Efficient Nonmyopic Active Search

Jiang, Malkomes, Converse, Shofner, Moseley, Garnett. ICML 2017

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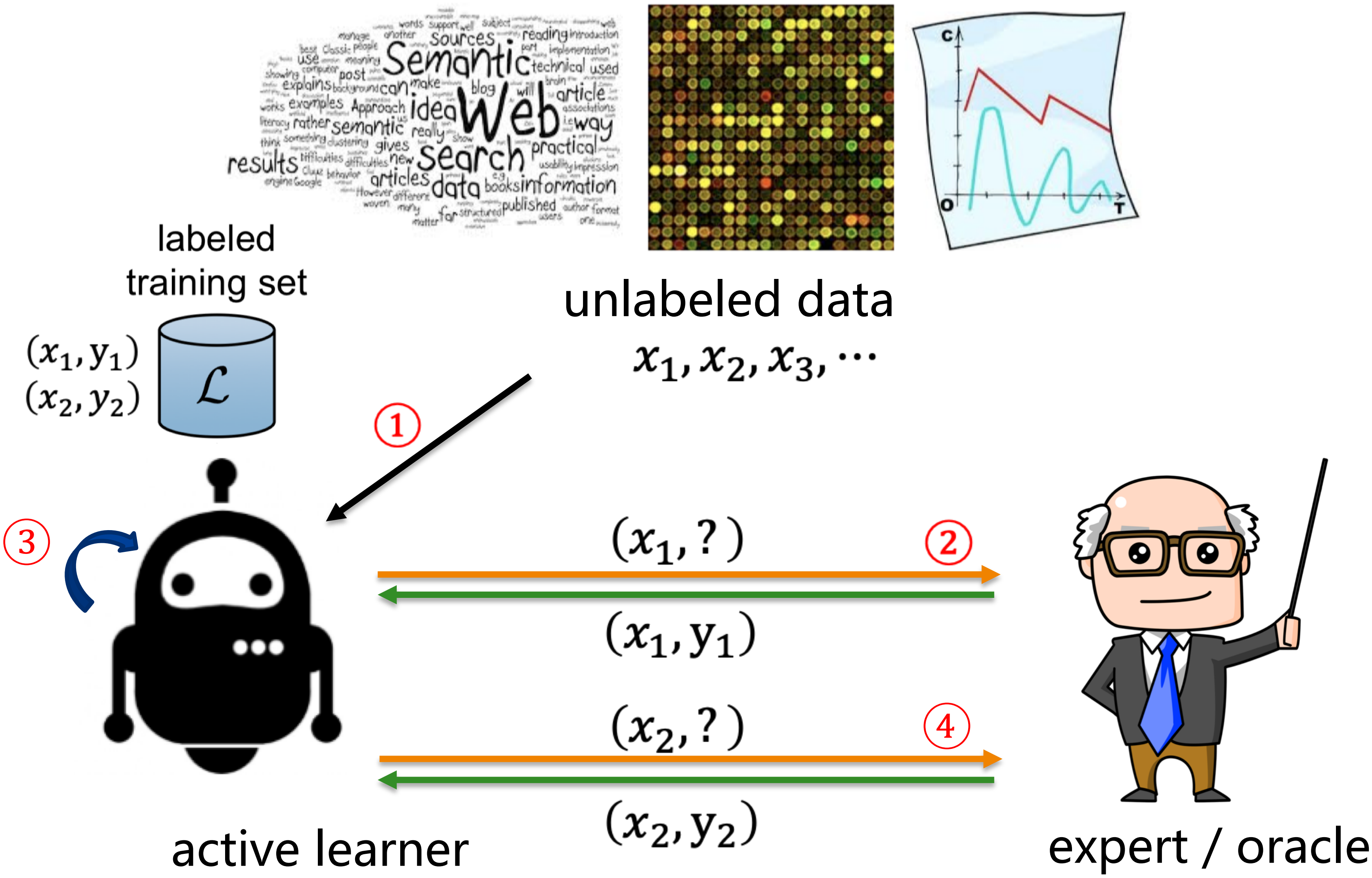
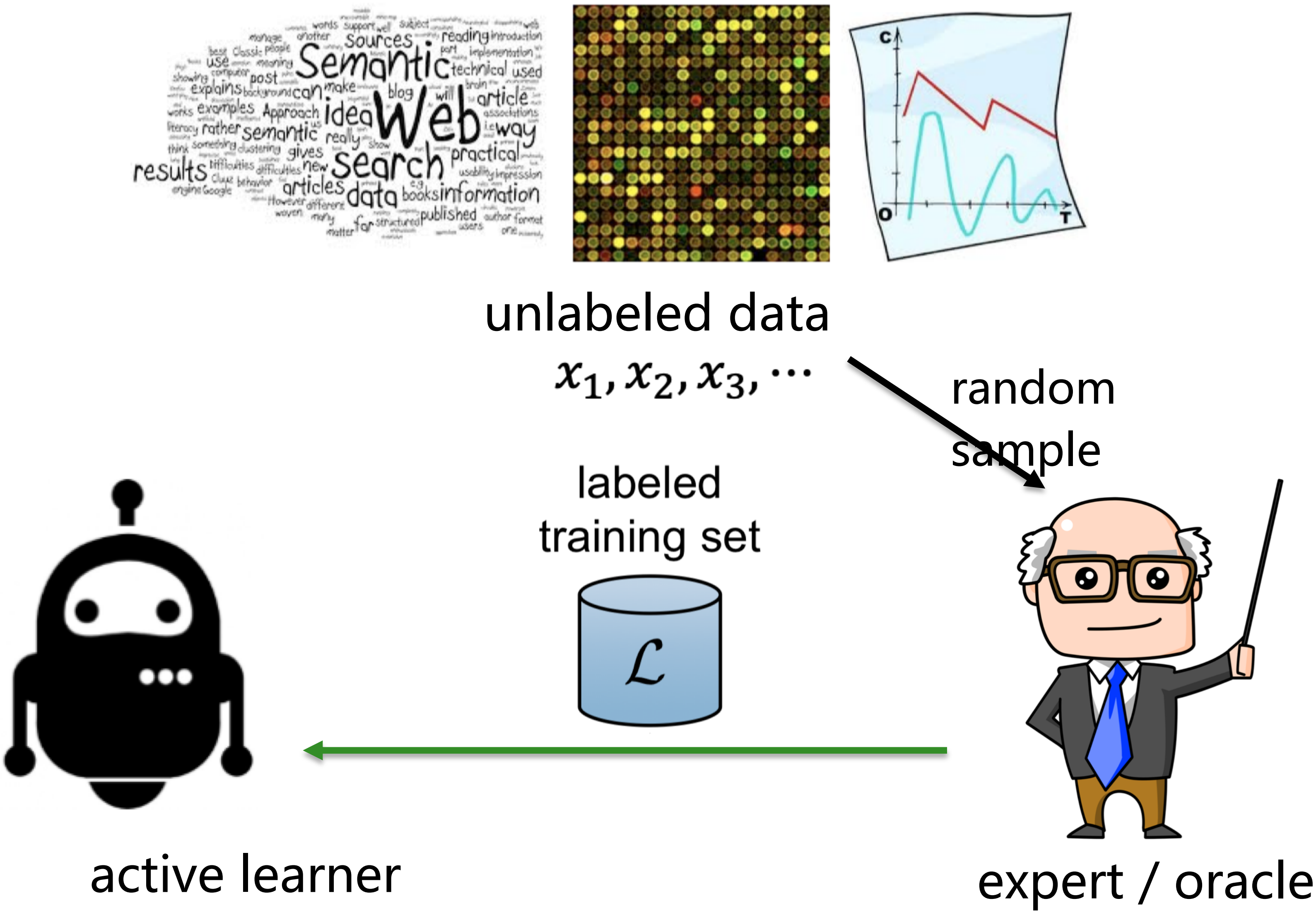
CSC 2547, Oct 18th

Active Learning



Supervised Learning



Why active learning matters?

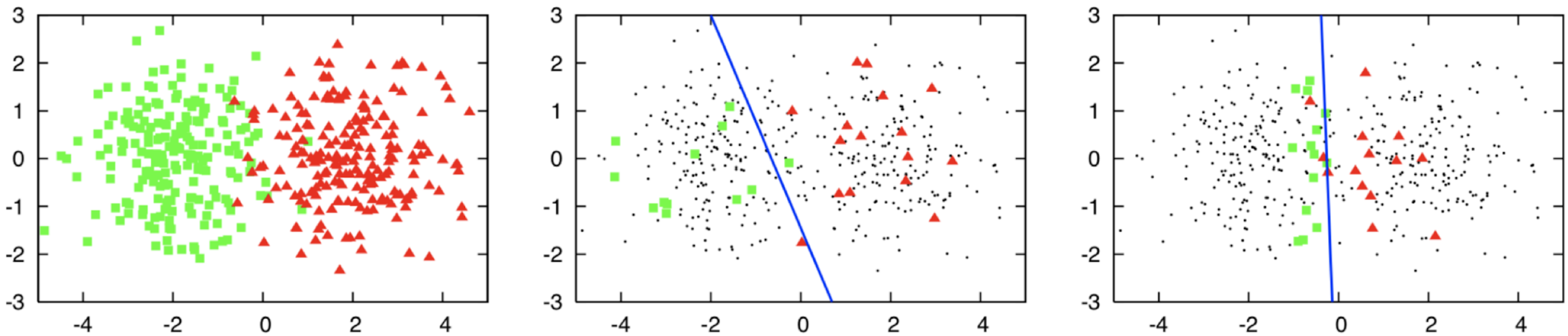
- Collecting data is much cheaper than annotating them
  - we have large-scale unlabeled data
- Labeling data is very difficult, time-consuming, or expensive

