

Neural Contextual Bandits for Personalized Recommendation



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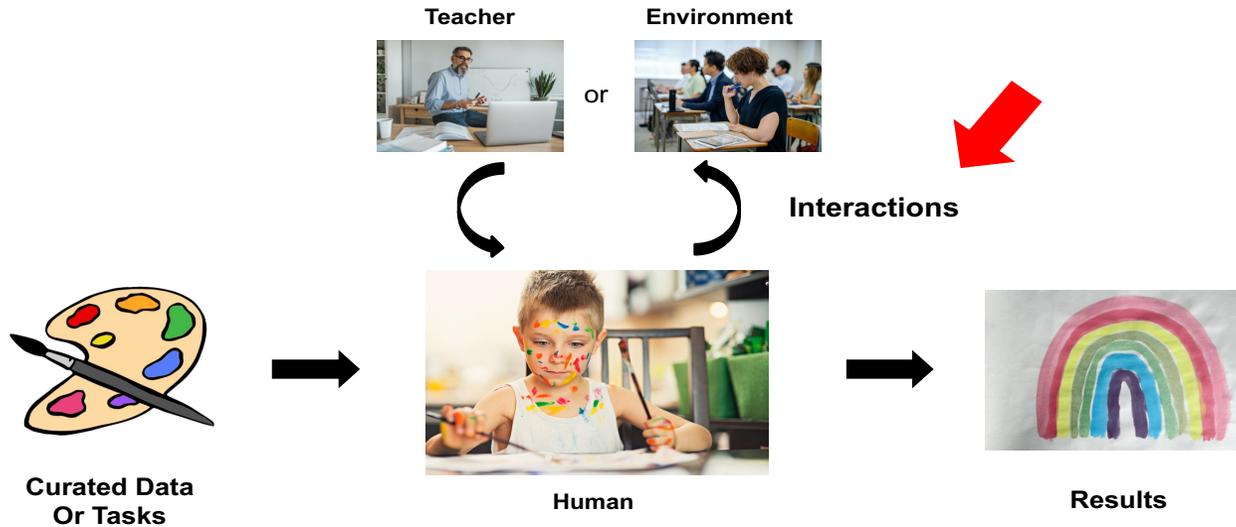
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Time: 9:00 AM – 12:30 PM, 13 May 2024

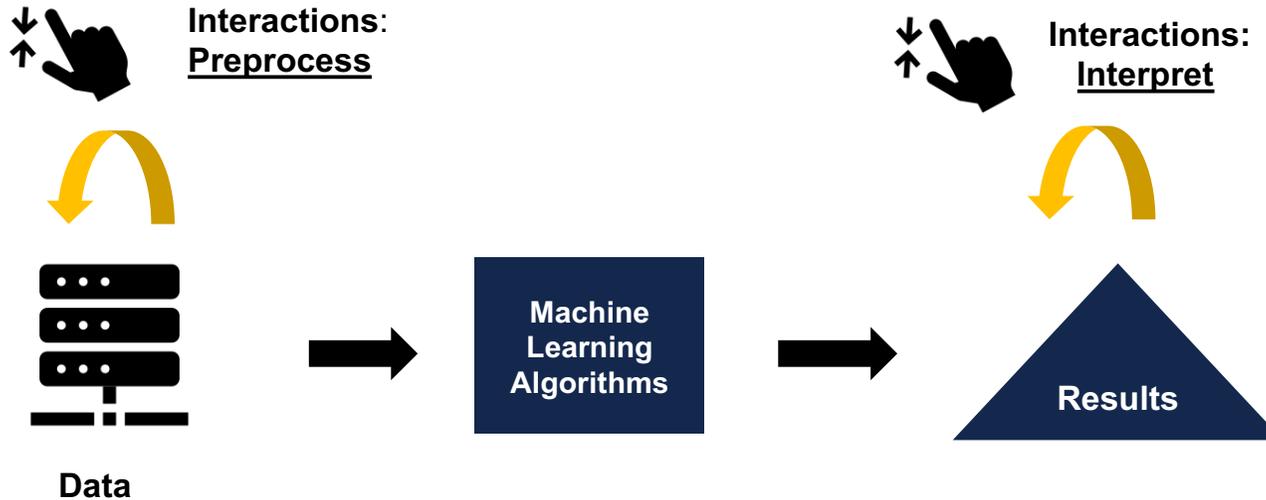
Location: Virgo 1, Resorts World Sentosa Convention Centre, Singapore

Website: www.banyikun.com/wwwtutorial/

Interactions in Machine Learning



**Interactive Learning
(Human)**



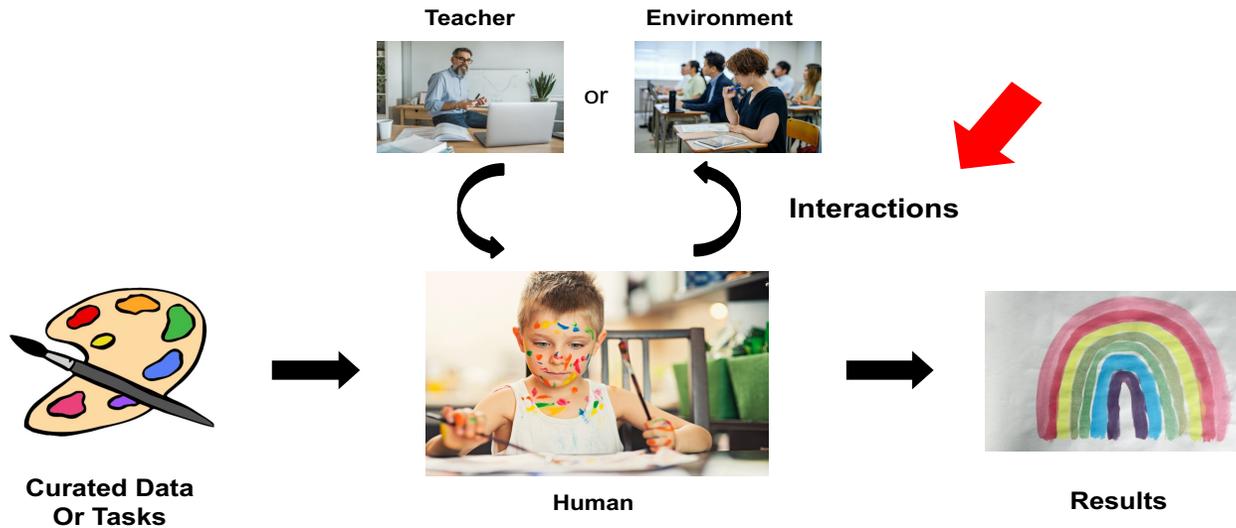
**Machine Learning
(Conventional)**



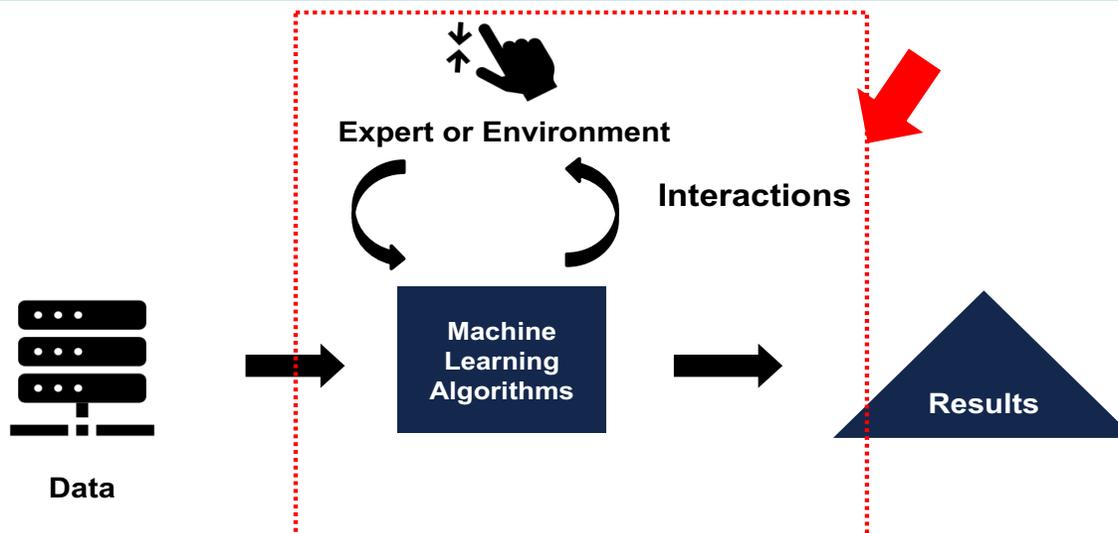
1. Ernst, Damien, and Arthur Louette. "Introduction to reinforcement learning." 2024.
2. Fails, Jerry Alan, and Dan R. Olsen Jr. "Interactive machine learning." *Proceedings of the 8th international conference on Intelligent user interfaces*. 2003.
3. Teso, Stefano, and Kristian Kersting. "Explanatory interactive machine learning." *Proceedings of the 2019 AAAI/ACM Conference on AI, Ethics, and Society*. 2019.



Interactions in Machine Learning



Interactive Learning
(Human)



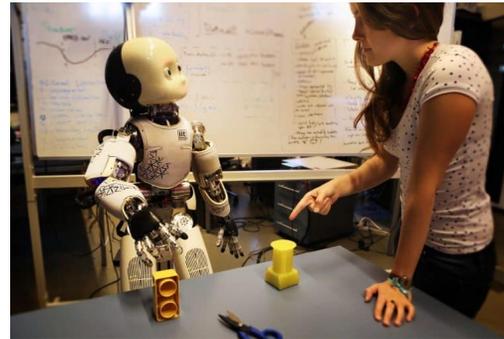
Interactive Machine Learning



- **Interactive Machine Learning (IML)** is the core of **Artificial Intelligence (AI)**.



(1) **Recommender Systems**



(2) **Robot Learning**

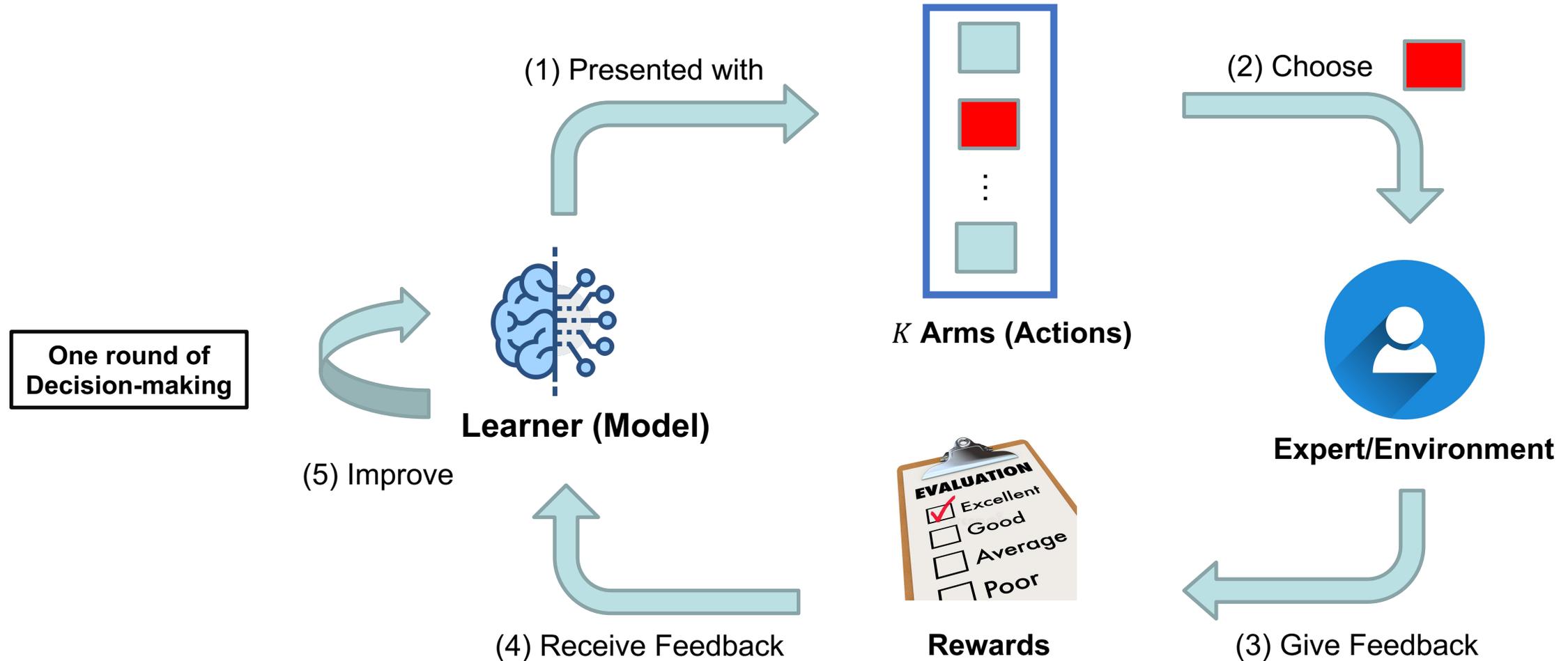


(3) **Language Model**

Sequential Decision-Making: Bandits Formulation



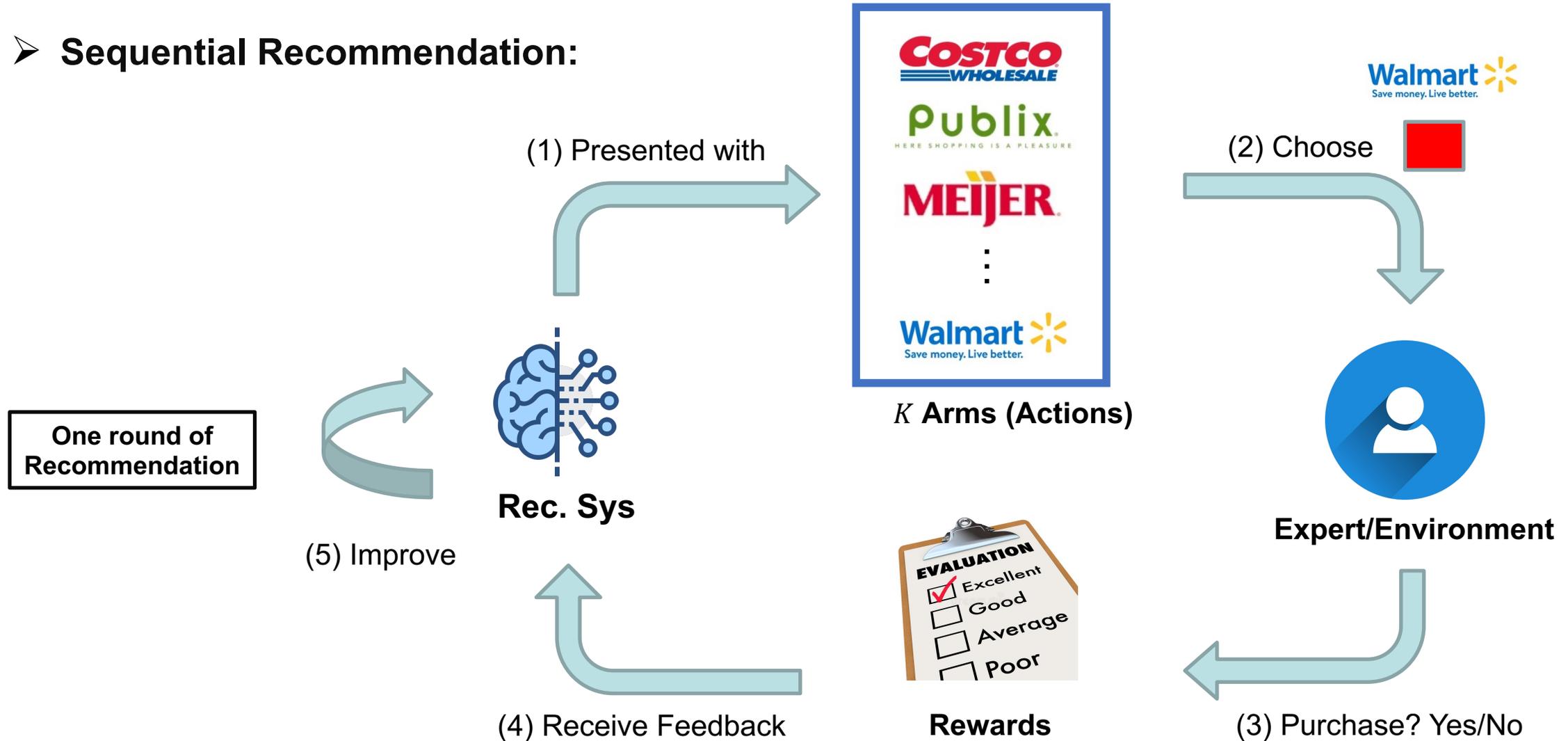
➤ Many IML scenarios can be formulated as **sequential decision-making**.



