D}_t, \{\tilde{f}_{z_s}\}_{s=1}^{S}\right)$$

Gaussian

ACQUISITION FUNCTION DETAILS

Back to the: EIG on algorithm output

We can similarity write:

$$\mathrm{EIG}_t(x) = H[p(O_{\mathcal{A}} \mid \mathcal{D}_t)] - \mathbb{E}_{p(y_x \mid \mathcal{D}_t)}[H[p(O_{\mathcal{A}} \mid \mathcal{D}_t \cup \{(x, y_x)\})]]$$

entropy of posterior distribution over algorithm output

minus

expected entropy of posterior distribution over algorithm output,
… if we were to make a query at x

ACQUISITION FUNCTION DETAILS

Back to the: EIG on algorithm output

We can similarity write:

$$\mathrm{EIG}_t(x) = H[p(O_{\mathcal{A}} \mid \mathcal{D}_t)] - \mathbb{E}_{p(y_x \mid \mathcal{D}_t)}[H[p(O_{\mathcal{A}} \mid \mathcal{D}_t \cup \{(x, y_x)\})]]$$

$$= \mathrm{H}\left[y_x \mid \mathcal{D}_t\right] - \mathbb{E}_{p(O_{\mathcal{A}} \mid \mathcal{D}_t)}\left[\mathrm{H}\left[y_x \mid \mathcal{D}_t, O_{\mathcal{A}}\right]\right]$$

ACQUISITION FUNCTION DETAILS

Back to the: EIG on algorithm output

We can similarity write:

$$\mathrm{EIG}_t(x) = H[p(O_{\mathcal{A}} \mid \mathcal{D}_t)] - \mathbb{E}_{p(y_x \mid \mathcal{D}_t)}[H[p(O_{\mathcal{A}} \mid \mathcal{D}_t \cup \{(x, y_x)\})]]$$

$$= \mathrm{H}\left[y_x \mid \mathcal{D}_t\right] - \mathbb{E}_{p(O_{\mathcal{A}} \mid \mathcal{D}_t)}\left[\mathrm{H}\left[y_x \mid \mathcal{D}_t, O_{\mathcal{A}}\right]\right]$$

Difficult

ACQUISITION FUNCTION DETAILS

Back to the: EIG on algorithm output

We can similarity write:

$$\mathrm{EIG}_t(x) = H[p(O_{\mathcal{A}} \mid \mathcal{D}_t)] - \mathbb{E}_{p(y_x \mid \mathcal{D}_t)}[H[p(O_{\mathcal{A}} \mid \mathcal{D}_t \cup \{(x, y_x)\})]]$$

$$= \mathrm{H}[y_x \mid \mathcal{D}_t] - \mathbb{E}_{p(O_{\mathcal{A}} \mid \mathcal{D}_t)}[\mathrm{H}[y_x \mid \mathcal{D}_t, O_{\mathcal{A}}]]$$

Note that:

$$\begin{aligned} p(y_x \mid \mathcal{D}_t, O_{\mathcal{A}}) &= \int p(y_x, e_{\mathcal{A}} \mid \mathcal{D}_t, O_{\mathcal{A}}) \, \mathrm{d}e_{\mathcal{A}} \\ &= \int p(y_x \mid \mathcal{D}_t, e_{\mathcal{A}}, O_{\mathcal{A}}) \, p(e_{\mathcal{A}} \mid O_{\mathcal{A}}, \mathcal{D}_t) \, \mathrm{d}e_{\mathcal{A}} \\ &= \mathbb{E}_{p(e_{\mathcal{A}} \mid O_{\mathcal{A}}, \mathcal{D}_t)} [p(y_x \mid \mathcal{D}_t, e_{\mathcal{A}})]. \end{aligned}$$

ACQUISITION FUNCTION DETAILS

Back to the: EIG on algorithm output

We can similarity write:

$$\mathrm{EIG}_t(x) = H[p(O_{\mathcal{A}} \mid \mathcal{D}_t)] - \mathbb{E}_{p(y_x \mid \mathcal{D}_t)}[H[p(O_{\mathcal{A}} \mid \mathcal{D}_t \cup \{(x, y_x)\})]]$$

$$= \mathrm{H}\left[y_x \mid \mathcal{D}_t\right] - \mathbb{E}_{p(O_{\mathcal{A}} \mid \mathcal{D}_t)}\left[\mathrm{H}\left[y_x \mid \mathcal{D}_t, O_{\mathcal{A}}\right]\right]$$

Note that:

$$p(y_x \mid \mathcal{D}_t, O_{\mathcal{A}}) = \int p(y_x, e_{\mathcal{A}} \mid \mathcal{D}_t, O_{\mathcal{A}})\, \mathrm{d}e_{\mathcal{A}}$$

$$= \int p(y_x \mid \mathcal{D}_t, e_{\mathcal{A}}, O_{\mathcal{A}})\, p(e_{\mathcal{A}} \mid O_{\mathcal{A}}, \mathcal{D}_t)\, \mathrm{d}e_{\mathcal{A}}$$

$$= \mathbb{E}_{p(e_{\mathcal{A}} \mid O_{\mathcal{A}}, \mathcal{D}_t)}\left[p\left(y_x \mid \mathcal{D}_t, e_{\mathcal{A}}\right)\right].$$

Gaussian

Back to the: EIG on algorithm output

We can similarity write:

$$\mathrm{EIG}_t(x) = H[p(O_{\mathcal{A}} \mid \mathcal{D}_t)] - \mathbb{E}_{p(y_x \mid \mathcal{D}_t)}[H[p(O_{\mathcal{A}} \mid \mathcal{D}_t \cup \{(x, y_x)\})]]$$

$$= \mathrm{H}\left[y_x \mid \mathcal{D}_t\right] - \mathbb{E}_{p(O_{\mathcal{A}} \mid \mathcal{D}_t)}\left[\mathrm{H}\left[y_x \mid \mathcal{D}_t, O_{\mathcal{A}}\right]\right]$$

$$= \mathrm{H}\left[y_x \mid \mathcal{D}_t\right] - \mathbb{E}_{p(O_{\mathcal{A}} \mid \mathcal{D}_t)}\left[\mathrm{H}\left[\mathbb{E}_{p(e_{\mathcal{A}} \mid O_{\mathcal{A}}, \mathcal{D}_t)}\left[p\left(y_x \mid \mathcal{D}_t, e_{\mathcal{A}}\right)\right]\right]\right]$$