Active learning helps model learn more efficiently (compared to random sampling)

Uncertainty Sampling

- Query examples that the learner are most uncertain about (i.e., instances near the decision boundary of the model)

Binary: query the instance whose posterior probability of being positive is nearest 0.5



400 instances sampled from 2 class Gaussians

random sampling
30 labeled instances
(accuracy=0.7)

uncertainty sampling
30 labeled instances
(accuracy=0.9)

$$x^* \triangleq \arg\min_x \left|\Pr(y=1 \mid x, \mathcal{D}) - {}^1\!/_2\right|$$

[Lewis & Gale, SIGIR'94]

Uncertainty Sampling

- For multiclass problems
  - *least confidence*

$$x^*_{LC} = \underset{x}{\operatorname{argmax}} \; 1 - P_\theta(\hat{y}|x)$$

$$\hat{y} = \operatorname{argmax}_y P_\theta(y|x)$$

  - *margin sampling*

$$x^*_M = \underset{x}{\operatorname{argmin}} \, P_\theta(\hat{y}_1|x) - P_\theta(\hat{y}_2|x)$$

$\hat{y}_1$ and $\hat{y}_2$ are the first and second most probable class labels

  - *entropy*

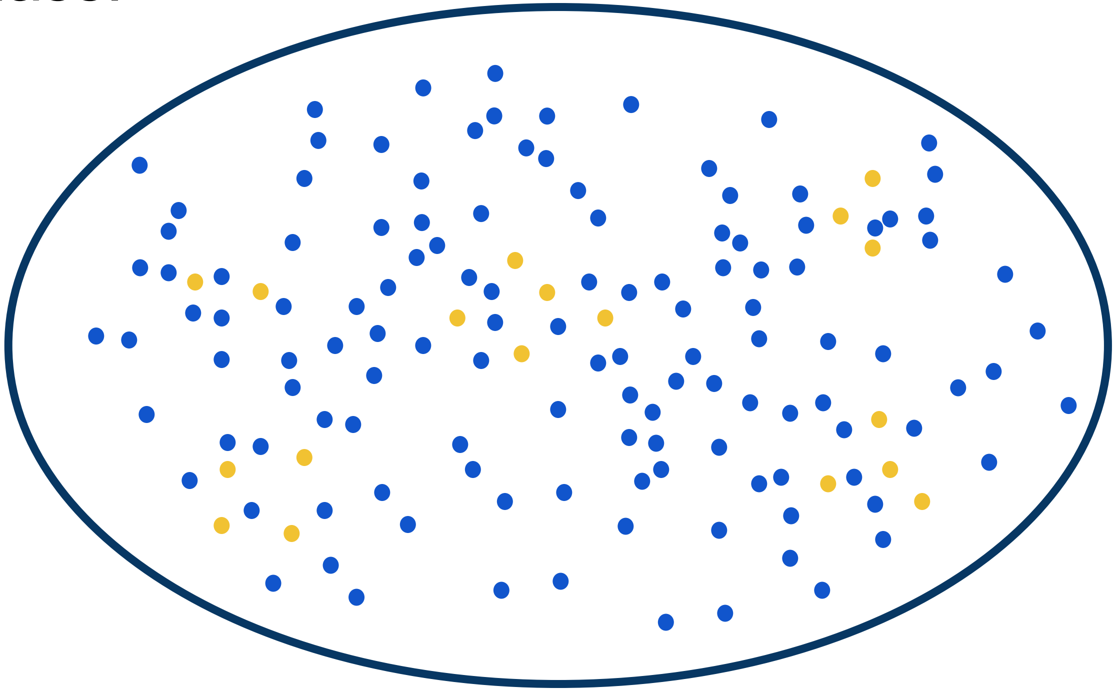
$$x^*_H = \underset{x}{\operatorname{argmax}} - \sum_i P_\theta(y_i|x) \log P_\theta(y_i|x)$$

Other Query Strategies

- Query-By-Committee (QBC)
  - maintain a committee for voting query candidates
- Expected Model Change
  - impart the greatest change to the current model
- Expected Error Reduction
  - how much its generalization error is likely to be reduced
- Variance Reduction
  - minimizing output variance
- Density-Weighted Methods
  - modifying the input distribution and pick informative instances (uncertain and representative)

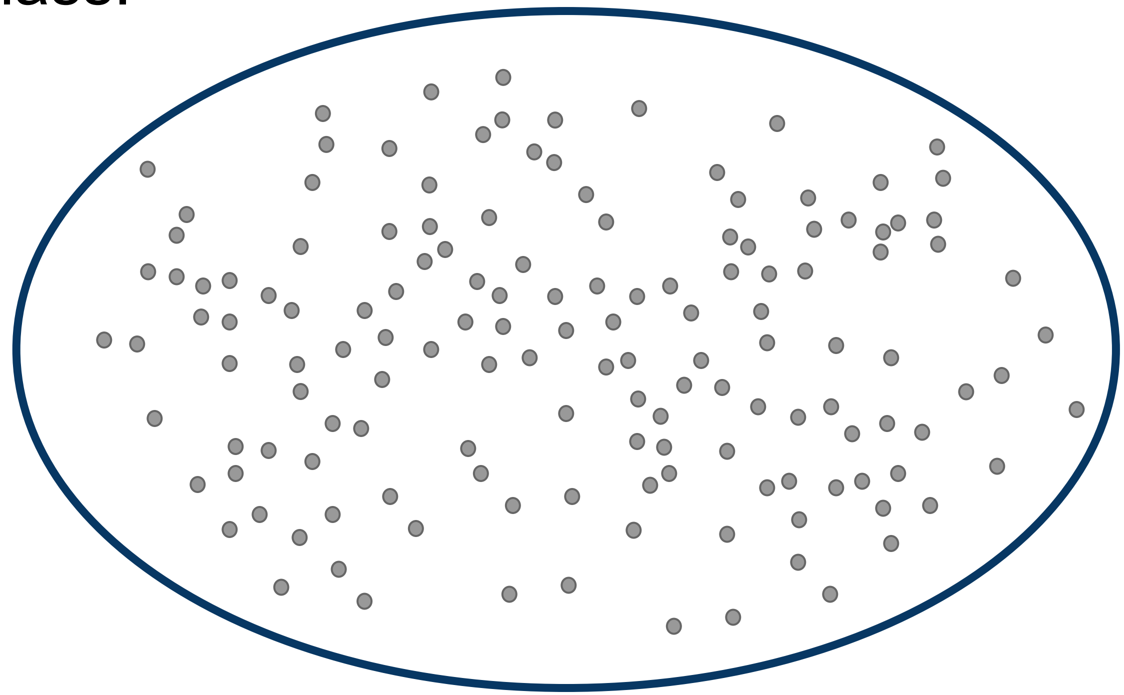
Active Search

sequentially inspecting data to discover members of a rare, desired class.



Active Search

sequentially inspecting data to discover members of a rare, desired class.



What is the best policy to select between data points such that we can find more of the *target* class in a given number of queries?

Active Search

- Given a finite domain of elements $\mathcal{X} \triangleq \{x_i\}$
- target set $\mathcal{R} \subset \mathcal{X}$
- budget t

Goal: Maximizing the utility function in budget t

$$u(\mathcal{D}) \triangleq \sum_{y_i \in \mathcal{D}} y_i$$

where

$$\mathcal{D} \triangleq \{(x_i, y_i)\} \quad y \triangleq \mathbb{1}\{x \in \mathcal{R}\}$$

Optimal Bayesian Policy

- Assume we have a probabilistic classification model that provides

$$\Pr(y = 1 \mid x, \mathcal{D})$$

- The optimal policy

$$x_i^* \triangleq \operatorname*{arg\,max}_{x_i \in \mathcal{X} \setminus \mathcal{D}_{i-1}} \mathbb{E}\big[u(\mathcal{D}_t) \mid x_i, \mathcal{D}_{i-1}\big]$$

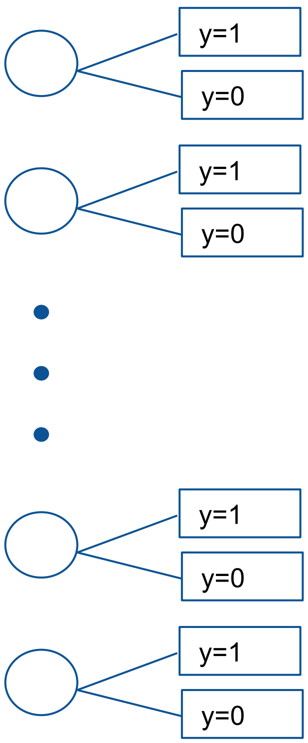
- How to solve above Equation?