Sequential Recommendation: Bandits Formulation



➤ Sequential Recommendation:



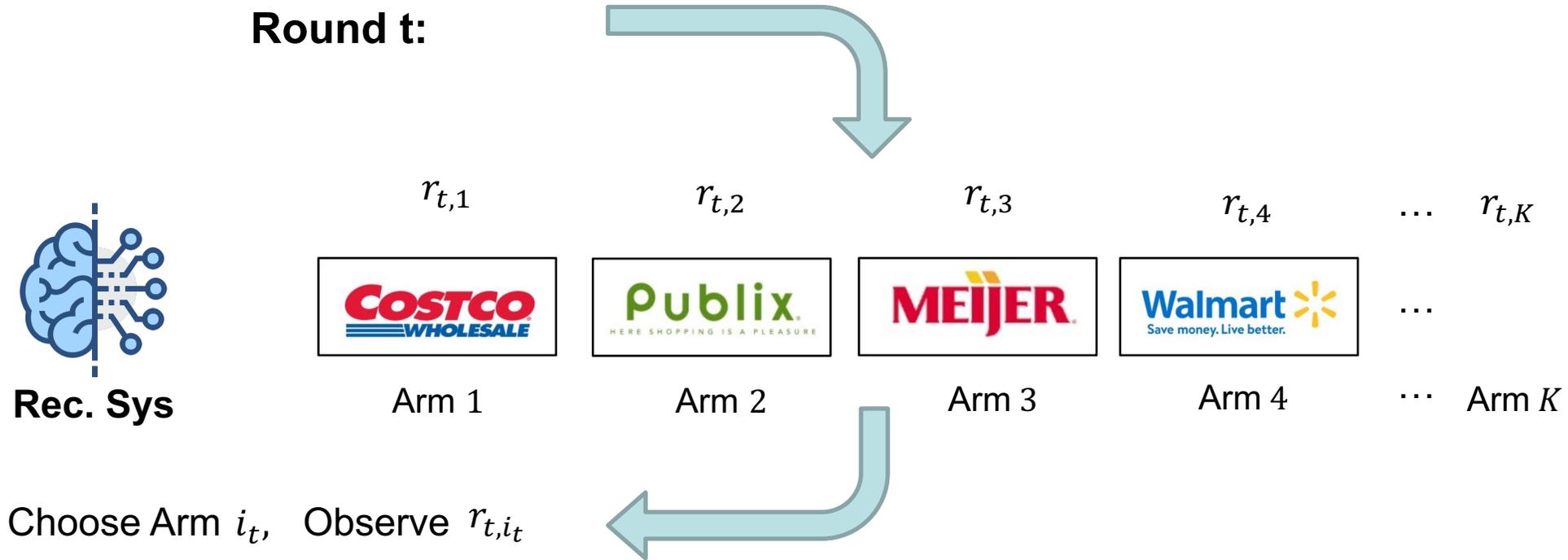
One round of Recommendation

- Ernst, Damien, and Arthur Louette. "Introduction to reinforcement learning." 2024.
- Fails, Jerry Alan, and Dan R. Olsen Jr. "Interactive machine learning." *Proceedings of the 8th international conference on Intelligent user interfaces*. 2003.
- Teso, Stefano, and Kristian Kersting. "Explanatory interactive machine learning." *Proceedings of the 2019 AAAI/ACM Conference on AI, Ethics, and Society*. 2019.



Sequential Recommendation: Objective

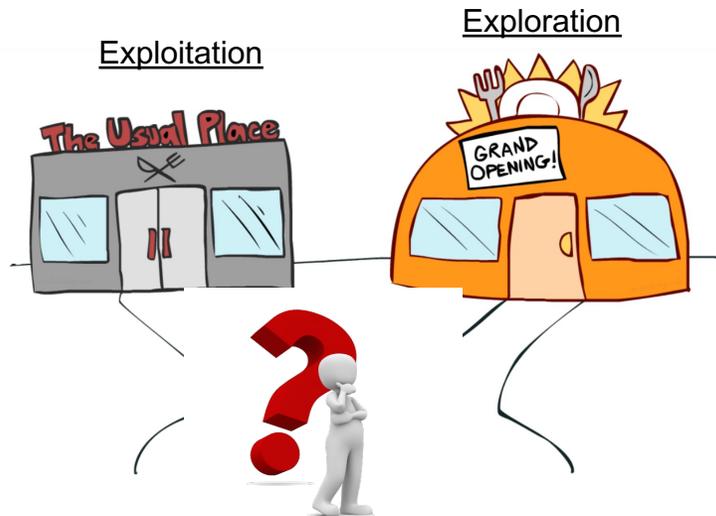
Goal: Maximize $\sum_{t=1}^T \mathbb{E}[r_{t,i_t}]$ Or Minimize $\sum_{t=1}^T (\mathbb{E}[r_{t,i_t^*}] - \mathbb{E}[r_{t,i_t}])$, where $i_t^* = \arg \max_{i \in [K]} \mathbb{E}[r_{t,i}]$.



Exploitation VS Exploration in Sequential Decision-Making



- Dilemma of **exploitation** and **exploration** is ubiquitous in human decision-making.

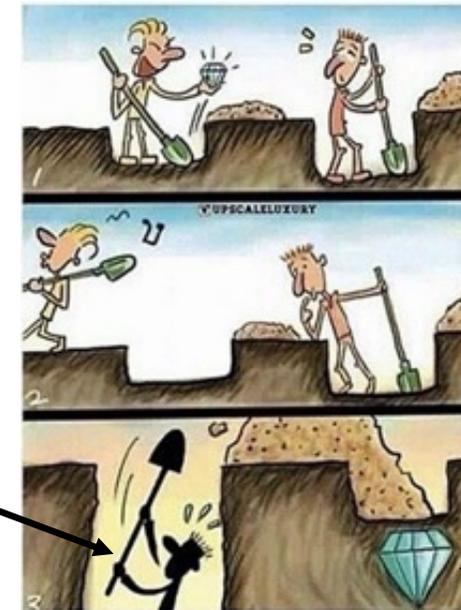


(1)

Exploitation:

Exploit past data or observations.
E.g., estimation by a greedy model

VS



(2)

Exploration:

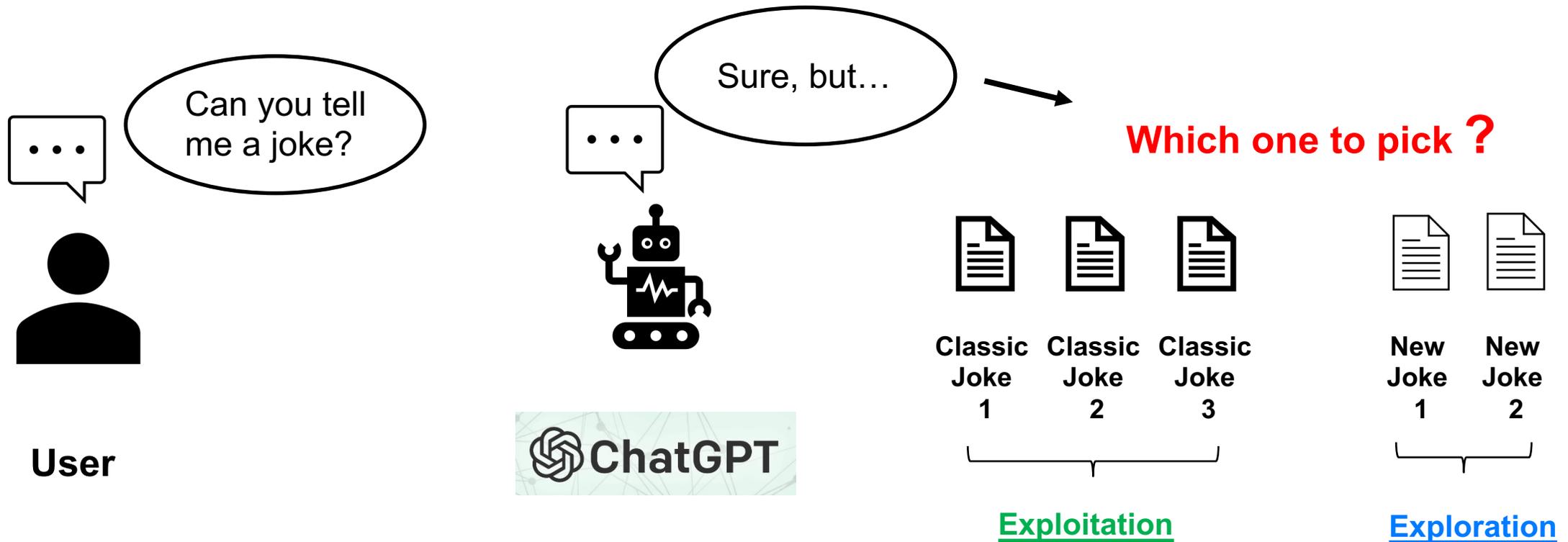
Explore new knowledge for long-term benefit.
E.g., take uncertain actions



Exploitation VS Exploration in Sequential Recommendation



- Dilemma of **exploitation** and **exploration** is a fundamental problem in **sequential decision-making**.



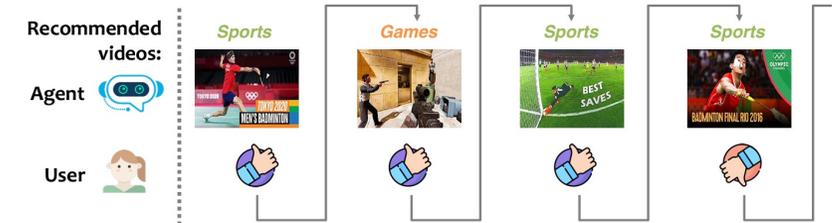
Advantages of Bandit-based Methods



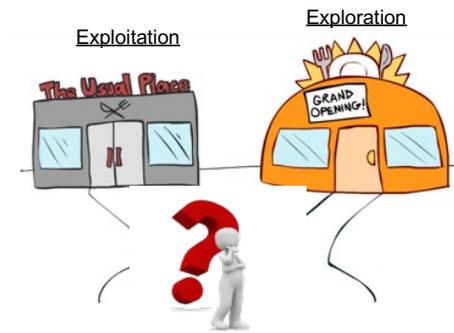
➤ No Requirement for Large Collected Data.

A	✓	✗	✓	✓
B		✓	✗	✗
C	✓	✓	✗	
D	✗		✓	
E	✓	✓	?	✗

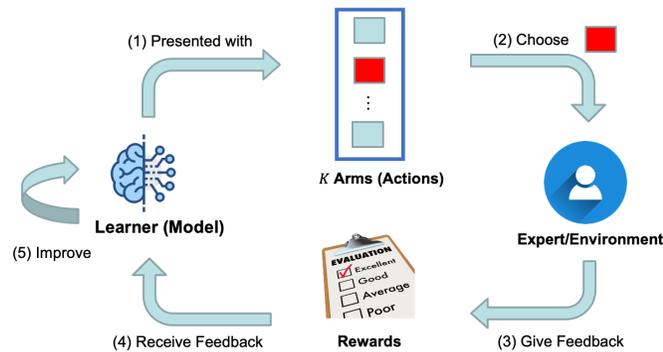
➤ Adapt over Time.

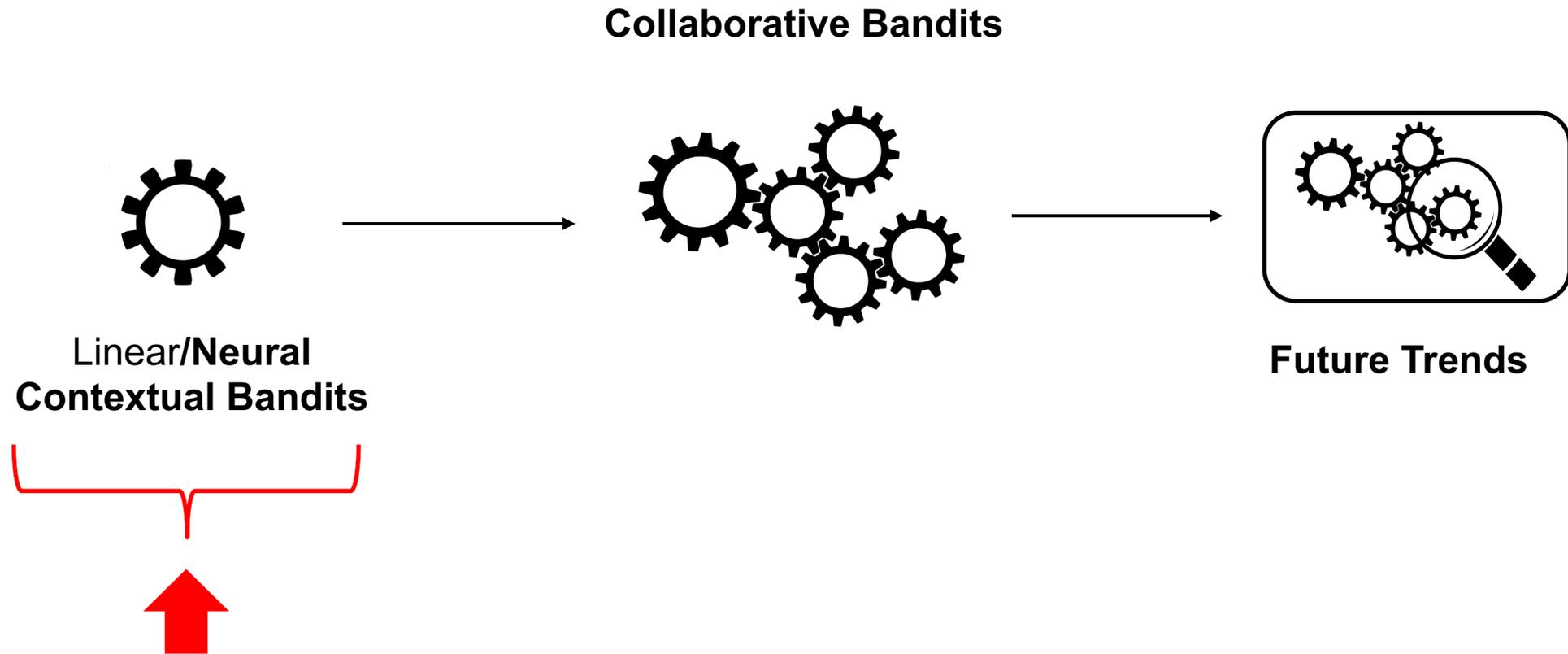


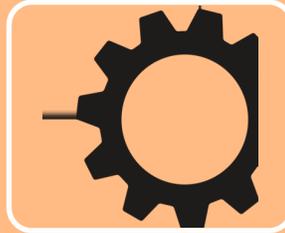
➤ Explicit Exploration.