Optimal Bayesian Policy

Optimal Policy for the last query ($i = t$) :

- Intuition
  - There is no need to explore
  - The optimal decision should be greedy

Time step i = t
[n - (t-1)] nodes are unlabeled

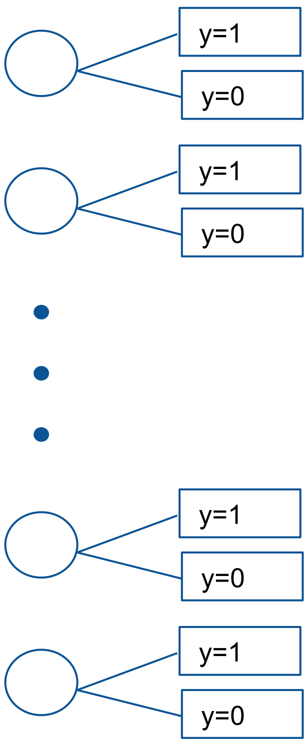


Optimal Bayesian Policy

Optimal Policy for the last query ($i = t$) :

- Intuition
  - There is no need to explore
  - The optimal decision should be greedy
- Solving Bayesian Policy equation confirms

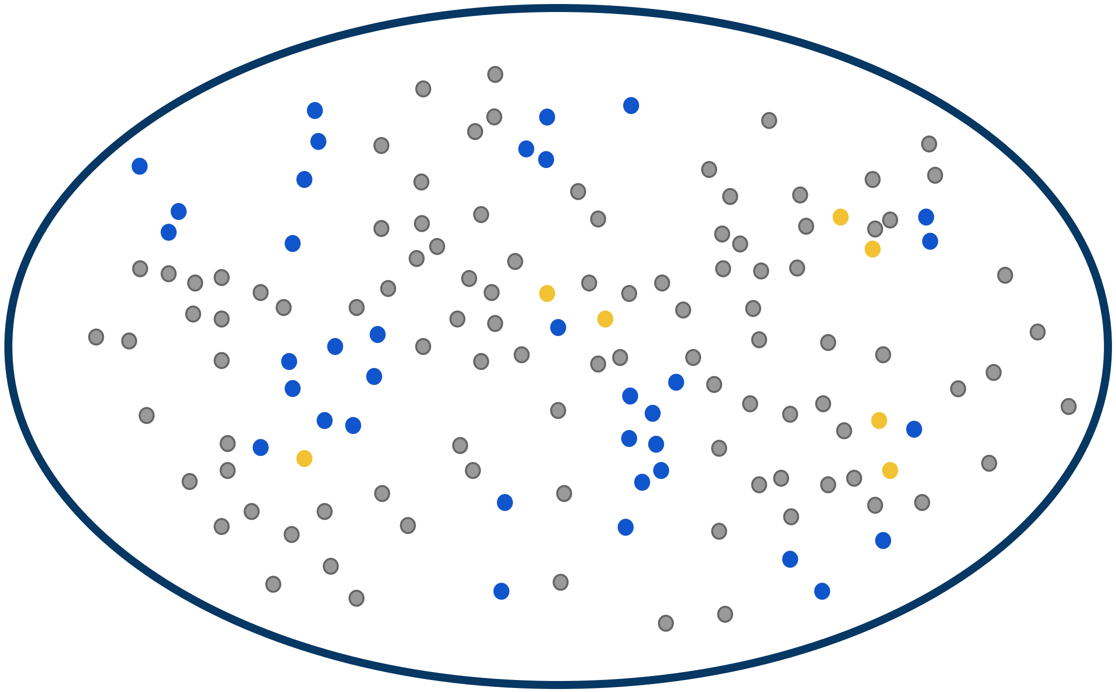
Time step i = t
[n - (t-1)] nodes are unlabeled



$$\mathbb{E}\left[u(\mathcal{D}_t) \mid x_t, \mathcal{D}_{t-1}\right] = u(\mathcal{D}_{t-1}) + \Pr(y_t = 1 \mid x_t, \mathcal{D}_{t-1})$$

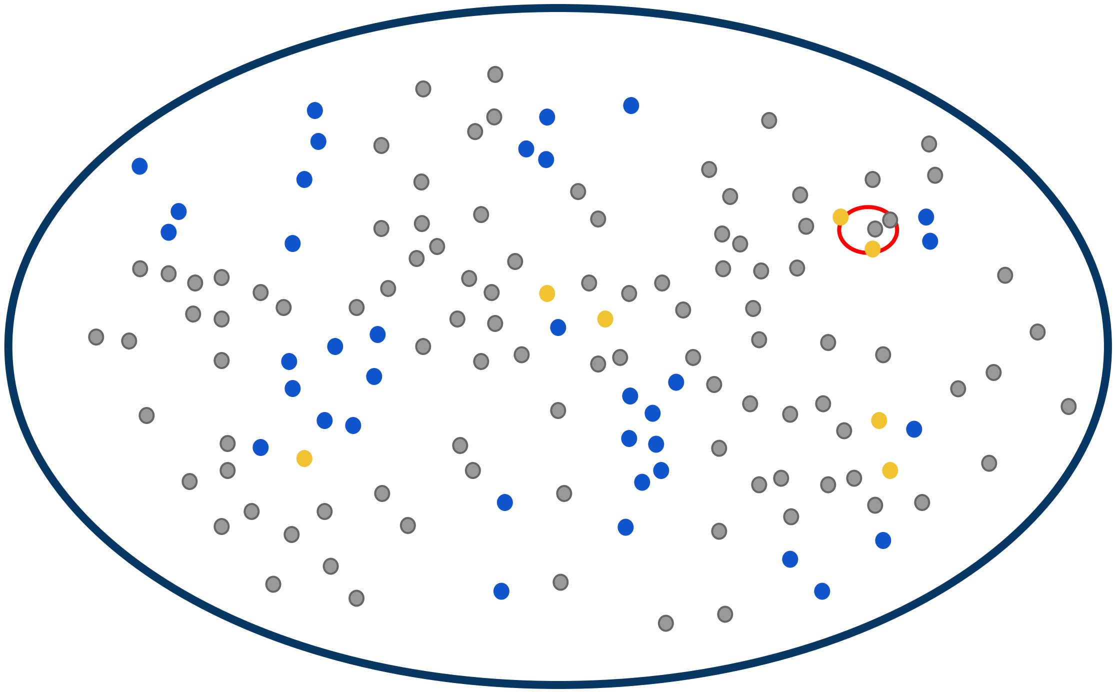
Optimal Bayesian Policy (Example)

last query for our example:



Optimal Bayesian Policy (Example)

last query for our example:

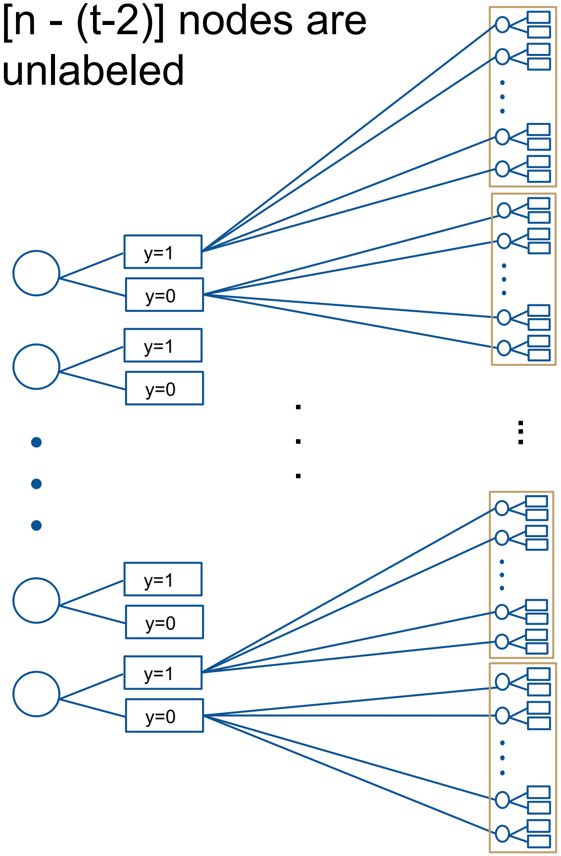


Optimal Bayesian Policy

Optimal Policy when two queries are left
$(i = t - 1)$

- policy is not as trivial
- the probability model changes after the first choice

Time step i = t-1
[n - (t-2)] nodes are unlabeled



Optimal Bayesian Policy

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Solving Bayesian Policy equation

$$\mathbb{E}\left[u(\mathcal{D}_t) \mid x_{t-1}, \mathcal{D}_{t-2}\right] = u(\mathcal{D}_{t-2}) + \\ \Pr(y_{t-1} = 1 \mid x_{t-1}, \mathcal{D}_{t-2}) + \\ \mathbb{E}_{y_{t-1}}\left[\max_{x_t} \Pr(y_t = 1 \mid x_t, \mathcal{D}_{t-1})\right]$$

Time step i = t-1
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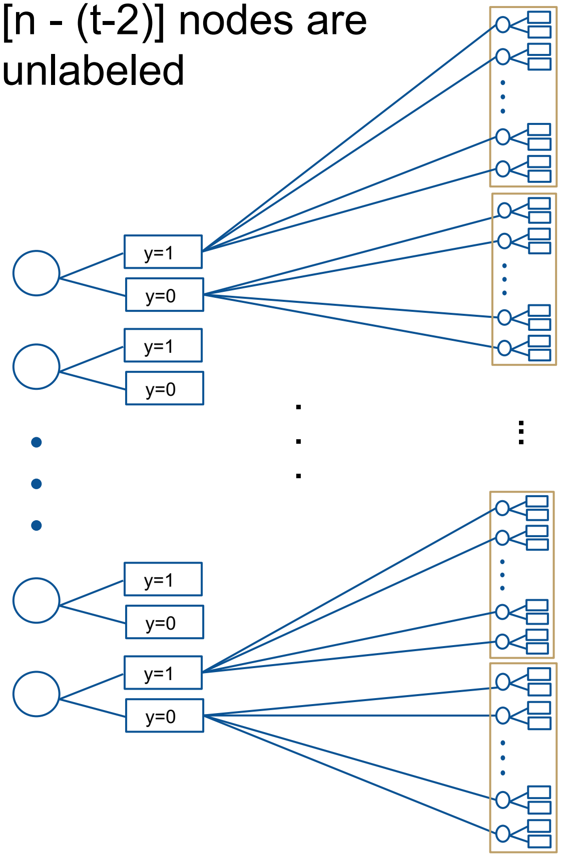

(n-(t-2)) * 2 * (n-(t-1) * 2) computation

Optimal Bayesian Policy

Optimal Policy when two queries are left $(i = t - 1)$

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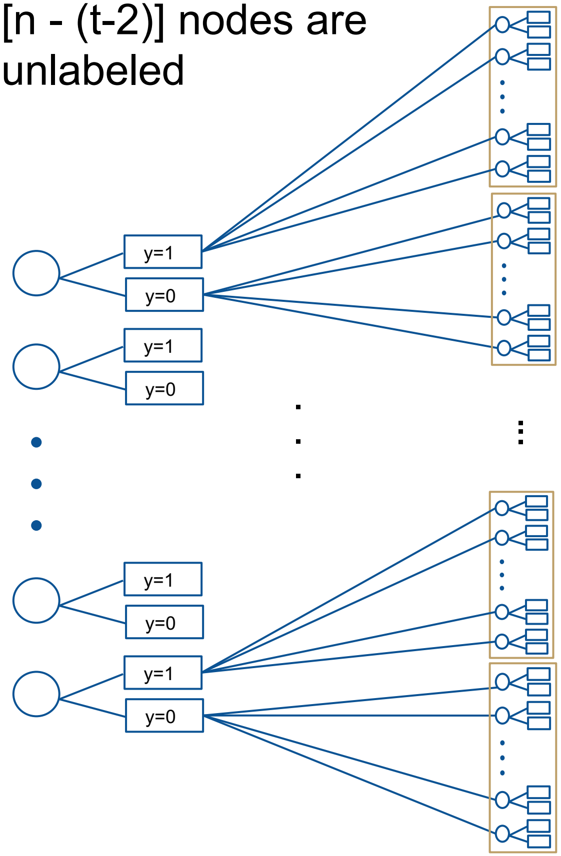
Solving Bayesian Policy equation

$$\mathbb{E}\left[u(\mathcal{D}_t) \mid x_{t-1}, \mathcal{D}_{t-2}\right] = u(\mathcal{D}_{t-2}) + \Pr(y_{t-1} = 1 \mid x_{t-1}, \mathcal{D}_{t-2}) + \mathbb{E}_{y_{t-1}}\left[\max_{x_t} \Pr(y_t = 1 \mid x_t, \mathcal{D}_{t-1})\right]$$

Exploitation

Time step i = t-1
[n - (t-2)] nodes are unlabeled



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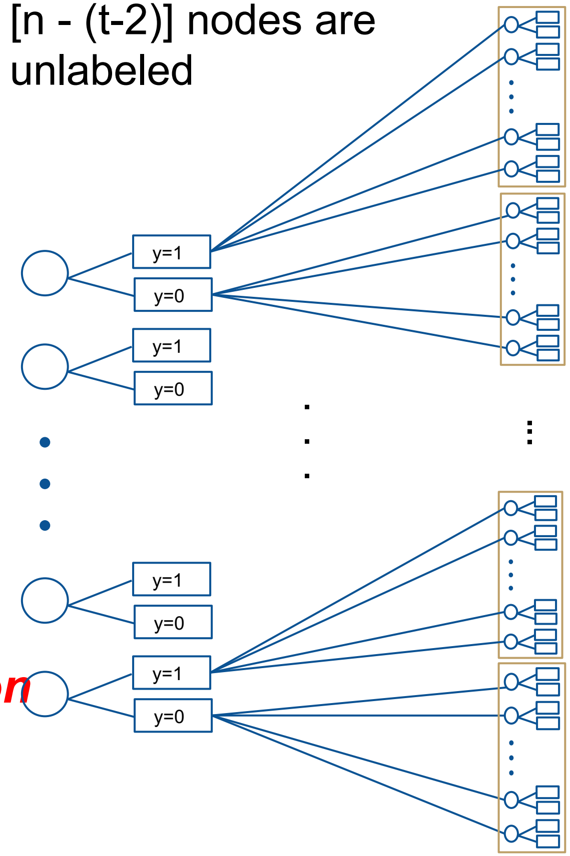
Exploration

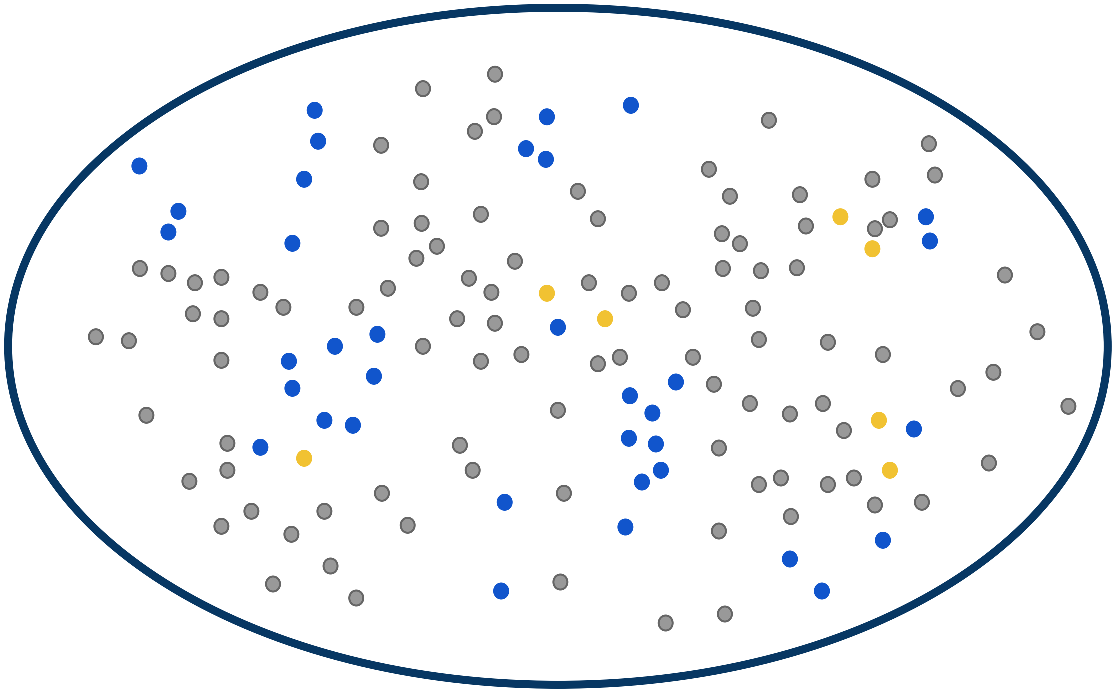
Time step i = t-1
[n - (t-2)] nodes are unlabeled



(n-(t-2)) * 2 * (n-(t-1) * 2)
computation

Optimal Bayesian Policy (Example)

Two queries are left:



Optimal Bayesian Policy (Example)

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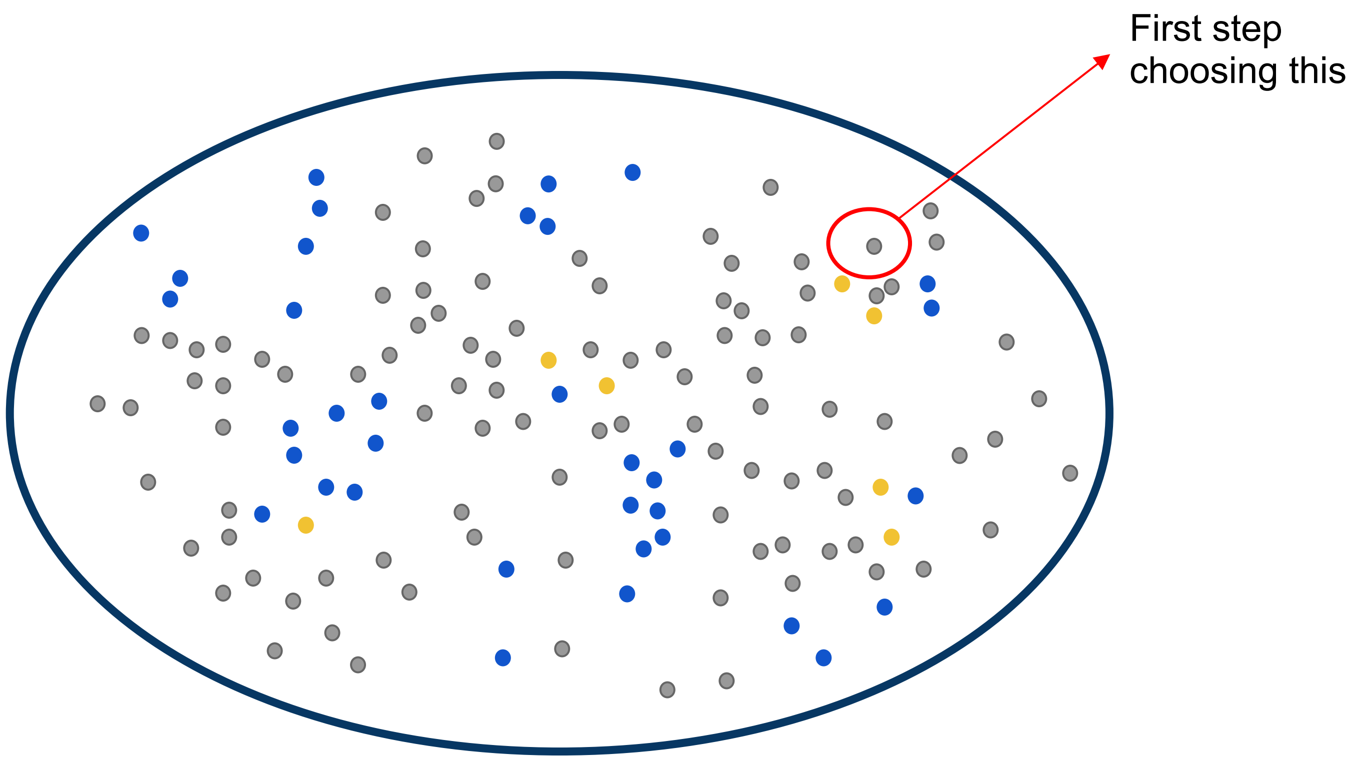