One round of Decision-making

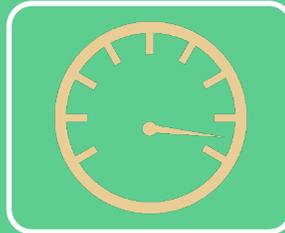






Fundamental Exploration

- Upper Confidence Bound
- Thompson Sampling
- Exploration Network



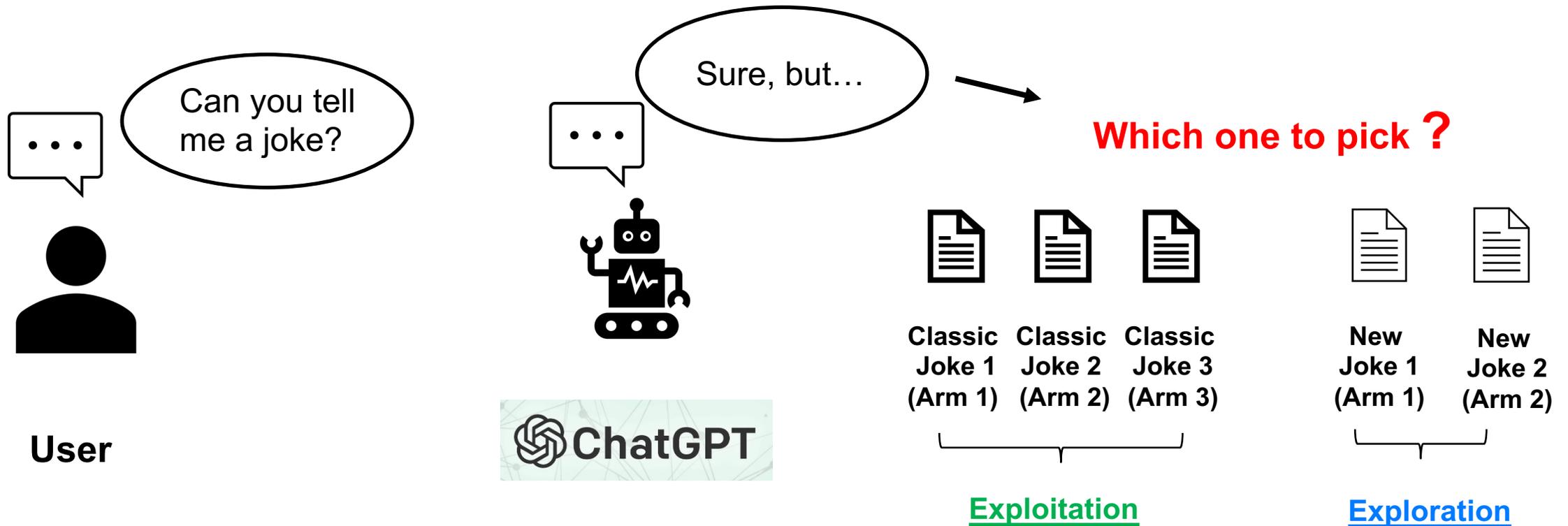
Efficient Exploration

- Neural Linear UCB
- Neural Network with Perturbed Reward
- Inverse Weight Gap Strategy

Background



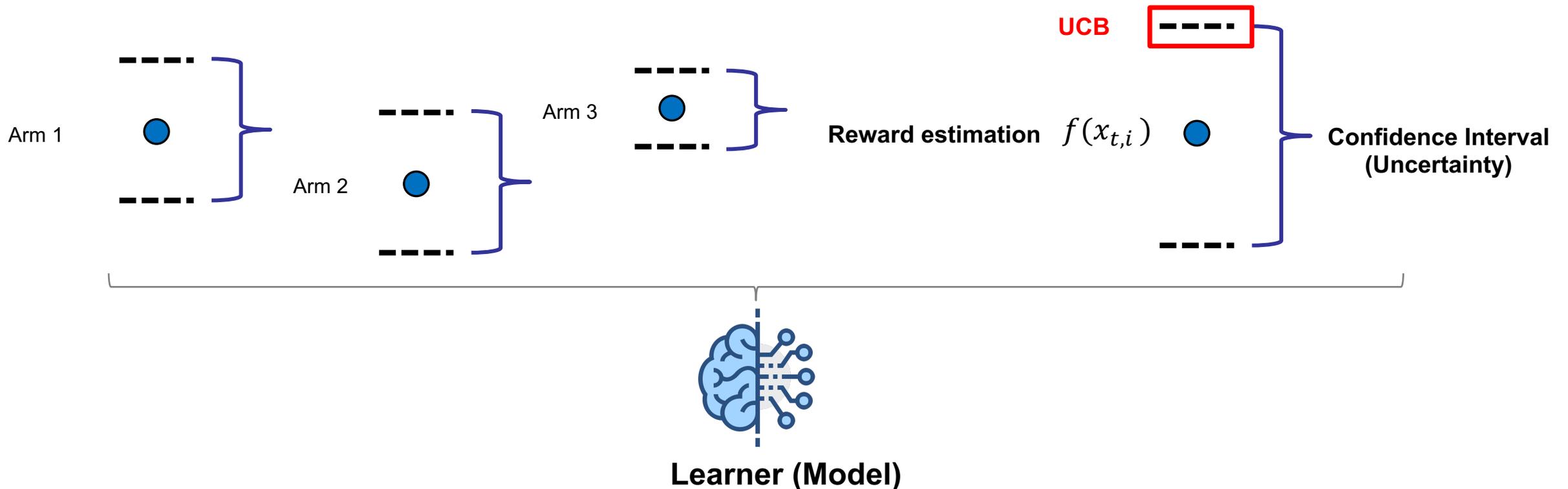
- Popular existing exploration strategies.
 - ❑ **ϵ -greedy**: With probability $1 - \epsilon$, greedily choose one arm according to history; Otherwise, choose an arm randomly.



➤ Popular existing exploration strategies.

❑ **ϵ -greedy**: With probability $1 - \epsilon$, greedily choose one arm according to history; Otherwise, choose an arm randomly.

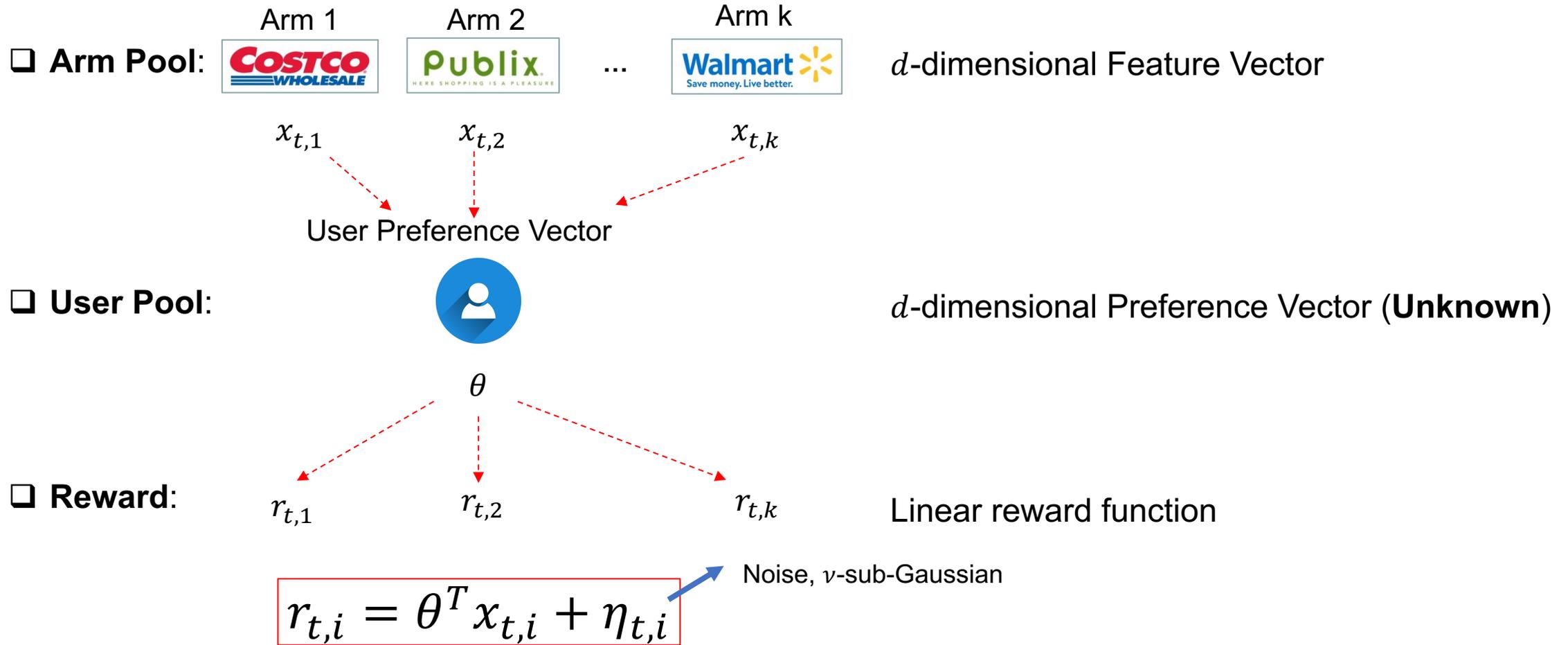
❑ **Upper Confidence Bound [1]**:



Linear Bandits: Joint Problem Definition



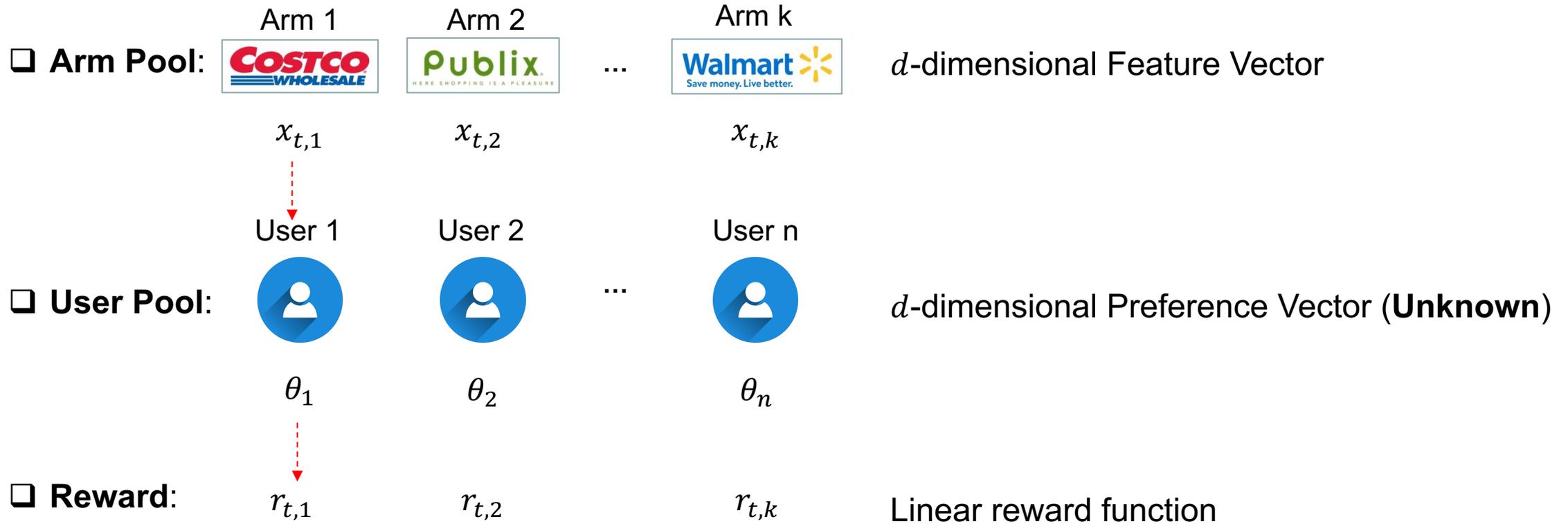
In round t : A user is serving



Linear Bandits: Disjoint Problem Definition



In round t : A user is serving



Given User j ,

$$r_{t,i} = \theta_j^T x_{t,i} + \eta_{t,i}$$

Noise, ν -sub-Gaussian



Linear UCB: Algorithm

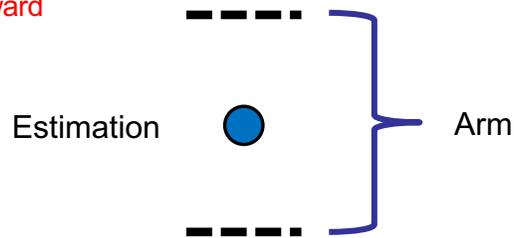


Joint Linear Models

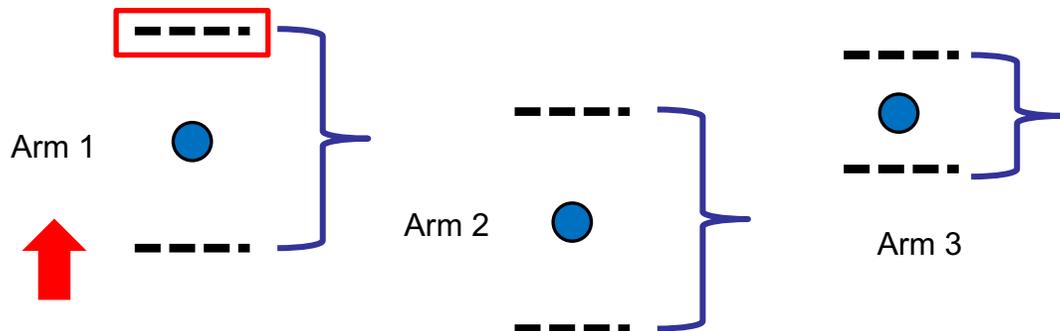
Confidence Interval:

$$|\hat{r}_{t,a} - x_{t,a}^\top \theta^*| \leq (\alpha + 1) s_{t,a}$$

Estimated Expected Reward



$$a_t \stackrel{\text{def}}{=} \arg \max_{a \in \mathcal{A}_t} \left(x_{t,a}^\top \hat{\theta}_a + \alpha \sqrt{x_{t,a}^\top \mathbf{A}_a^{-1} x_{t,a}} \right),$$



Estimated by Ridge Regression

```

for  $t = 1, 2, 3, \dots, T$  do  -- A user is serving in each round
   $\theta_t \leftarrow A^{-1}b$ 
  Observe  $K$  features,  $x_{t,1}, x_{t,2}, \dots, x_{t,K} \in \mathbb{R}^d$ 
  for  $a = 1, 2, \dots, K$  do
     $p_{t,a} \leftarrow \theta_t^\top x_{t,a} + \alpha \sqrt{x_{t,a}^\top A^{-1} x_{t,a}}$  {Computes
    upper confidence bound}
  end for
  Choose action  $a_t = \arg \max_a p_{t,a}$  with ties broken
  arbitrarily
  Observe payoff  $r_t \in \{0, 1\}$ 
   $A \leftarrow A + x_{t,a_t} x_{t,a_t}^\top$ 
   $b \leftarrow b + x_{t,a_t} r_t$ 
end for
  
```

(Item 1) (Item 2) ...

Exploitation

Exploration

Estimated by Ridge Regression



➤ Confidence Interval:

Estimated by Ridge Regression

With high probability,

$$|\hat{r}_{t,a} - x_{t,a}^\top \theta^*| \leq (\alpha + 1) s_{t,a}.$$

where

$$s_{t,a} = \sqrt{x_{t,a}^\top A_t^{-1} x_{t,a}} \in \mathbb{R}_+$$

$$\begin{aligned} \hat{r}_{t,a} - x_{t,a}^\top \theta^* &= x_{t,a}^\top \theta_t - x_{t,a}^\top \theta^* \\ &= x_{t,a}^\top A_t^{-1} b_t - x_{t,a}^\top A_t^{-1} (I_d + D_t^\top D_t) \theta^* \\ &= x_{t,a}^\top A_t^{-1} D_t^\top y_t - x_{t,a}^\top A_t^{-1} (\theta^* + D_t^\top D_t \theta^*) \\ &= \underbrace{x_{t,a}^\top A_t^{-1} D_t^\top (y_t - D_t \theta^*)}_{\text{Bounded by Conf. Interval}} - \underbrace{x_{t,a}^\top A_t^{-1} \theta^*}_{\text{Bounded by Conf. Interval}}, \end{aligned}$$

Bounded by Conf. Interval

Bounded by Conf. Interval

➤ Regret Upper Bound

$$O\left(\sqrt{Td \ln^3(KT \ln(T)/\delta)}\right).$$

The Number of Rounds

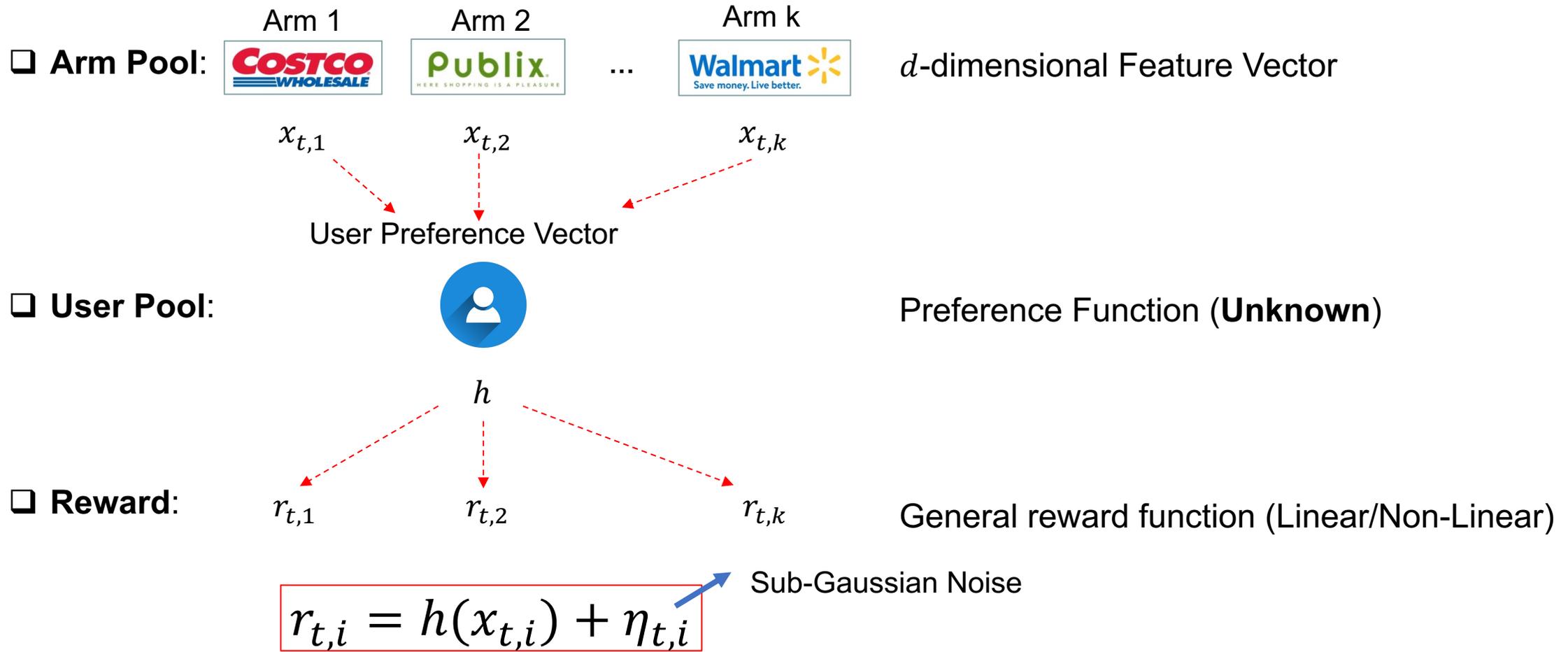
The Number of Items

Dimensionality of Item Context Vector

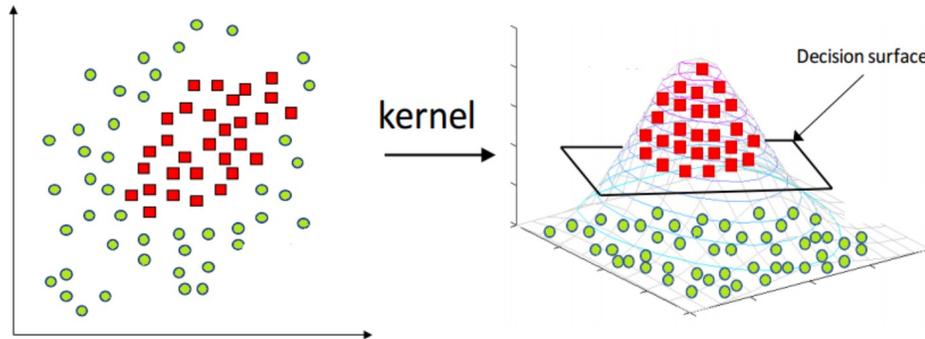
Neural Bandits: Problem Formulation



In round t :



- A **sufficiently wide neural network** behaves like a **linearized model** governed by the derivative of network with respect to its parameters (**Gradient**).