Optimal Bayesian Policy (Example)

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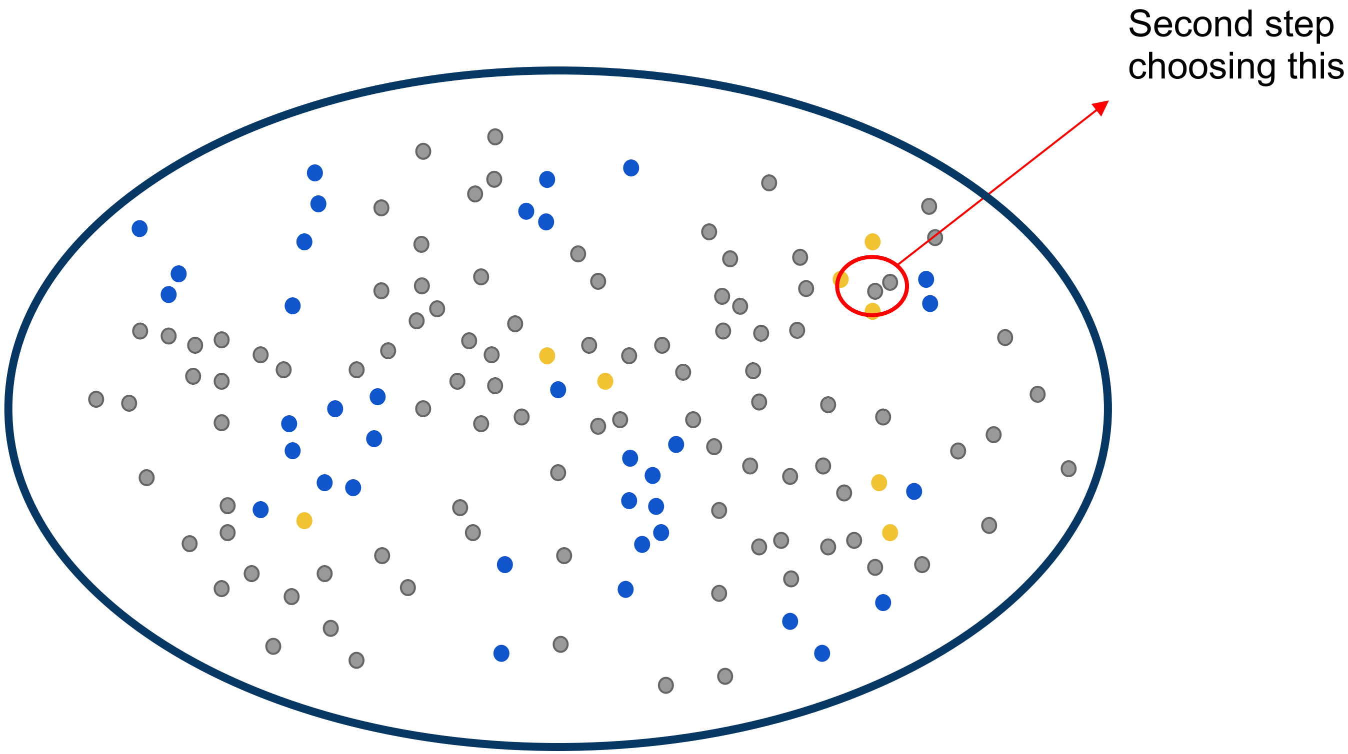


Optimal Bayesian Policy

Bayesian Policy equation (General Form)

$$\mathbb{E}\big[u(\mathcal{D}_t) \mid x_i, \mathcal{D}_{i-1}\big] = u(\mathcal{D}_{i-1}) + \underbrace{\Pr(y_i = 1 \mid x_i, \mathcal{D}_{i-1})}_{\text{exploitation, } < 1} + \underbrace{\mathbb{E}_{y_i}\Big[\max_{x'} \mathbb{E}\big[u(\mathcal{D}_t \setminus \mathcal{D}_i) \mid x', \mathcal{D}_i\big]\Big]}_{\text{exploration, } < t-i}$$

Time complexity: $\mathcal{O}\big((2n)^{\ell}\big)$

- where ℓ is the lookahead $\ell = t - i + 1$
- n is the total number of unlabeled point

Optimal Bayesian Policy

Bayesian Policy equation (General Form)

$$\mathbb{E}\big[u(\mathcal{D}_t) \mid x_i, \mathcal{D}_{i-1}\big] = u(\mathcal{D}_{i-1}) + \underbrace{\Pr(y_i = 1 \mid x_i, \mathcal{D}_{i-1}) +}_{\text{exploitation, } \leq 1} \underbrace{\mathbb{E}_{y_i}\Big[\max_{x'} \mathbb{E}\big[u(\mathcal{D} \setminus \mathcal{D}_i) \mid x', \mathcal{D}_i\big]\Big]}_{\text{exploration, } < t-i}$$

Time complexity: $O((2n)^{\ell})$

- where ℓ is the lookahead $\ell = t - i + 1$
- n is the total number of unlabeled point

infeasible

Hardness of Approximation

There is no *polynomial-time* active search policy with a constant factor approximation ratio for optimizing the expected utility.

Myopic Approach

- **1-step ahead myopic**

$$x_i^* = \arg\max_{x_i} \mathbb{E}[u(\mathcal{D}_i)|x_i, \mathcal{D}_{i-1}]$$

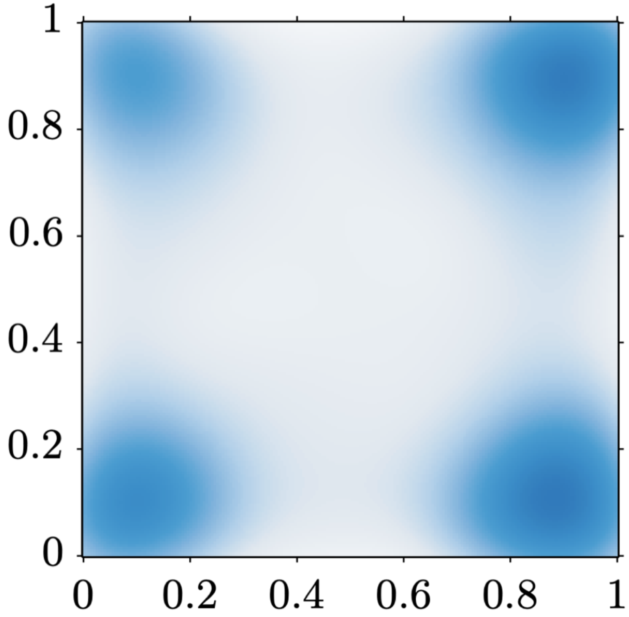
- **2-step ahead myopic**

$$x_i^* = \arg\max_{x_i} \mathbb{E}[u(\mathcal{D}_{i+1})|x_i, \mathcal{D}_{i-1}]$$

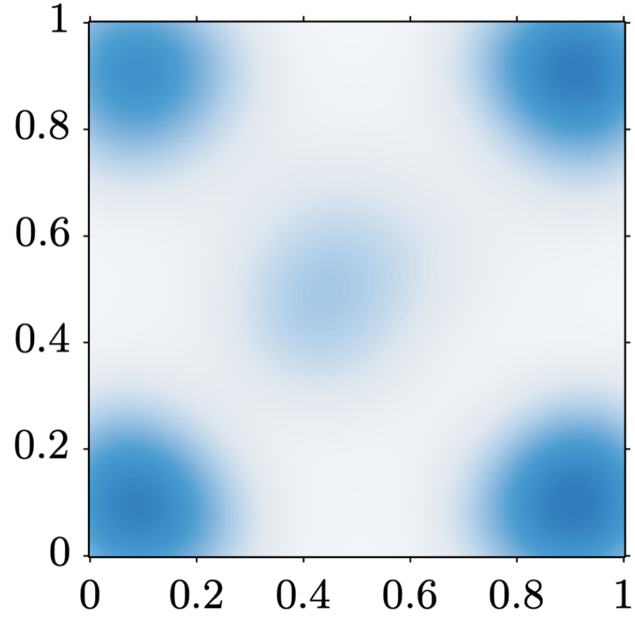
Toy Example

$$I \triangleq [0,1]^2$$

- Target: all points within Euclidean distance $1/4$ from either the center or any corner of I



uncertainty sampling



1-step optimal

Experiments (Active Search)

- Dataset: CiteSeer citation network (38079 nodes)
- Target: Papers appearing in NeurIPS (2198 in total, 5.2%)
- Features: extracted by PCA

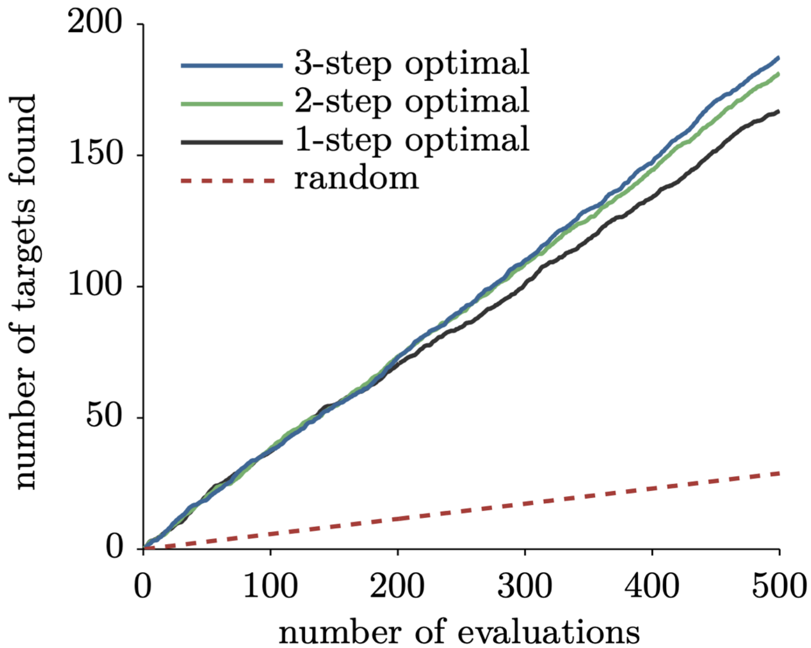


Figure 3: Cumulative number of targets found during 1 000 steps of several active querying schemes on the CiteSeer^x data. The dashed red line shows the expected performance of random sampling.

- 1-step: 167 targets
- 2-step: 180 targets
- 3-step: 187 targets
- 6.5 times better than random search

Search-space pruning

- Pruning improves the search efficiency
- Still exponential

Table 1: The average time (in seconds) taken for one iteration of the ℓ-step lookahead optimal search policy on the CiteSeer^{x} data, for $1 \leq \ell \leq 4$. Some times are approximate. For reference, the one-step policy took an average of 2.24×10^{-3} s per iteration.

	$\ell = 2$	$\ell = 3$	$\ell = 4$
pruning	0.228 s	15.0 s	745 s
no pruning	166 s	≈146 days	≈30 500 years
speedup	731	8.42×10^5	1.29×10^9

Approximating Bayesian Optimal Policy

Reminder: Bayesian Optimal Policy

$$
\begin{aligned}
\mathbb{E}\big[u(\mathcal{D}_t) \mid x_i, \mathcal{D}_{i-1}\big] = u(\mathcal{D}_{i-1}) + \\
\Pr(y_i = 1 \mid x_i, \mathcal{D}_{i-1}) + \\
\underbrace{\mathbb{E}_{y_i}\Big[\max\nolimits_{x'} \mathbb{E}\big[u(\mathcal{D}_t \setminus \mathcal{D}_i) \mid x', \mathcal{D}_i\big]\Big]}_{\text{exploration, } < t-i}
\end{aligned}
$$

Approximating Bayesian Optimal Policy

$$\begin{aligned}\mathbb{E}\big[u(\mathcal{D}_t) \mid x_i, \mathcal{D}_{i-1}\big] \approx u(\mathcal{D}_{i-1}) &+ \\ \Pr(y_i = 1 \mid x_i, \mathcal{D}_{i-1}) &+ \\ &\underbrace{\mathbb{E}_{y_i}\Big[\textstyle\sum'_{t-i} \Pr\big(y = 1 \mid x, \mathcal{D}_i\big)\Big]}_{\text{exploration, } < t-i}\end{aligned}$$

assume that any remaining points, in our budget will be selected simultaneously in one big batch

Approximating Bayesian Optimal Policy

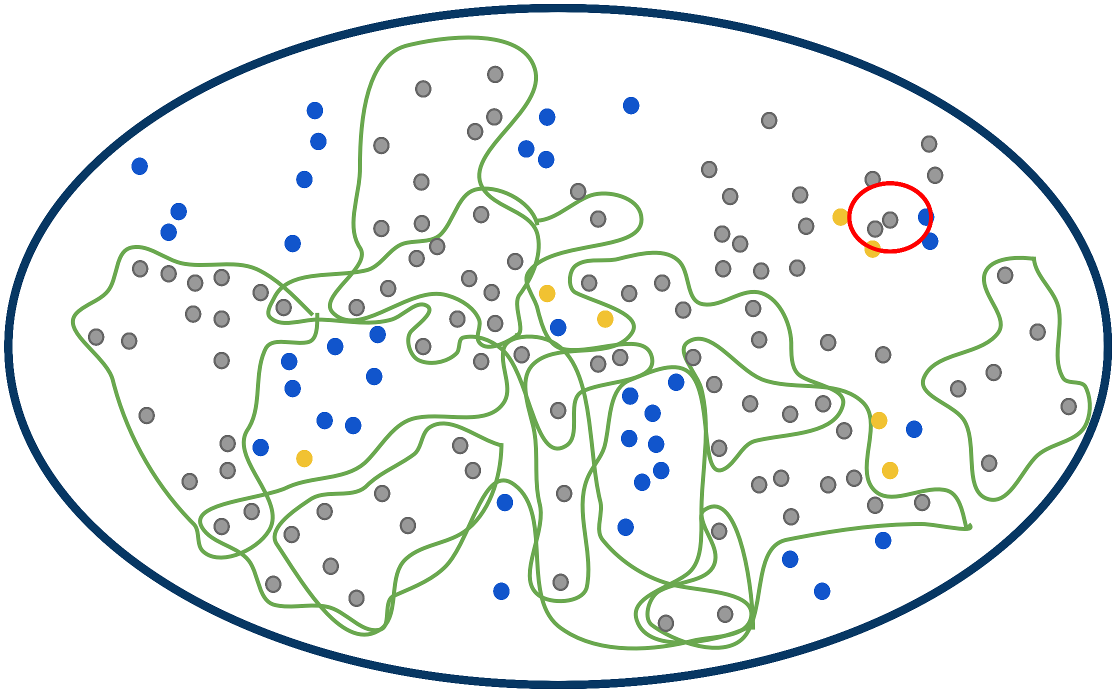
We will call this policy **efficient nonmyopic search (ENS)**.

$$
\begin{aligned}
\mathbb{E}\big[u(\mathcal{D}_t) \mid x_i, \mathcal{D}_{i-1}\big] \approx\; & u(\mathcal{D}_{i-1}) + \\
& \Pr(y_i = 1 \mid x_i, \mathcal{D}_{i-1}) + \\
& \underbrace{\mathbb{E}_{y_i}\Big[\textstyle\sum'_{t-i} \Pr\big(y = 1 \mid x, \mathcal{D}_i\big)\Big]}_{\text{exploration, } < t-i}
\end{aligned}
$$

Time complexity: $\mathcal{O}(n^2 \log n)$

ENS (Example)

at ith query ($t-i$ nodes are left to be labelled)



ENS (Example)

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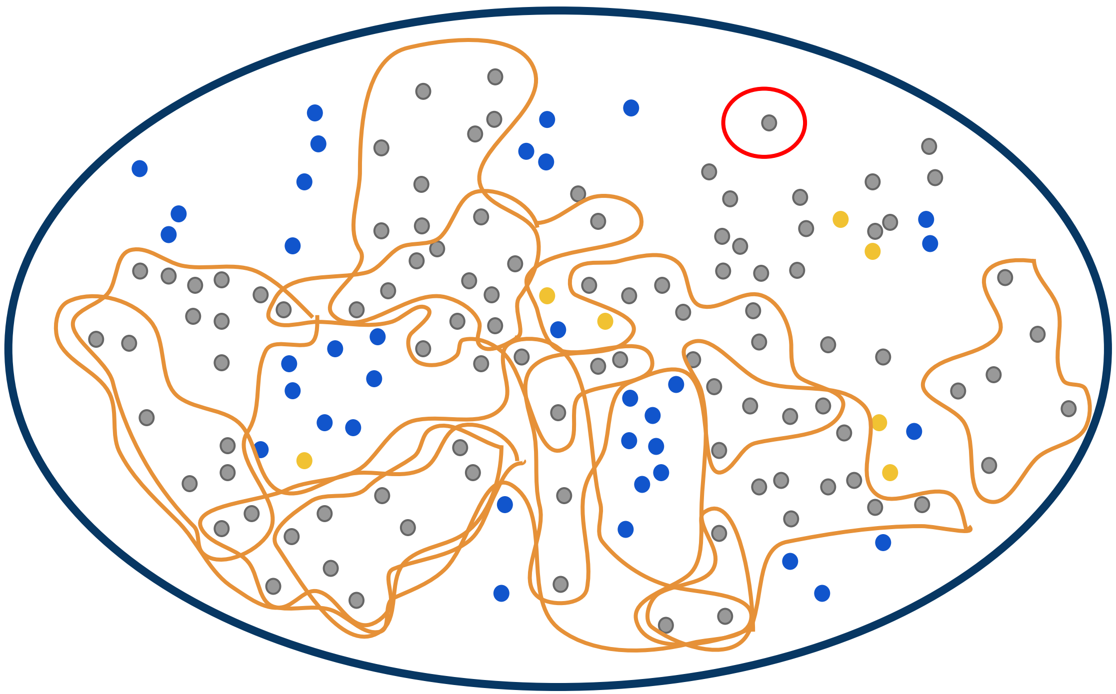


Until we find the x with maximum utility...

Efficient nonmyopic search (ENS)

When does ENS become the exact Bayesian optimal policy?

Efficient nonmyopic search (ENS)

When does ENS become the exact Bayesian optimal policy?