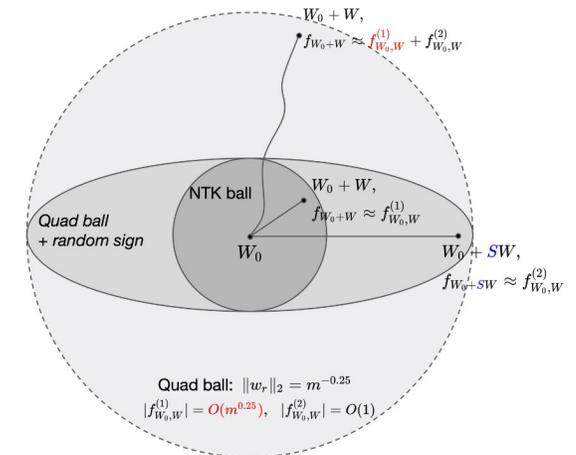


<https://www.geeksforgoeks.org/major-kernel-functions-in-support-vector-machine-svm/>

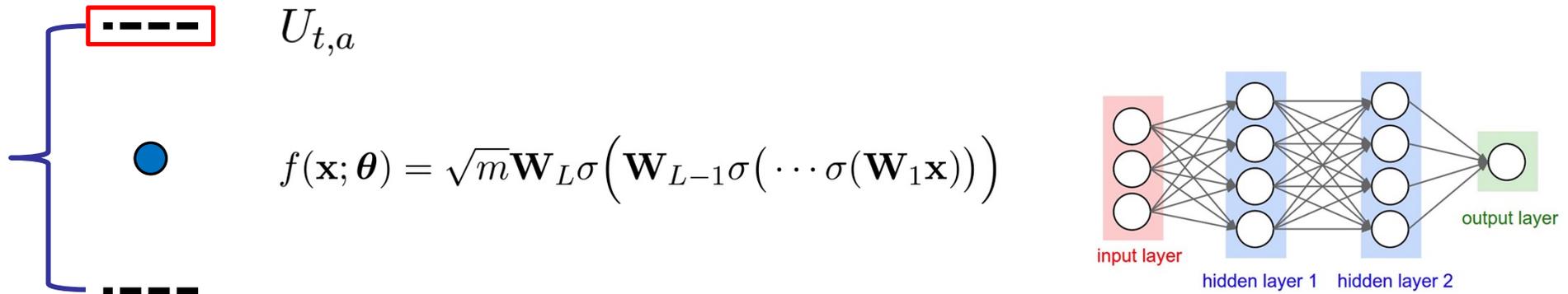
Neural Tangent Kernel

$$\Theta(x, x'; \theta) = \nabla_{\theta} f(x; \theta) \cdot \nabla_{\theta} f(x'; \theta).$$

- With near-**infinite width**, Neural network behaves like a **kernel predictor** with Neural Tangent Kernel (NTK)



Neural UCB: Method



Gradient of f

$$U_{t,a} = \underbrace{f(\mathbf{x}_{t,a}; \boldsymbol{\theta}_{t-1})}_{\text{mean}} + \gamma_{t-1} \underbrace{\sqrt{\mathbf{g}(\mathbf{x}_{t,a}; \boldsymbol{\theta}_{t-1})^\top \mathbf{Z}_{t-1}^{-1} \mathbf{g}(\mathbf{x}_{t,a}; \boldsymbol{\theta}_{t-1}) / m}}_{\text{variance}}$$

Compared with LinUCB (Li et al. 2010)

$$U_{t,a} = \underbrace{\langle \mathbf{x}_{t,a}, \boldsymbol{\theta}_{t-1} \rangle}_{\text{mean}} + \gamma_{t-1} \underbrace{\sqrt{\mathbf{x}_{t,a}^\top \mathbf{Z}_{t-1}^{-1} \mathbf{x}_{t,a}}}_{\text{variance}}$$

Neural UCB: Workflow



➤ In each round, a user is serving

for $t = 1, \dots, T$ **do** K arms (Items)

 Observe $\{\mathbf{x}_{t,a}\}_{a=1}^K$ Exploration

for $a = 1, \dots, K$ **do** Exploitation

 Compute $U_{t,a} = f(\mathbf{x}_{t,a}; \boldsymbol{\theta}_{t-1}) + \gamma_{t-1} \sqrt{\mathbf{g}(\mathbf{x}_{t,a}; \boldsymbol{\theta}_{t-1})^\top \mathbf{Z}_{t-1}^{-1} \mathbf{g}(\mathbf{x}_{t,a}; \boldsymbol{\theta}_{t-1}) / m}$

 Let $a_t = \operatorname{argmax}_{a \in [K]} U_{t,a}$

end for

 Play a_t and observe reward r_{t,a_t}

 Compute $\mathbf{Z}_t = \mathbf{Z}_{t-1} + \mathbf{g}(\mathbf{x}_{t,a_t}; \boldsymbol{\theta}_{t-1}) \mathbf{g}(\mathbf{x}_{t,a_t}; \boldsymbol{\theta}_{t-1})^\top / m$ Similar to Linear Regression

 Let $\boldsymbol{\theta}_t = \operatorname{TrainNN}(\lambda, \eta, J, m, \{\mathbf{x}_{i,a_i}\}_{i=1}^t, \{r_{i,a_i}\}_{i=1}^t, \boldsymbol{\theta}_0)$ Train Neural Networks

 Compute

$$\gamma_t = \sqrt{1 + C_1 m^{-1/6} \sqrt{\log m} L^4 t^{7/6} \lambda^{-7/6} \cdot \left(\nu \sqrt{\log \frac{\det \mathbf{Z}_t}{\det \lambda \mathbf{I}}} + C_2 m^{-1/6} \sqrt{\log m} L^4 t^{5/3} \lambda^{-1/6} - 2 \log \delta + \sqrt{\lambda} S \right)}$$

+ $(\lambda + C_3 t L) \left[(1 - \eta m \lambda)^{J/2} \sqrt{t/\lambda} + m^{-1/6} \sqrt{\log m} L^{7/2} t^{5/3} \lambda^{-5/3} (1 + \sqrt{t/\lambda}) \right]$.

end for

Confidence Radius

Neural Function Approximation Error



- Definition of **NTK Matrix** on all observed contexts of T rounds.

$$\tilde{\mathbf{H}}_{i,j}^{(1)} = \Sigma_{i,j}^{(1)} = \langle \mathbf{x}^i, \mathbf{x}^j \rangle, \quad \mathbf{A}_{i,j}^{(l)} = \begin{pmatrix} \Sigma_{i,i}^{(l)} & \Sigma_{i,j}^{(l)} \\ \Sigma_{i,j}^{(l)} & \Sigma_{j,j}^{(l)} \end{pmatrix},$$

$$\Sigma_{i,j}^{(l+1)} = 2\mathbb{E}_{(u,v) \sim N(\mathbf{0}, \mathbf{A}_{i,j}^{(l)})} [\sigma(u)\sigma(v)],$$

$$\tilde{\mathbf{H}}_{i,j}^{(l+1)} = 2\tilde{\mathbf{H}}_{i,j}^{(l)} \mathbb{E}_{(u,v) \sim N(\mathbf{0}, \mathbf{A}_{i,j}^{(l)})} [\sigma'(u)\sigma'(v)] + \Sigma_{i,j}^{(l+1)}.$$

Then, $\mathbf{H} = (\tilde{\mathbf{H}}^{(L)} + \Sigma^{(L)})/2$ is called the *neural tangent kernel (NTK) matrix* on the context set.

- Analyze dynamics of gradient and NTK regression.

Assumption: $\mathbf{H} \succeq \lambda_0 \mathbf{I}$.

- Satisfied if no two observed arm contexts are parallel.

Lemma: When neural network is wide enough,

$$\begin{aligned} h(\mathbf{x}^i) &= \langle \mathbf{g}(\mathbf{x}^i; \boldsymbol{\theta}_0), \boldsymbol{\theta}^* - \boldsymbol{\theta}_0 \rangle, && \text{Linear function w.r.t. Gradient} \\ \sqrt{m} \|\boldsymbol{\theta}^* - \boldsymbol{\theta}_0\|_2 &\leq \sqrt{2\mathbf{h}^\top \mathbf{H}^{-1} \mathbf{h}}, && (5.1) \end{aligned}$$

for all $i \in [TK]$.





Assumption: $\mathbf{H} \succeq \lambda_0 \mathbf{I}$.

$$\sqrt{m} \|\boldsymbol{\theta}^* - \boldsymbol{\theta}_0\|_2 \leq \sqrt{2\mathbf{h}^\top \mathbf{H}^{-1} \mathbf{h}},$$

$$S = \sqrt{2\mathbf{h}^\top \mathbf{H}^{-1} \mathbf{h}}$$

Satisfied if *no* two contexts in $\{\mathbf{x}^i\}_{i=1}^{TK}$ are parallel.

$$h(\mathbf{x}^i) = \langle \mathbf{g}(\mathbf{x}^i; \boldsymbol{\theta}_0), \boldsymbol{\theta}^* - \boldsymbol{\theta}_0 \rangle,$$

$$\tilde{d} = \frac{\log \det(\mathbf{I} + \mathbf{H}/\lambda)}{\log(1 + TK/\lambda)}$$

Theorem

LinUCB:
 $\tilde{O}(d\sqrt{T})$

Let $\mathbf{h} = [h(\mathbf{x}^i)]_{i=1}^{TK} \in \mathbb{R}^{TK}$. Set $J = \tilde{\Theta}(TL/\lambda)$,
 $\eta = \Theta((mTL + m\lambda)^{-1})$ and $S = 2\sqrt{\mathbf{h}^\top \mathbf{H}^{-1} \mathbf{h}}$. Under the
overparameterized setting ($m \gg 1$), with probability at least $1 - \delta$,

$$R_T = \tilde{O}\left(\sqrt{\tilde{d}T} \sqrt{\max\{\tilde{d}, S^2\}}\right).$$

Upper Bound of Neural Parameters

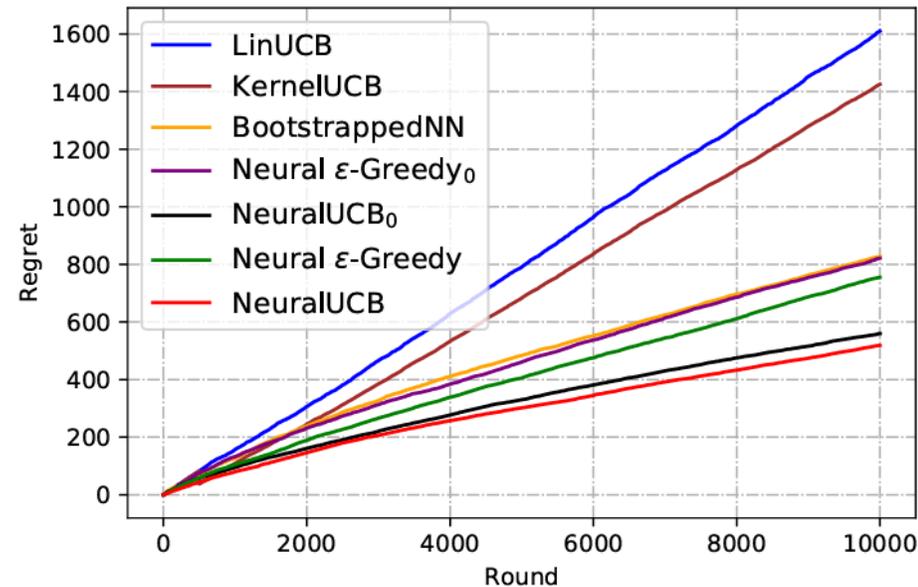
Effective dimension in NTK Space



Neural UCB: Empirical Evaluation



- NeuralUCB uses neural networks for exploitation, and gradient to explore.
- NeuralUCB achieve $\tilde{O}(\sqrt{T})$ regret upper bound, similar to LinearUCB.
- NeuralUCB generally outperforms linear contextual bandits.



Thompson Sampling

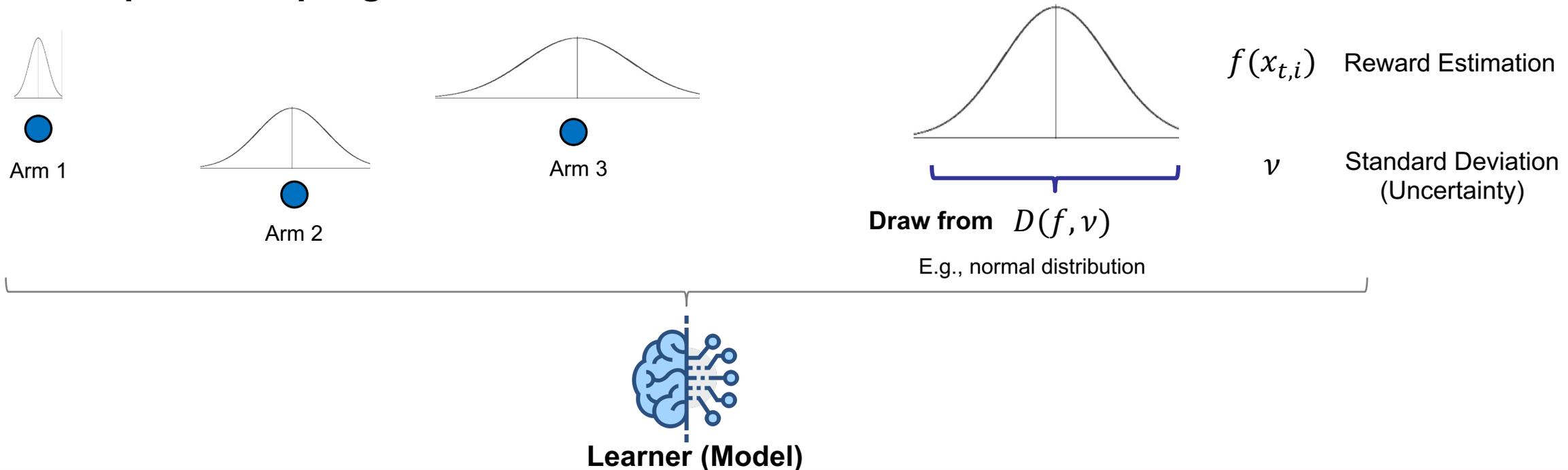


➤ Popular existing exploration strategies.

❑ **ϵ -greedy**: With probability $1 - \epsilon$, greedily choose one arm according to history; Otherwise, choose an arm randomly.