- if after observing $\mathcal{D}_i$, the labels of all remaining unlabeled points are conditionally independent

Nonmyopic Behavior

$$I \triangleq [0,1]^2$$

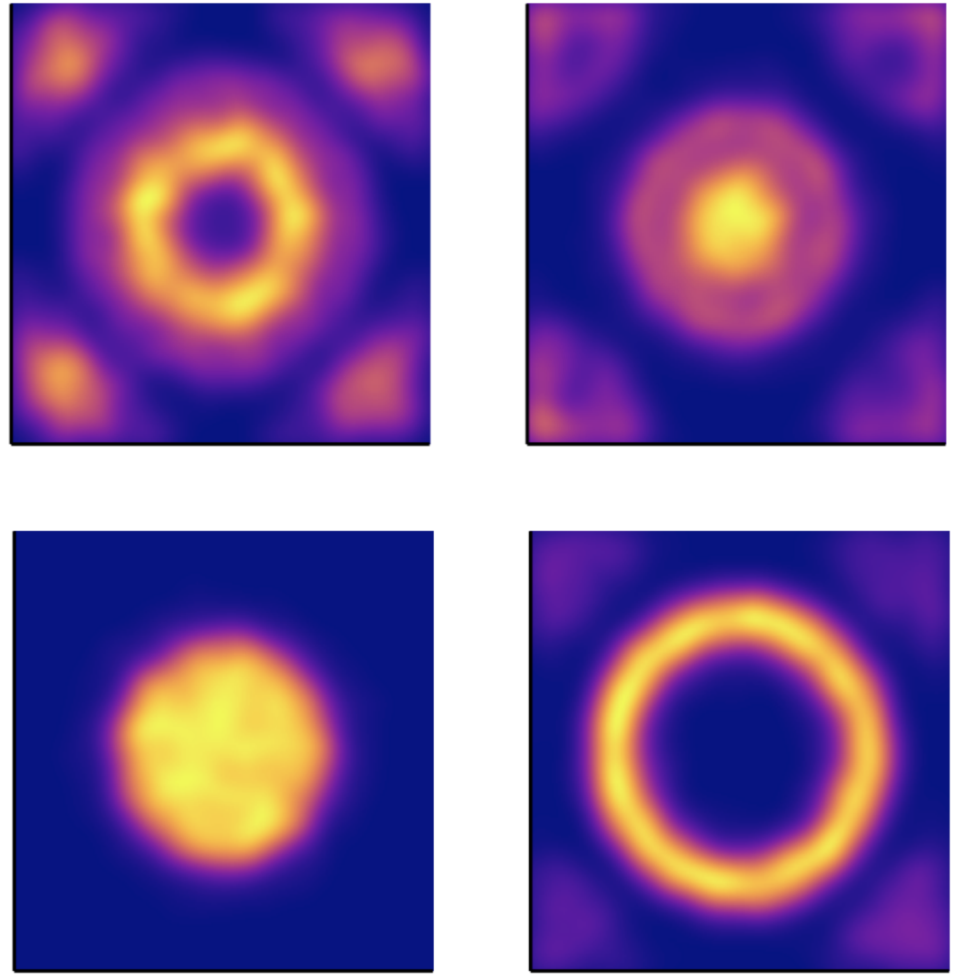
- Target:

  all points within Euclidean distance $1/4$ from either the center or any corner of I

- Budget: 200

ENS:

2-step lookahead:



first 100 points **last 100 points**

Experiment

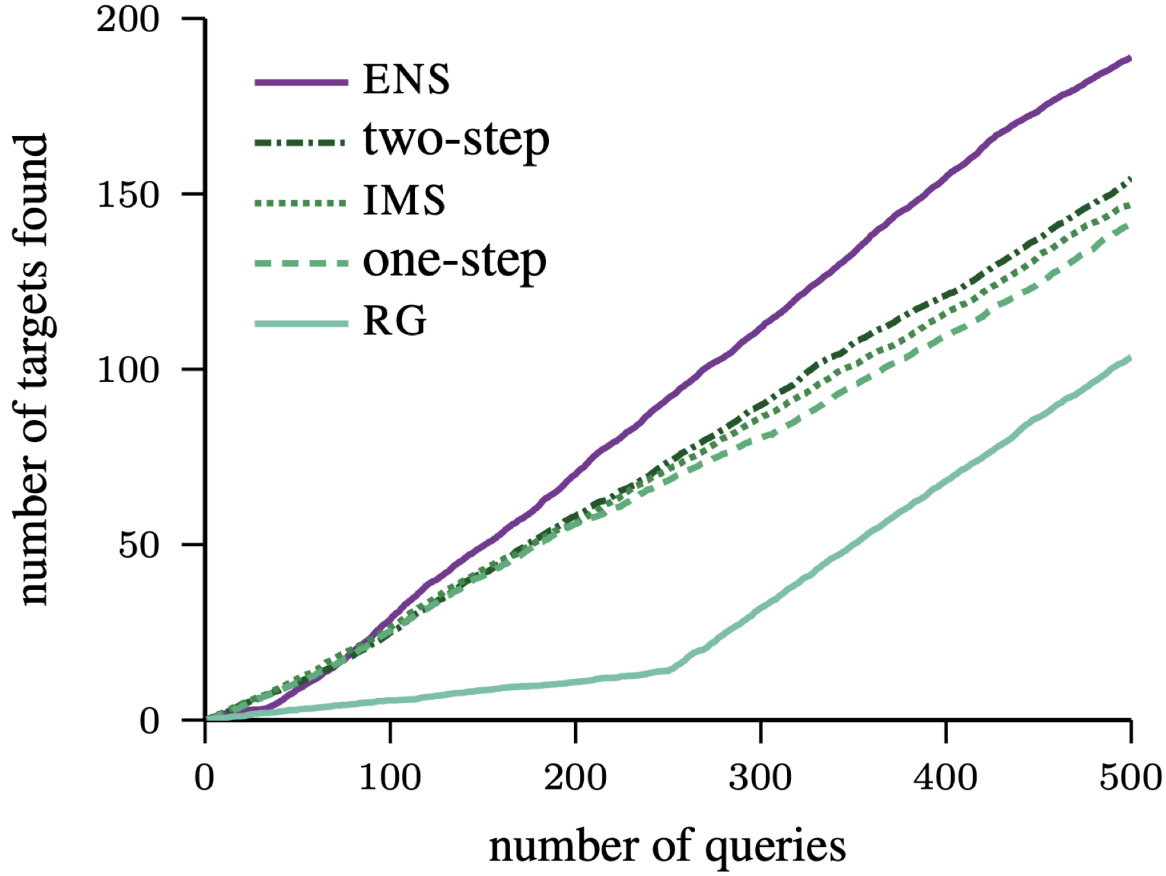
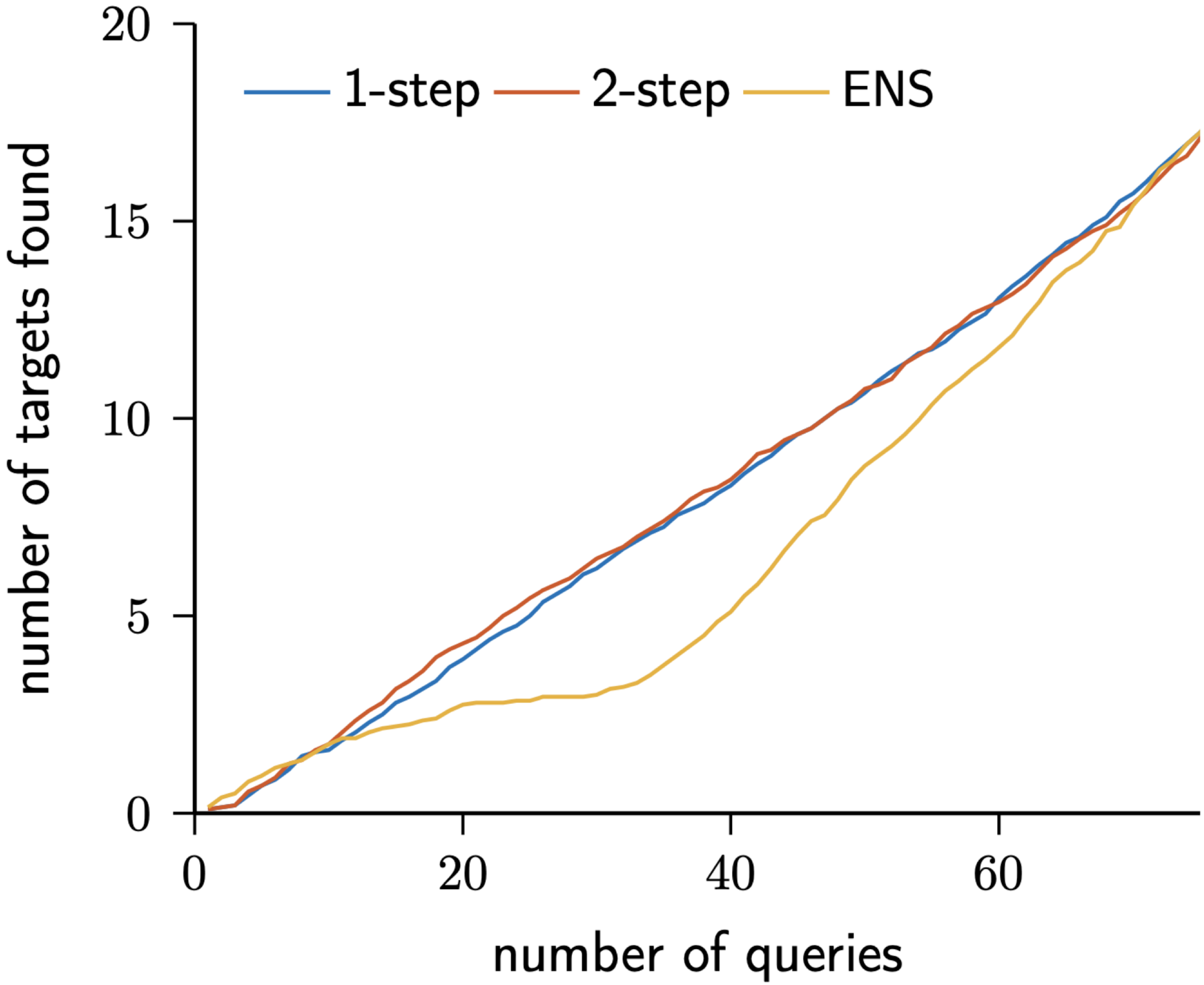


Figure 2: The learning curve of our policy and other baselines on the CiteSeer^x dataset.

Zoom



1-step
2-step
ENS
number of targets found
number of queries
0
5
10
15
20
0
20
40
60

Experiment

CiteSeer^x data

	query number				
policy	100	300	500	700	900
RG	19.7	60.0	104	140	176
IMS	26.3	86.3	147	214	281
one-step	25.5	80.5	141	209	273
two-step	24.9	89.8	155	220	287
ENS–900	25.9	94.3	163	239	**308**
ENS–700	28.0	105	188	**259**	
ENS–500	28.7	**112**	**189**		
ENS–300	26.4	105			
ENS–100	**30.7**				

Limitations

- Bayesian optimal policy and myopic methods (when lookahead step is large) are sample inefficient
- Assume the conditional independence of unlabelled data (ENS)
    - limited performance when budget is very small
- Can not deal with the continuous search space
- Difficult to generalize other more general setting
    - Bayesian Optimization, Multi-bandits, Reinforcement Learning

Takeaways

- Optimal Bayesian Policy (intractable)
- Myopic approach for approximating the optimal policy
  - Less-myopic approximations perform better
- Efficient nonmyopic search (ENS) improves the search efficiency but rely on strong assumptions

Related Work

1) ENS in batch mode (query a batch of points at a time)
    a) efficiency improvement
    b) theoretical guarantee of performance - not that worse compared to query one at a time (Jiang et al., 2018)

1) Bayesian Optimization (BO)
    a) AS can be seen as a special case of BO - **with binary observations and cumulative reward**
    b) Non-myopic policies for BO in the regression setting (Ling et al., 2016)
    c) ENS is similar to GLASS algorithm (González et al., 2016)

1) Multi-armed bandit
    a) electing an item can understood as “pulling an arm”
    b) items are correlated and cannot be played twice
    c) ENS is similar to *knowledge gradient* policy (Frazier et al., 2008)

References

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[3] Jiang, S., Malkomes, G., Converse, G., Shofner, A., Moseley, B., & Garnett, R. (2017, August). **Efficient nonmyopic active search**. In ICML 2017

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[5] González, J., Osborne, M. & Lawrence, N., 2016, May. **GLASSES: Relieving the myopia of Bayesian optimisation.** In Artificial Intelligence and Statistics

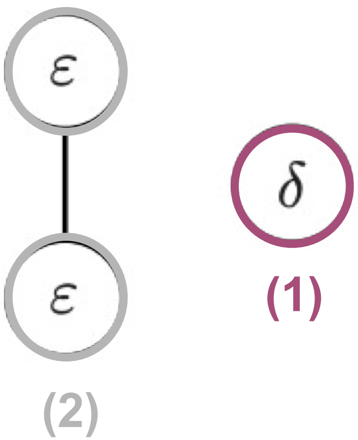
[6] Hasan Z. & Hidru D. Slide for Efficient nonmyopic batch active search. https://bayesopt .github.io/slides/2016/ContributedGarnett.pdf

[7] Jiang, S. Slide for Efficient nonmyopic batch active search. https://bayesopt.github.io/ slides/2016/ContributedGarnett.pdf

Q & A

Appendix: Myopic Approach

simple greedy one-step policy vs **two-step look ahead**:



one-step:

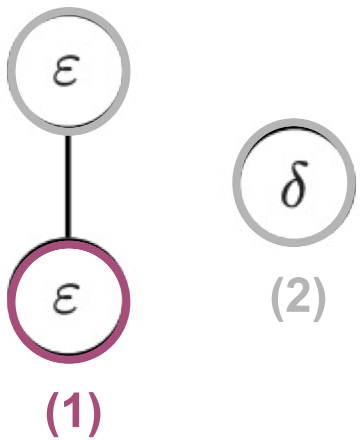
$$x_1* = \text{argmax}_{x_1}\,\mathbb{E}[u(\mathcal{D}_1)|x_1,\mathcal{D}_0] = \text{right point}$$

$$x_2* = \text{left point}$$

$$\mathbb{E}(u(\mathcal{D}_2)) = \delta + \epsilon$$

Appendix: Myopic Approach

simple greedy one-step policy vs **two-step look ahead**:



one-step:

$$\mathbb{E}(u(\mathcal{D}_2)) = \delta + \epsilon$$

two-step(left):

$$\begin{aligned}\mathbb{E}\big[u(\mathcal{D}_t) \mid x_{t-1}, \mathcal{D}_{t-2}\big] = u(\mathcal{D}_{t-2}) &+ \\ \Pr(y_{t-1} = 1 \mid x_{t-1}, \mathcal{D}_{t-2}) &+ \\ \mathbb{E}_{y_{t-1}}\Big[\max_{x_t} \Pr(y_t = 1 \mid x_t, \mathcal{D}_{t-1})\Big]\end{aligned}$$

$$\begin{aligned}\mathbb{E}[u(\mathcal{D}_2)|x_1, \mathcal{D}_0] &= u(\mathcal{D}_0) + Pr(y_1 = 1|x_1, \mathcal{D}_0) + \\ &\quad \mathbb{E}_{y_1}[\max_{x_2} Pr(y_2 = 1|x_2, \mathcal{D}_1)] \\ &= 0 + \epsilon + Pr(y1 = 0) * [\max_{x_2} Pr(y_2 = 1|x_2, \mathcal{D}_1)] + \\ &\quad Pr(y1 = 1) * [\max_{x_2} Pr(y_2 = 1|x_2, \mathcal{D}_1)] \\ &= \epsilon + (1 - \epsilon) * \delta + \epsilon \times 1 \\ &= 2\epsilon + (1 - \epsilon) \times \delta\end{aligned}$$

Appendix: Myopic Approach

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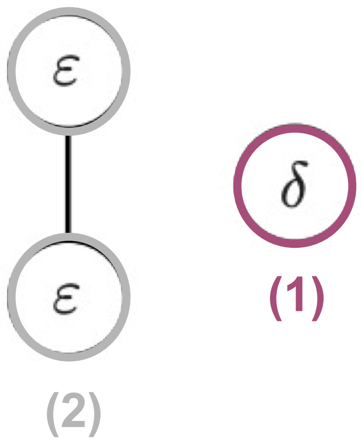


one-step:

$$\mathbb{E}(u(\mathcal{D}_2)) = \delta + \epsilon$$

two-step (left):

$$\begin{aligned}\mathbb{E}[u(\mathcal{D}_2)|x_1, \mathcal{D}_0] &= 2\epsilon + (1-\epsilon) \times \delta \\ &= \epsilon + \delta + \epsilon(1-\delta)\end{aligned}$$

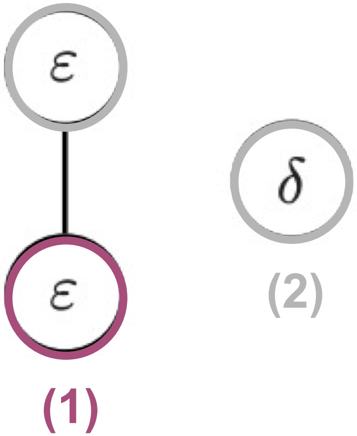
two-step (right):

$$\begin{aligned}\mathbb{E}\big[u(\mathcal{D}_t) \mid x_{t-1}, \mathcal{D}_{t-2}\big] = u(\mathcal{D}_{t-2}) +& \\ \Pr(y_{t-1} = 1 \mid x_{t-1}, \mathcal{D}_{t-2}) +& \\ \mathbb{E}_{y_{t-1}}\big[\max_{x_t} \Pr(y_t = 1 \mid x_t, \mathcal{D}_{t-1})\big]&\end{aligned}$$

$$\begin{aligned}\mathbb{E}[u(\mathcal{D}_2)|x_1, \mathcal{D}_0] &= u(\mathcal{D}_0) + Pr(y_1 = 1|x_1, \mathcal{D}_0) + \\ &\quad \mathbb{E}_{y_1}[\max_{x_2} Pr(y_2 = 1|x_2, \mathcal{D}_1)] \\ &= 0 + \delta + Pr(y1 = 0) * [\max_{x_2} Pr(y_2 = 1|x_2, \mathcal{D}_1)] + \\ &\quad Pr(y1 = 1) * [\max_{x_2} Pr(y_2 = 1|x_2, \mathcal{D}_1)] \\ &= \delta + (1-\delta) * \epsilon + \delta \times \epsilon \\ &= \epsilon + \delta\end{aligned}$$

Appendix: Myopic Approach

simple greedy one-step policy vs **two-step look ahead**:



one-step:

$$\mathbb{E}(u(\mathcal{D}_2)) = \delta + \epsilon$$

two-step(left):

$$\begin{aligned}\mathbb{E}[u(\mathcal{D}_2)|x_1, \mathcal{D}_0] &= 2\epsilon + (1-\epsilon) \times \delta \\ &= \epsilon + \delta + \epsilon(1-\delta)\end{aligned}$$

two-step(right):

$$\mathbb{E}[u(\mathcal{D}_2)|x_1\, \mathcal{D}_0] = \epsilon + \delta$$