❑ **Upper Confidence Bound.**

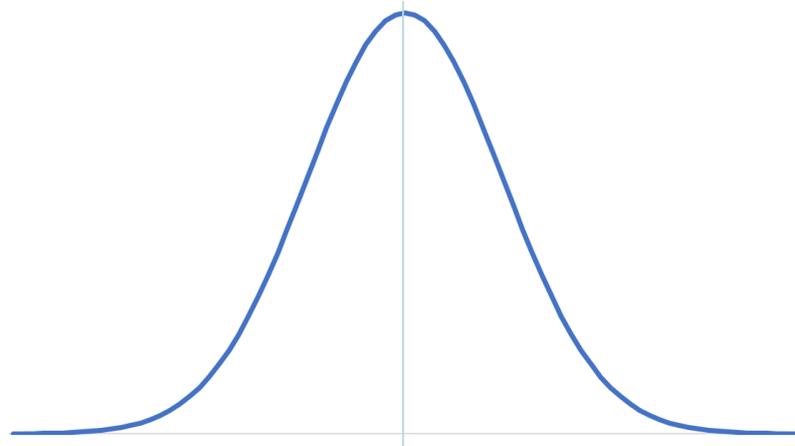
❑ **Thompson Sampling:**



Linear Thompson Sampling



Reward Distribution (Gaussian Prior)



User Preference Parameter (Unknown)

$$\mathcal{N}(b_i(t)^T \mu, v^2)$$

Arm context



Arm

for all $t = 1, 2, \dots$, **do**

Sample $\tilde{\mu}(t)$ from distribution $\mathcal{N}(\hat{\mu}, v^2 B^{-1})$.

Play arm $a(t) := \arg \max_i b_i(t)^T \tilde{\mu}(t)$, and observe reward r_t .

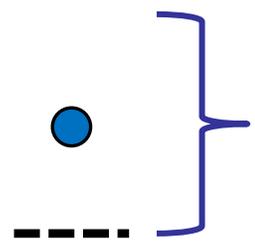
Update $B = B + b_{a(t)}(t)b_{a(t)}(t)^T$, $f = f + b_{a(t)}(t)r_t$, $\hat{\mu} = B^{-1}f$.

end for

Estimated User Preference

Sampled Reward

Estimated By Ridge Regression



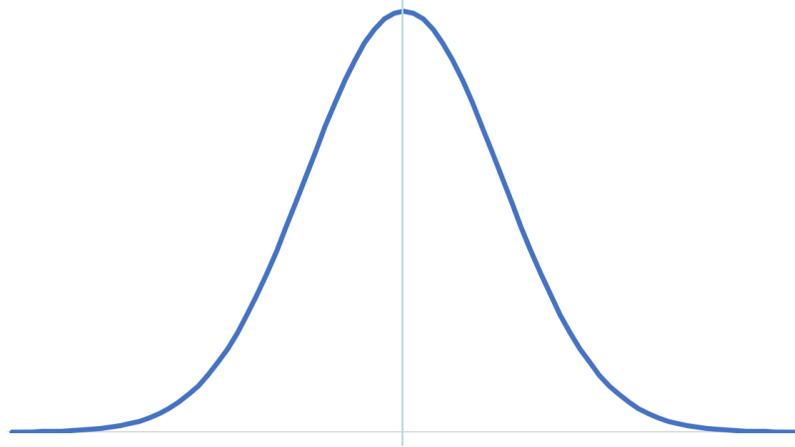
Confidence Interval



Neural Thompson Sampling



Reward Distribution (Gaussian Prior)



$$N(h(x_{t,k}), v^2)$$

Expected Reward and Variance

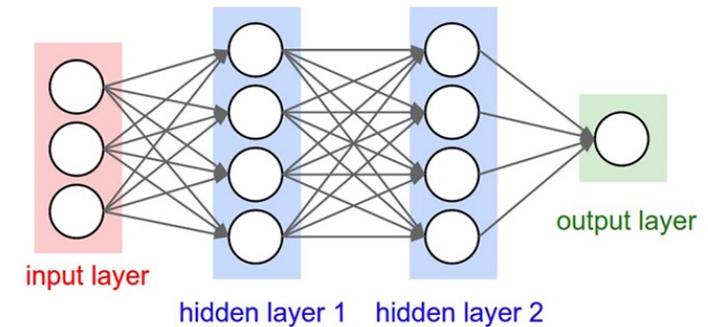


Arm

Estimated Distribution:

$$\mathcal{N}(f(\mathbf{x}_{t,k}; \boldsymbol{\theta}_{t-1}), \nu^2 \sigma_{t,k}^2)$$

$$f(\mathbf{x}; \boldsymbol{\theta}) = \sqrt{m} \mathbf{W}_L \sigma(\mathbf{W}_{L-1} \sigma(\dots \sigma(\mathbf{W}_1 \mathbf{x})))$$



Neural Thompson Sampling



- In each round, a user is serving

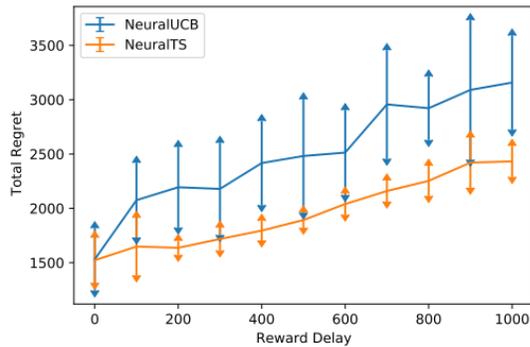
```
for  $t = 1, \dots, T$  do K arms
  for  $k = 1, \dots, K$  do
     $\sigma_{t,k}^2 = \lambda \mathbf{g}^\top(\mathbf{x}_{t,k}; \boldsymbol{\theta}_{t-1}) \mathbf{U}_{t-1}^{-1} \mathbf{g}(\mathbf{x}_{t,k}; \boldsymbol{\theta}_{t-1}) / m$  Similar to Linear Regression
    Sample estimated reward  $\tilde{r}_{t,k} \sim \mathcal{N}(f(\mathbf{x}_{t,k}; \boldsymbol{\theta}_{t-1}), \nu^2 \sigma_{t,k}^2)$ 
    Mean Variance
  end for
  Pull arm  $a_t$  and receive reward  $r_{t,a_t}$ , where  $a_t = \operatorname{argmax}_a \tilde{r}_{t,a}$ 
  Set  $\boldsymbol{\theta}_t$  to be the output of gradient descent for solving (2.3)
   $\mathbf{U}_t = \mathbf{U}_{t-1} + \mathbf{g}(\mathbf{x}_{t,a_t}; \boldsymbol{\theta}_t) \mathbf{g}(\mathbf{x}_{t,a_t}; \boldsymbol{\theta}_t)^\top / m$ 
end for
```

Compared to NeuralUCB:

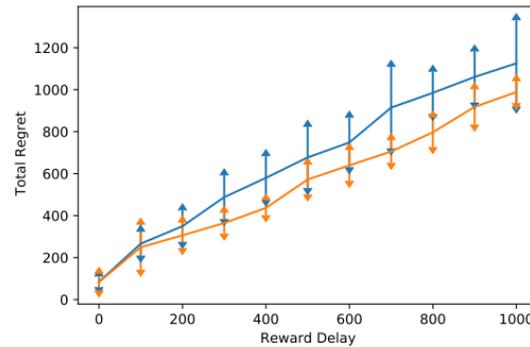
$$U_{t,a} = f(\mathbf{x}_{t,a}; \boldsymbol{\theta}_{t-1}) + \gamma_{t-1} \sqrt{\mathbf{g}(\mathbf{x}_{t,a}; \boldsymbol{\theta}_{t-1})^\top \mathbf{Z}_{t-1}^{-1} \mathbf{g}(\mathbf{x}_{t,a}; \boldsymbol{\theta}_{t-1}) / m}$$



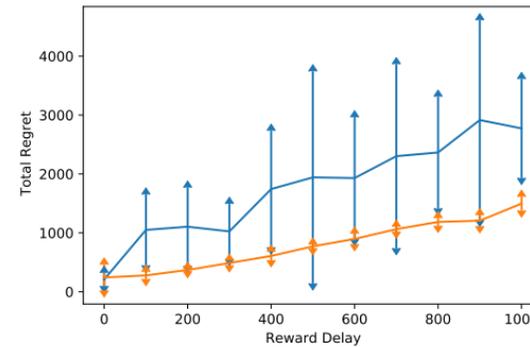
Neural Thompson Sampling



(a) MNIST

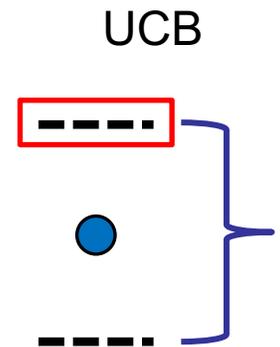
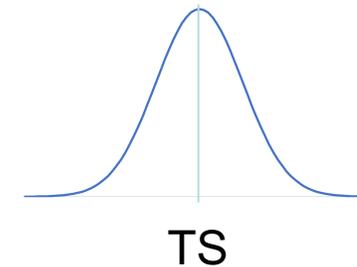


(b) Mushroom



(c) Shuttle

- NeuralTS and NeuralUCB have **similar performance** when network is trained every iteration.
- NeuralTS is more robust than NeuralUCB when network is trained **in batch**.
- NeuralTS introduces more **robustness** in exploration.



- UCB-based and TS-based exploration highly rely on large-deviation-based **statistical confidence interval**.

□ **Ideal scenario:**

● **Expected reward**

● **Estimated Reward**



Symmetric



➤ UCB-based and TS-based exploration highly rely on large-deviation-based **statistical confidence bound**.

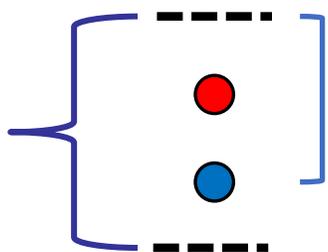
□ In practice, may be:



Expected reward

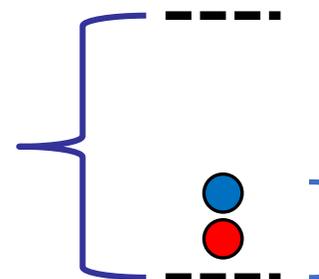


Estimated Reward



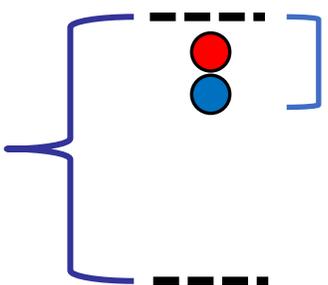
80% Pr

And



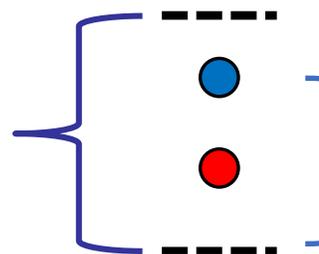
20% Pr

Asymmetric



10% Pr

And



90% Pr

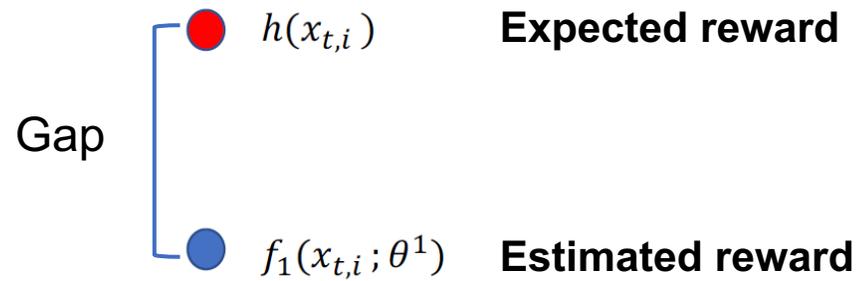




➤ Why making exploration?

□ Because we cannot make accurate prediction on a subset of data.

➤ **Goal of exploration:** Fill the **gap** between **expected reward** and **estimated reward**.



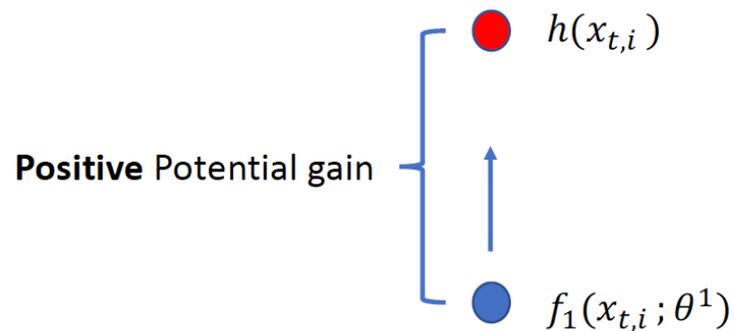
EE-Net: Exploration Direction



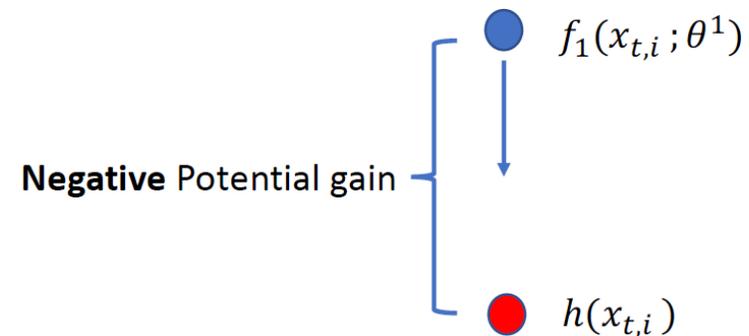
- **Two types of exploration:** “Upward” exploration and “downward” Exploration.

● $h(x_{t,i})$ Expected reward

● $f_1(x_{t,i}; \theta^1)$ Estimation



Case 1: Upward Exploration



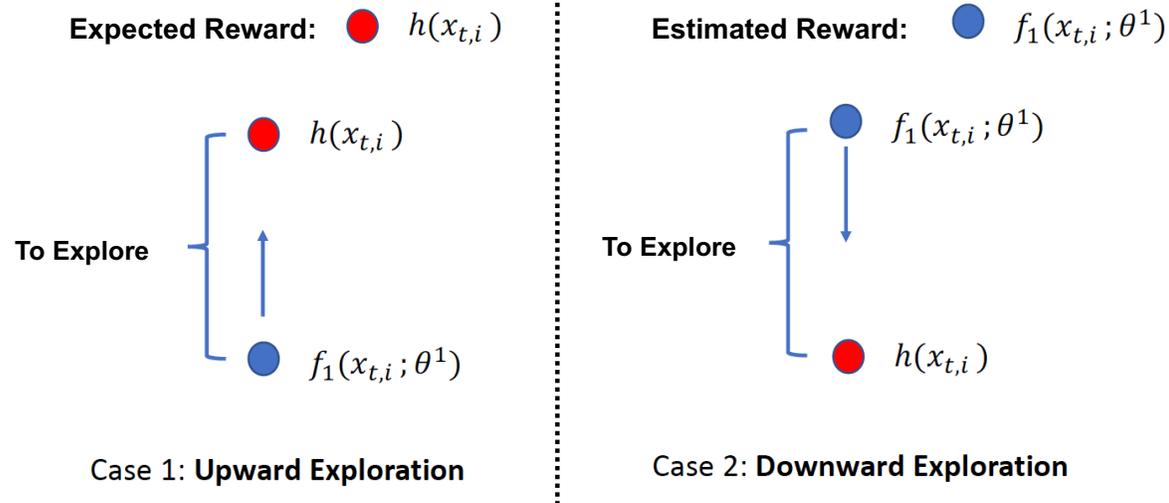
Case 2: Downward Exploration

Underestimation

Overestimation



Adapt to Exploration Direction is Challenging



Challenge:
Not 50% vs 50% !

Datasets	Upward Exploration	Downward Exploration
Mnist	76.3%	23.7%
Disin	29.1%	70.9%
MovieLens	58.6%	41.4%
Yelp	55.3%	44.7%



Pessimistic Model (Human)



Optimistic Model (Human)



- Motivation: Can we have an **adaptive** exploration strategy for both “upward” and “downward” exploration?
- **Proposed solution**: We propose to use **another neural network to learn** the gap between expected reward and estimated reward (**potential gain**) **incorporating exploration direction**.



- Motivation: Can we have an **adaptive** exploration strategy for both “upward” and “downward” exploration?
- **Proposed solution**: We propose to use **another neural network to learn** the gap between expected reward and estimated reward (**potential gain**) **incorporating exploration direction**.
- **Exploitation neural network** f_1 to estimate reward:
 - Given an arm $x_{t,i}$,
$$f_1(x_{t,i}; \theta^1) = \mathbf{W}_L \sigma(\mathbf{W}_{L-1} \sigma(\dots \sigma(\mathbf{W}_1 \cdot)))$$
 - $f_1(x_{t,i}; \theta^1)$ is to **estimate expected reward** represented by some unknown function $h(x_{t,i})$.
 - In round t , θ^1 is **trained on data of past $t - 1$ rounds**, using **gradient descent**.



- **Exploration neural network f_2** (novel component) to estimate potential gain:
 - Given an arm $x_{t,i}$ and its estimation $f_1(x_{t,i}; \theta^1)$, **expected potential gain** is defined as:

$$h(x_{t,i}) - f_1(x_{t,i}; \theta^1),$$

where $h(x_{t,i})$ is the expected reward.

- Thus, given the received reward $r_{t,i}$, **potential gain** is defined as:

$$r_{t,i} - f_1(x_{t,i}; \theta^1),$$

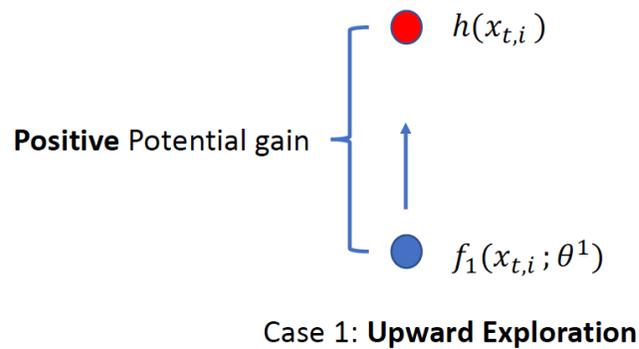
where $\mathbb{E}[r_{t,i}] = h(x_{t,i})$.

- Potential gain has a good property: **Indicating exploration direction.**

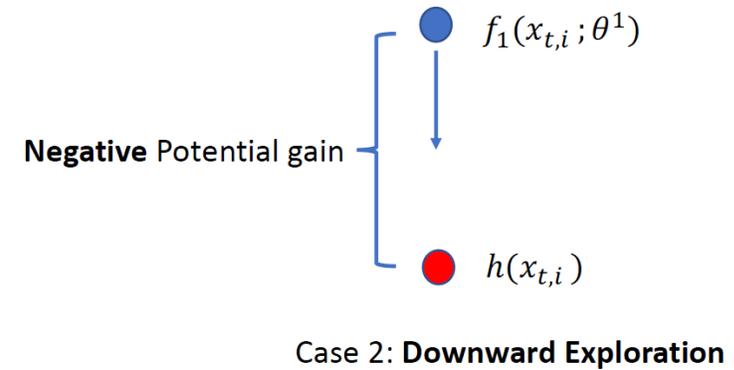


- **Exploration neural network f_2** (novel component) to estimate potential gain:
 - Potential gain has good property: **indicating exploration direction.**

$$h(x_{t,i}) - f_1(x_{t,i}; \theta^1) > 0$$



$$h(x_{t,i}) - f_1(x_{t,i}; \theta^1) < 0$$





➤ **Exploration neural network f_2** (novel component) to estimate potential gain:

- Label of f_2 : $r_{t,i} - f_1(x_{t,i};)$

$$f_2(x_{t,i}; \theta^2) = \mathbf{W}_L \sigma(\mathbf{W}_{L-1} \sigma(\dots \sigma(\mathbf{W}_1 \cdot)))$$

- What is input of f_2 ?



- **Exploration neural network f_2** (novel component) to estimate potential gain:
 - Input of f_2 : **Gradient of f_1 with respect to θ^1** :

$$\nabla_{\theta^1} f(x_{t,i}; \theta^1)$$

- **Rational:**

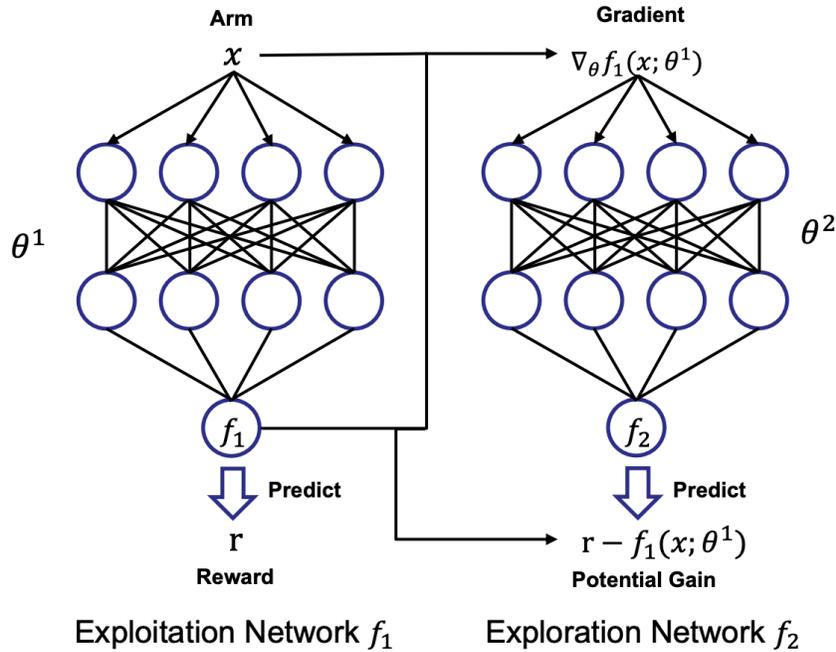
- Incorporate both **feature of input** and **discriminative information of f_1** .
- Based on [2,3], f_1 has the following confidence bound:

$$|h(\mathbf{x}_{t,i}) - f_1(\mathbf{x}_{t,i}; \theta_{t-1}^1)| \leq \Psi(\nabla_{\theta_{t-1}^1} f_1(\mathbf{x}_{t,i}; \theta_{t-1}^1)),$$

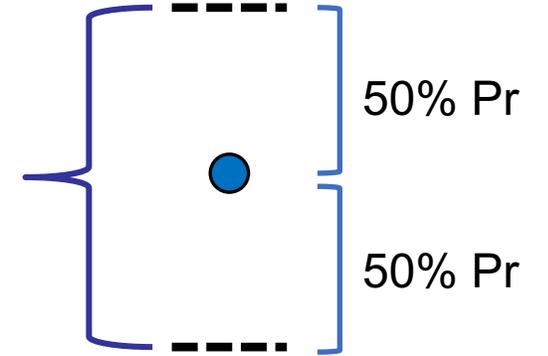
Here, **instead of choosing a fixed form Ψ , we use f_2 to learn it.**

- In this way, θ^2 is trained on $\{\nabla_{\theta^1} f(x_{t,i}; \theta_{t-1}^1)\}_{t=1}^t$ to **store historical information.**

EE-Net: Overview

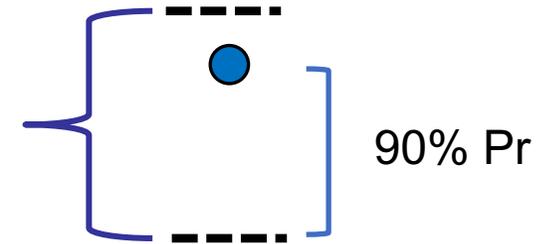


Statistical
Confidence Interval



Symmetric and Fixed

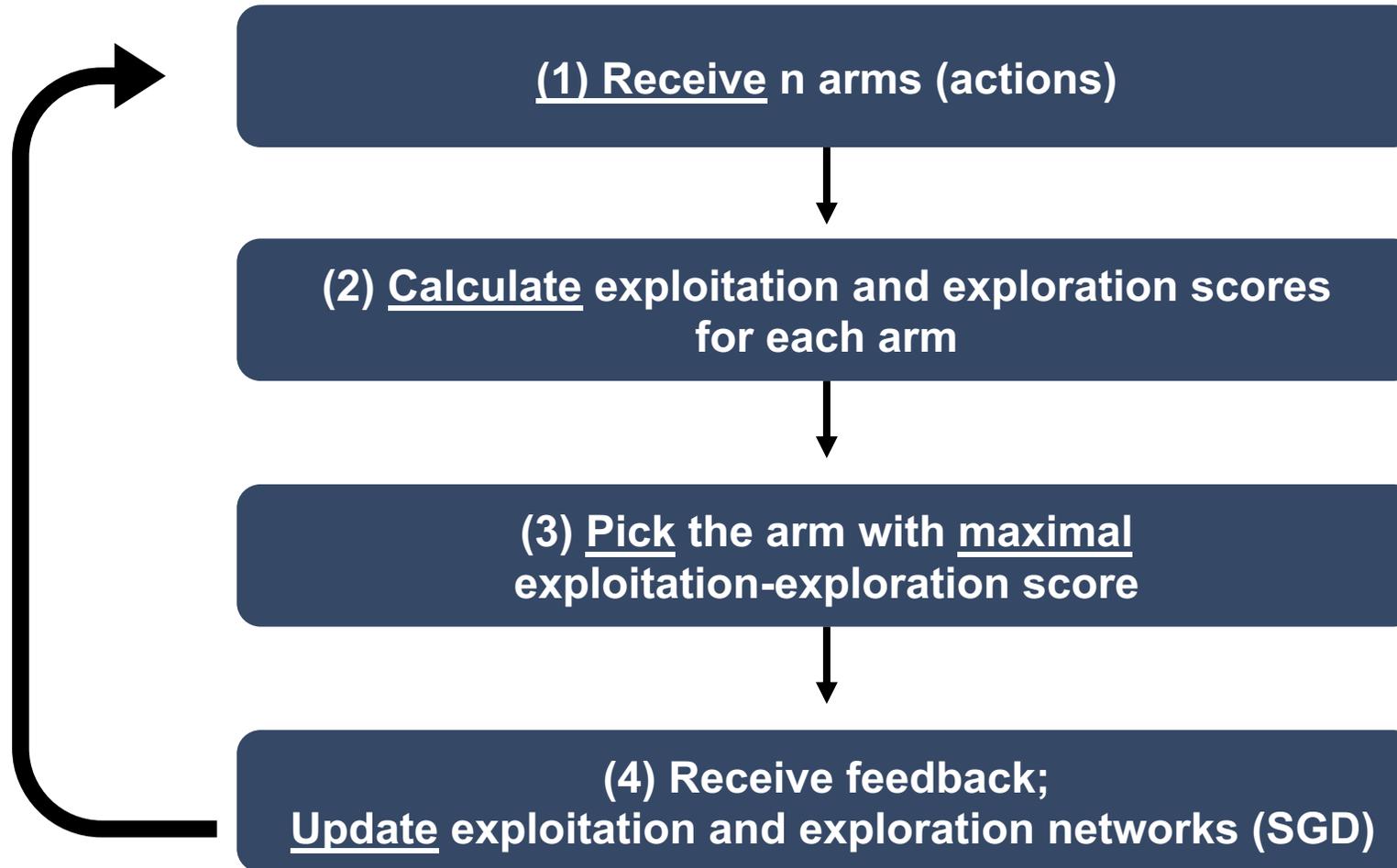
Confidence Interval
learned by neural network
(Our approach)



Asymmetric and Adaptive

Methods	"Upward" Exploration	"Downward" Exploration
ϵ -Greedy	×	×
NeuralUCB	✓	×
NeuralTS	Randomly	Randomly
EE-Net	✓	✓

1. Ban, Yikun, et al. "EE-Net: Exploitation-Exploration Neural Networks in Contextual Bandits." ICLR 2022.
2. Ban, Yikun, et al. "Neural Exploitation and Exploration of Contextual Bandits." JMLR 2024.

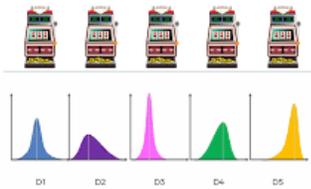


EE-Net: Theoretical Analysis

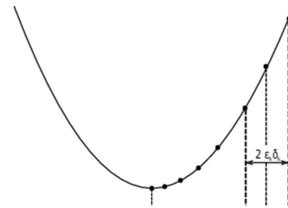


➤ Proof Workflow of NeuralUCB [1] and NeuralTS [2]:

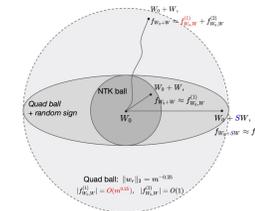
Gradient Descent in Bandits



Gradient Descent on Ridge Regression



NTK Regression

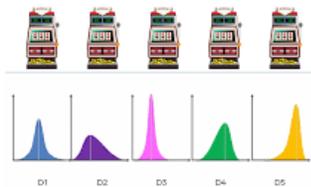


Expected Reward

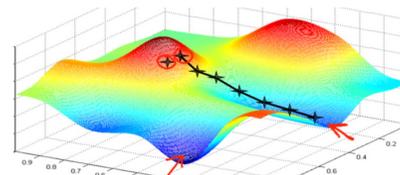


➤ Proof Workflow of EE-Net [3,4]:

Gradient Descent in Bandits



Online Gradient Descent



Expected Reward



1. Zhou, Dongruo, Lihong Li, and Quanquan Gu. "Neural contextual bandits with ucb-based exploration." ICML, 2020.
2. Zhang, Weitong, et al. "Neural thompson sampling." ICLR 2021.
3. Ban, Yikun, et al. "EE-Net: Exploitation-Exploration Neural Networks in Contextual Bandits." ICLR 2022.
4. Ban, Yikun, et al. "Neural Exploitation and Exploration of Contextual Bandits." JMLR 2024.



Assumption 1: For any $t \in [T], i \in [n], \|\mathbf{x}_{t,i}\|_2 = 1$, and $r_{t,i} \in [0, 1]$.

- Assumption 1 is standard and mild in analysis of over-parameterized neural networks.
- **No assumption** on distribution of arm contexts.
- Then, we have the following **average error bound for exploration network f_2** :

Lemma1. For any $\delta \in (0, 1), R > 0$, suppose m satisfies the conditions in Theorem 6. In round $t \in [T]$, let

$$\hat{i} = \arg \max_{i \in [k]} \left(f_1(\mathbf{x}_{t,\hat{i}}; \boldsymbol{\theta}_{t-1}^1) / \sqrt{m} + f_2(\phi(\mathbf{x}_{t,\hat{i}}); \boldsymbol{\theta}_{t-1}^2) / \sqrt{m} \right).$$

Then, with probability at least $1 - \delta$, we have

$$\begin{aligned} & \frac{1}{T} \sum_{t=1}^T \mathbb{E}_{r_{t,\hat{i}}} \left[\min \left\{ \left| f_2(\phi(\mathbf{x}_{t,\hat{i}}); \boldsymbol{\theta}_{t-1}^2) / \sqrt{m} - (r_{t,\hat{i}} - f_1(\mathbf{x}_{t,\hat{i}}; \boldsymbol{\theta}_{t-1}^1) / \sqrt{m}) \right|, 1 \right\} \right] \\ & \leq \underbrace{\sqrt{\frac{\Psi(\boldsymbol{\theta}_0^2, R)}{T}}}_{(1)} + \underbrace{\mathcal{O}\left(\frac{3LR}{\sqrt{2T}}\right)}_{(2)} + \underbrace{\sqrt{\frac{2 \log(\mathcal{O}(1)/\delta)}{T}}}_{(3)}. \end{aligned} \quad (5.3)$$

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➤ **(1) Complexity term Ψ : Infimum of regression error** caused by function class $B(\boldsymbol{\theta}^2, R)$:

$$B(\boldsymbol{\theta}_0^2, R) = \left\{ \tilde{\boldsymbol{\theta}}^2 \in \mathbb{R}^p : \|\tilde{\boldsymbol{\theta}}^2 - \boldsymbol{\theta}_0^2\|_2 \leq \mathcal{O}\left(\frac{R}{\sqrt{m}}\right) \right\}. \quad \Psi(\boldsymbol{\theta}_0^2, R) = \inf_{\tilde{\boldsymbol{\theta}}^2 \in B(\boldsymbol{\theta}_0^2, R)} \sum_{t=1}^T (f^2(\mathbf{x}_{t,\hat{i}}; \tilde{\boldsymbol{\theta}}^2) - r_{t,\hat{i}}^2)^2$$

➤ **(2) Price** of picking function class $B(\boldsymbol{\theta}^2, R)$ controlled by radius R .

➤ **(3) Confidence bound** for predictions of f_2 .

EE-Net: Regret Upper Bound



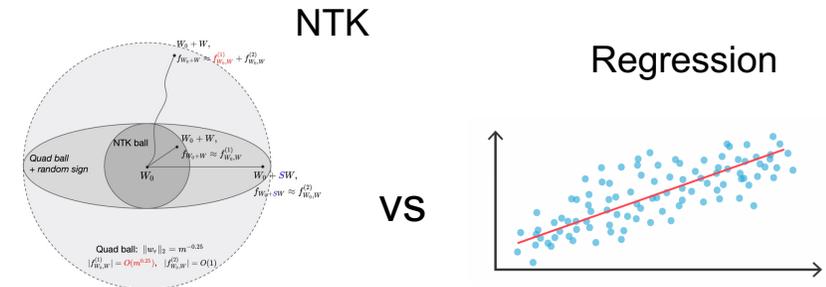
➤ Then, we have following regret upper bound $\tilde{O}(\sqrt{T})$ for EE-Net:

Theorem. Let f_1, f_2 follow the setting of f (Eq. (5.1)) with the same width m and depth L . Suppose $m \geq \Omega(\text{poly}(T, L, R, \log(1/\delta)))$, $\eta_1 = \eta_2 = \frac{\sqrt{\nu}R}{m\sqrt{T}}$ and $\Psi(\theta_0^2, R) \& \Psi^*(\theta_0^2, R) \leq \Psi$. Then, for any $\delta \in (0, 1)$, $R > 0$, with probability at least $1 - \delta$ over the initialization, there exists a constant ν , such that the pseudo regret of Algorithm 1 in T rounds satisfies

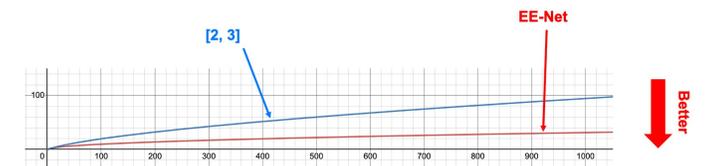
$$\mathbf{R}_T \leq \sqrt{T} \cdot \mathcal{O}\left(RL + \sqrt{\Psi} + 2\sqrt{2\log(\mathcal{O}(1)/\delta)}\right) + \mathcal{O}(1) \quad (5.2)$$

➤ Compared to existing works NeuralUCB [3] and NeuralTS [4]:

$$\mathbf{R}_T \leq \mathcal{O}\left(\sqrt{\tilde{d}T \log T + S^2}\right) \cdot \mathcal{O}\left(\sqrt{\tilde{d} \log T}\right), \quad \text{and} \quad \tilde{d} = \frac{\log \det(\mathbf{I} + \mathbf{H}/\lambda)}{\log(1 + Tn/\lambda)}$$



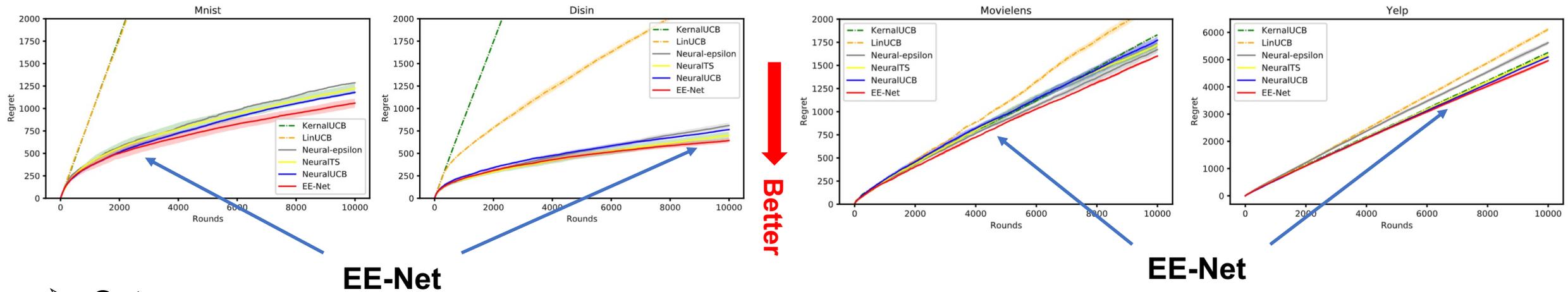
- 1) **[Better Interpretability]:** Have the similar complexity term but Ψ **easier to interpret**.
- 2) **[Contexts]:** Allow arm contexts to be **repeatedly observed**.
- 3) **[Tighter Bound]:** EE-Net **improves by a multiplicative factor $\log T$** .



1. Ban, Yikun, et al. "EE-Net: Exploitation-Exploration Neural Networks in Contextual Bandits." ICLR 2022.
2. Ban, Yikun, et al. "Neural Exploitation and Exploration of Contextual Bandits." JMLR 2024.
3. Zhou, Dongruo, Lihong Li, and Quanquan Gu. "Neural contextual bandits with ucb-based exploration." ICML, 2020.
4. Zhang, Weitong, et al. "Neural thompson sampling." ICLR 2021.



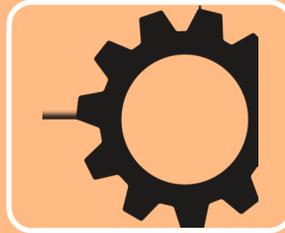
EE-Net: Empirical Experiments



➤ Setup:

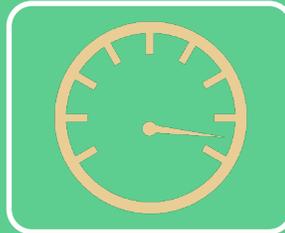
- ❑ Classification and recommendation dataset.
- ❑ 5 state-of-the-art baselines including ϵ -greedy, UCB, TS exploration strategy.
- ❑ All methods have the same exploitation network f_1 .

➤ **EE-Net** achieves **substantial improvements**, because **all improvements purely come from exploration!**



Fundamental Exploration

- Upper Confidence Bound
- Thompson Sampling
- Exploration Network



Efficient Exploration

- Neural Linear UCB
- Neural Network with Perturbed Reward
- Inverse Weight Gap Strategy





➤ In each round, a user is serving

```

for  $t = 1, \dots, T$  do
  receive feature vectors  $\{\mathbf{x}_{t,1}, \dots, \mathbf{x}_{t,K}\}$ 
  choose arm  $a_t = \operatorname{argmax}_{k \in [K]} \underbrace{\boldsymbol{\theta}_{t-1}^\top \phi(\mathbf{x}_{t,k}; \mathbf{w}_{t-1})}_{\text{Exploitation}} + \underbrace{\alpha_t \|\phi(\mathbf{x}_{t,k}; \mathbf{w}_{t-1})\|_{\mathbf{A}_{t-1}^{-1}}}_{\text{Exploration}}$ , and obtain
  reward  $\hat{r}_t$ 
  update  $\mathbf{A}_t$  and  $\mathbf{b}_t$  as follows:
     $\mathbf{A}_t = \mathbf{A}_{t-1} + \phi(\mathbf{x}_{t,a_t}; \mathbf{w}_{t-1})\phi(\mathbf{x}_{t,a_t}; \mathbf{w}_{t-1})^\top$ ,  $\mathbf{b}_t = \mathbf{b}_{t-1} + \hat{r}_t \phi(\mathbf{x}_{t,a_t}; \mathbf{w}_{t-1})$ ,
  update  $\boldsymbol{\theta}_t = \mathbf{A}_t^{-1} \mathbf{b}_t$ 
  if  $\text{mod}(t, H) = 0$  then
     $\mathbf{w}_t \leftarrow$  output of Algorithm 2
     $q = q + 1$ 
  else
     $\mathbf{w}_t = \mathbf{w}_{t-1}$ 
  end if
end for
Output  $\mathbf{w}_T$ 
  
```

Compared with LinUCB (Li et al. 2010)

$$U_{t,a} = \underbrace{\langle \mathbf{x}_{t,a}, \boldsymbol{\theta}_{t-1} \rangle}_{\text{mean}} + \gamma_{t-1} \underbrace{\sqrt{\mathbf{x}_{t,a}^\top \mathbf{Z}_{t-1}^{-1} \mathbf{x}_{t,a}}}_{\text{variance}}$$

$$\phi(\mathbf{x}; \mathbf{w}) = \sqrt{m} \sigma(\mathbf{W}_L \sigma(\mathbf{W}_{L-1} \cdots \sigma(\mathbf{W}_1 \mathbf{x}) \cdots)).$$

➤ Update Neural Network Parameter:

Loss function:

$$\mathcal{L}_q(\mathbf{w}) = \sum_{i=1}^{qH} (\boldsymbol{\theta}_i^\top \phi(\mathbf{x}_{i,a_i}; \mathbf{w}) - \hat{r}_i)^2.$$

- Gradient Descent.



Neural Bandit With Perturbed Reward

➤ In each round, a user is serving

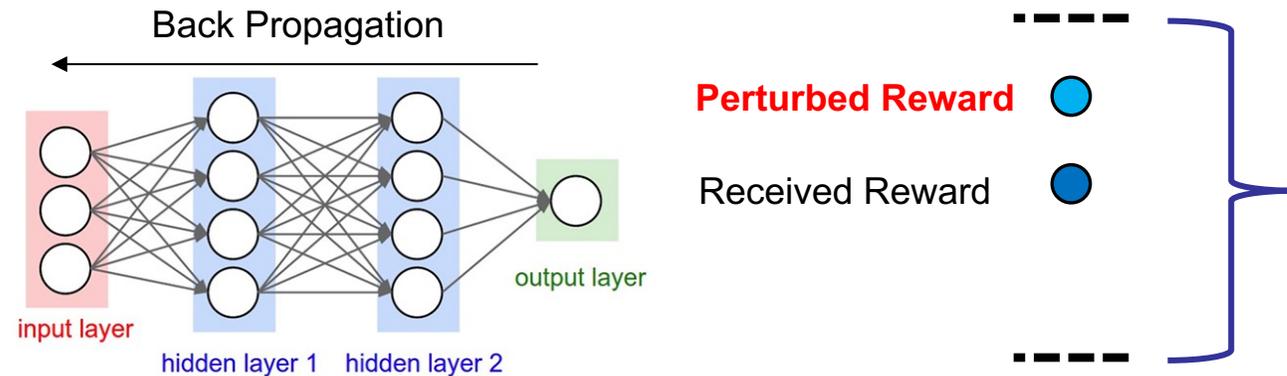
```

for  $t = 1, \dots, T$  do
  if  $t > K$  then Initialization: Pull each arm once
    Pull arm  $a_t$  and receive reward  $r_{t,a_t}$ , where  $a_t = \operatorname{argmax}_{i \in [K]} f(\mathbf{x}_i, \boldsymbol{\theta}_{t-1})$ . Selection Criterion
    Generate  $\{\gamma_s^t\}_{s \in [t]} \sim \mathcal{N}(0, \nu^2)$ . Perturbed Reward
    Set  $\boldsymbol{\theta}_t$  by the output of gradient descent for solving Eq (3.2).
  else
    Pull arm  $a_k$ .
  end if
end for
  
```

Reward Perturbation (Noise)

$$\min_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}) = \sum_{s=1}^t (f(\mathbf{x}_{a_s}; \boldsymbol{\theta}) - (r_{s,a_s} + \gamma_s^t))^2 / 2 + m\lambda \|\boldsymbol{\theta} - \boldsymbol{\theta}_0\|_2^2 / 2$$

Implicit Exploration:



Neural SquareCB: Inverse Gap Strategy



➤ In each round, a user is serving

```

for  $t = 1, 2, \dots, T$  do
    Receive contexts  $\mathbf{x}_{t,1}, \dots, \mathbf{x}_{t,K}$ , and compute  $\hat{y}_{t,a} = \tilde{f}^{(S)}(\theta; \mathbf{x}_{t,a}, \epsilon^{(1:S)})$ ,  $\forall a \in [K]$ 
    Let  $b = \arg \min_a \hat{y}_{t,a}$ ,  $p_{t,a} = \frac{1}{K + \gamma(\hat{y}_{t,b} - \hat{y}_{t,a})}$ , and  $p_{t,b} = 1 - \sum_{a \neq b} p_{t,a}$ 
    Sample arm  $a_t \sim p_t$  and observe output  $y_{t,a_t}$ 
    Update  $\theta_{t+1} = \Pi_{B_{\rho, \rho_1}^{\text{Frob}}(\theta_0)} \left( \theta_t - \eta_t \nabla \mathcal{L}_{\text{Sq}}^{(S)}(y_{t,a_t}, \{ \tilde{f}(\theta; \mathbf{x}_{t,a_t}, \epsilon_s) \}_{s=1}^S) \right)$ 
end for
    
```

Special Case: $y = 1 - r$

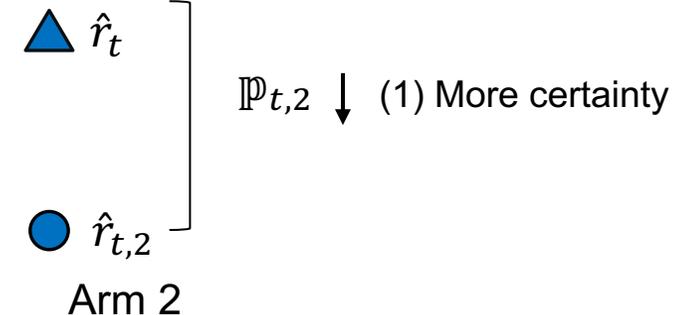
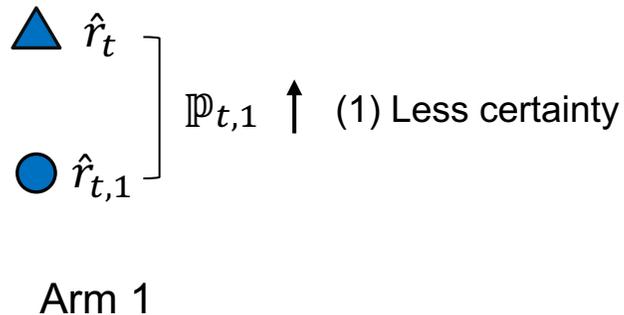
Estimated loss by neural networks

Equal to the arm with maximal reward

Inverse Weight Gap to form distribution for Selection

$$\hat{r}_t = \arg \max f(x_{t,i}; \theta_t)$$

$$\mathbb{P}_{t,i} \propto \frac{1}{\hat{r}_t - \hat{r}_{t,i}} \quad \text{Selection Probability}$$



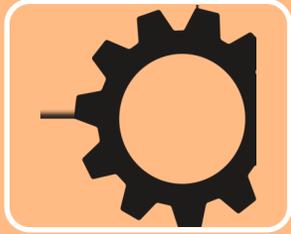
Neural SquareCB: Inverse Gap Strategy



Algorithm	Regret	Remarks
Neural UCB [Zhou et al., 2020]	$\tilde{O}(\tilde{d}\sqrt{T})$	Bound <u>depends on \tilde{d} and could be $\Omega(T)$ in worst case.</u>
Neural TS Zhang et al. [2021]	$\tilde{O}(\tilde{d}\sqrt{T})$	Bound <u>depends on \tilde{d} and could be $\Omega(T)$ in worst case.</u>
EE-Net [Ban et al., 2022b]	$\tilde{O}(\sqrt{T})$	<u>Assumes that the contexts at every round are drawn i.i.d and needs to store all the previous networks.</u>
NeuSquareCB (This work)	$\tilde{O}(\sqrt{KT})$	No dependence on \tilde{d} and holds even when the contexts are chosen adversarially.

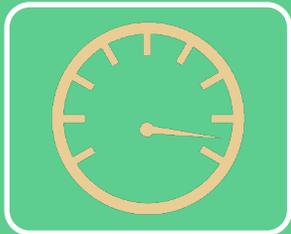
- Remove dependence of effective dimension.
- Minimize dependence on Neural Tangent Kernel.





Fundamental Exploration

- Neural UCB [1] -- An Extension of LinUCB to NTK Space
- Neural TS [2] -- An Extension of LinTS to NTK Space
- EE-Net [3] -- Another Neural Network for Exploration

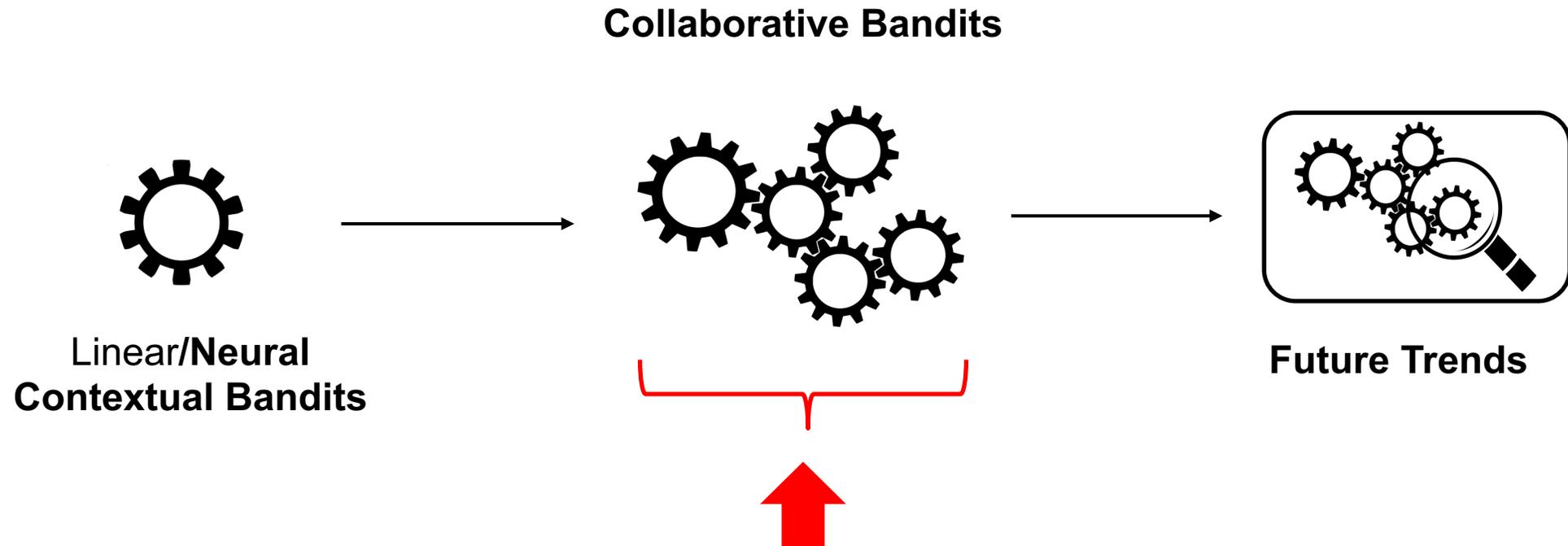


Efficient Exploration

- Neural Linear UCB [4] -- LinUCB with Neural Representation
- Neural Network with Perturbed Reward [5] -- Implicit Exploration by Perturbing Rewards
- Neural Square CB[6] -- Exploration using Inverse Weight Gap Strategy

1. Zhou, Dongruo, Lihong Li, and Quanquan Gu. "Neural contextual bandits with ucb-based exploration." ICML 2020.
2. Zhang, Weitong, Dongruo Zhou, Lihong Li, and Quanquan Gu. "Neural thompson sampling." ICLR 2021.
3. Ban, Yikun, Yuchen Yan, Arindam Banerjee, and Jingrui He. "Ee-net: Exploitation-exploration neural networks in contextual bandits." ICLR 2022.

4. Xu, Pan, et al. "Neural contextual bandits with deep representation and shallow exploration." ICLR 2022.
5. Jia, Yiling, Weitong Zhang, Dongruo Zhou, Quanquan Gu, and Hongning Wang. "Learning neural contextual bandits through perturbed rewards." ICLR 2022.
6. Deb, Rohan, Yikun Ban, Shiliang Zuo, Jingrui He, and Arindam Banerjee. "Contextual bandits with online neural regression." ICLR 2024.





Introduction

- Background & Motivations
- Challenges



Online Clustering of Bandits

- Clustering of Linear Bandits
- Clustering of Neural Bandits



Graph Bandit Learning with Collaboration

- User side: Graph Neural Bandits
- Arm side: Neural Bandit with Arm Group Graph
- Other Scenarios: Bandit Learning with Graph Feedback & Online Graph Classification with Neural Bandit



Bandits for Combo Recommendation

- Multi-facet Contextual Bandits

Collaborative Contextual Bandits: Background & Motivation



- ❑ Conventional approaches, e.g., **collaborative and content-based filtering**:

					
A		✓	✗	✓	✓
B			✓	✗	✗
C		✓	✓	✗	
D		✗		✓	
E		✓	✓	?	✗

(InCube Group)

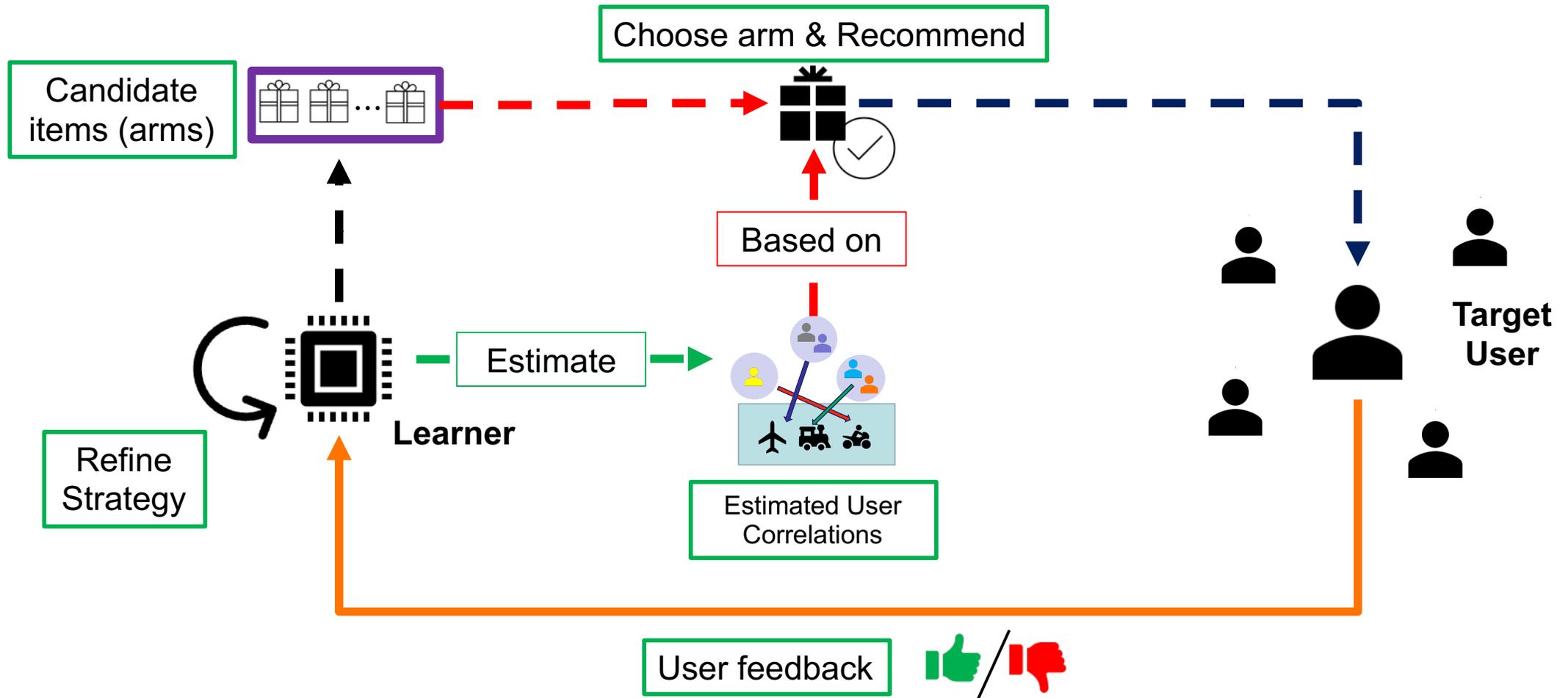
Challenges:

- ❑ **Cold-start** problem (Lack of history data);
- ❑ **Rapid change** of recommendation content and user interests.
- ❑ Dilemma of **Exploitation** and **Exploration**.

Collaborative Contextual Bandits: Background & Motivation



□ Online recommendation scenario (in each round):



Collaborative Contextual Bandits: Background & Motivation



□ The dilemma of exploitation and exploration:

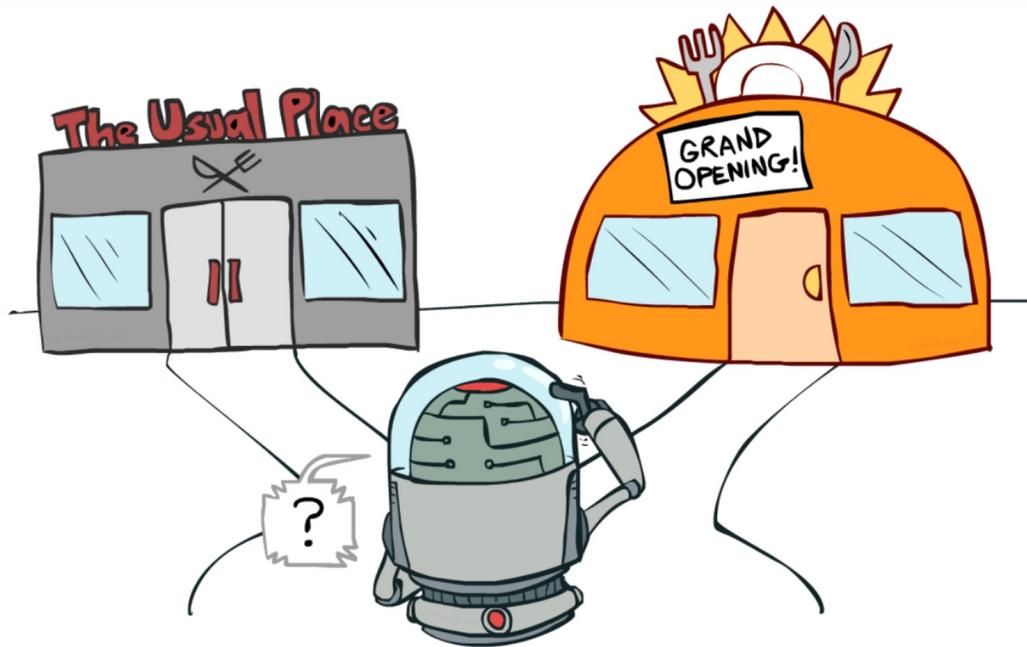
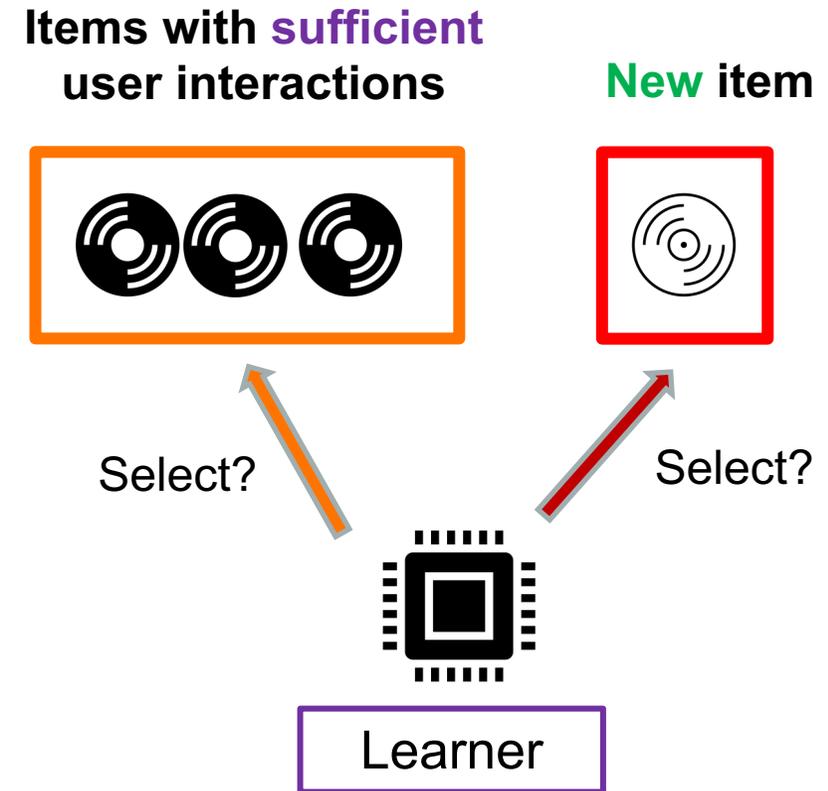


Figure: UC Berkeley CS 188, Introduction to Artificial Intelligence



- ❑ One user's decision is affected by other users.



- ❑ **Motivations:** Utilizing the **mutual influence / user collaborative effects** can
 - Improve **recommendation quality**.
 - Alleviate the **interaction scarcity** issue in terms of individual users.
 - Rapidly adapt to **new users / items** based on interactions with other users.

Collaborative Contextual Bandits: Challenges



□ **Challenge #1:** How to formally model user collaborations?

- User clusters [1, 2, 3, 4, 5, 6, 7], graphs with user nodes [10], etc.

□ **Challenge #2:** How to discover user correlations?

- Leveraging the **known** user correlation information from the environment [8, 9];
- User clustering based on their past interactions [2,3,4,5,7], exploitation-exploration graph construction [10].

□ **Challenge #3:** How to utilize user correlation to improve recommendation quality?

- Combination of linear estimations [1, 2, 3, 4, 5, 6], gradient-based meta-learning [7], graph neural networks [10], etc.

1. Gentile et. al., Online clustering of bandits. ICML 2014.

2. Li et. al., Improved algorithm on online clustering of bandits. IJCAI 2019.

3. Nguyen et. al., Dynamic clustering of contextual multi-armed bandits. CIKM 2014.

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6. Li et. al., Collaborative filtering bandits. SIGIR 2016.

7. Ban et. al., Meta clustering of neural bandits. In submission.

8. Nicolo Cesa-Bianchi et. al., A gang of bandits. NIPS 2013.

9. Wu et. al., Contextual bandits in a collaborative environment. SIGIR 2016.

10. Qi et. al., Graph neural bandits. KDD 2023.



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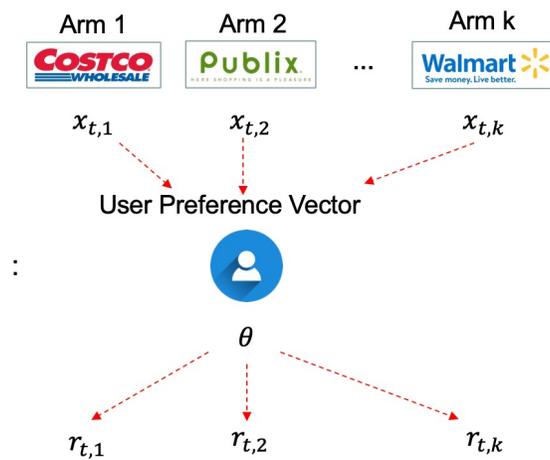


Bandits for Combo Recommendation

- Multi-facet Contextual Bandits

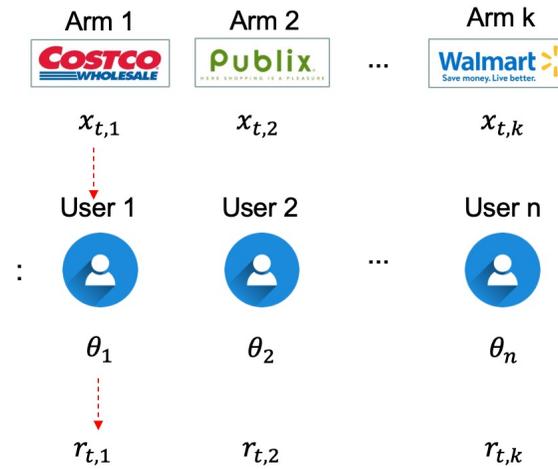
□ Two problem settings in standard MAB algorithms:

- Ignore user heterogeneity



(1) Joint Modeling

- Ignore user correlations



(2) Disjoint Modeling

□ For **trade-off** between user heterogeneity and user correlations:

- Objective #1: **Identify user clusters** in MAB;
- Objective #2: **Exploit the user clusters** to improve the recommendation.

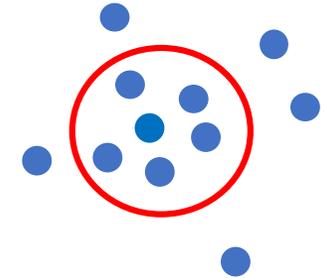
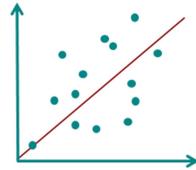


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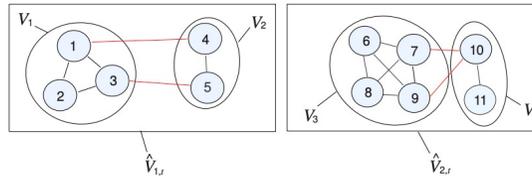
➤ Clustering of Linear Bandits:

❑ Under **linear** stochastic contextual bandit settings: $r = \langle \theta_u, x \rangle + \eta$.



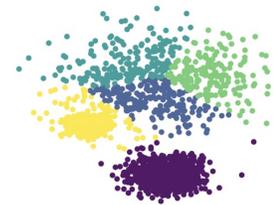
❑ User **correlation intensity** between u, u' is measured by $\|\theta_u - \theta_{u'}\|_2$.

1. User clusters with **identical preferences** [1, 2, 3, 4, 5] ($\forall u, u' \in \mathcal{N}: \theta_u = \theta_{u'}$).
 - Global clustering with evolving connected components



2. A generalized formulation: γ -cluster of users [6] ($\forall u, u' \in \mathcal{N}: \|\theta_u - \theta_{u'}\|_2 \leq \gamma$).

- Seed-based Local clustering

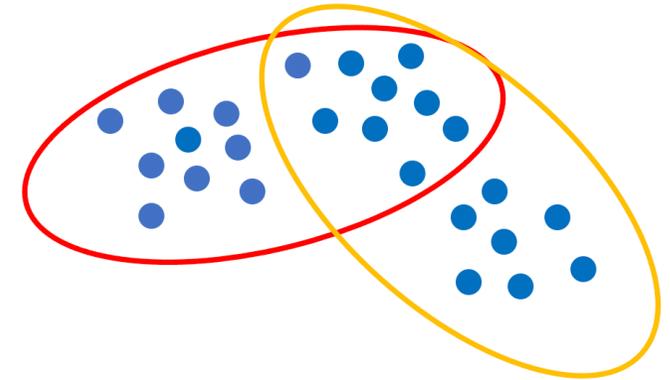


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➤ **Challenge 1: When to ensure a set of identified users is a true cluster?**

- ❑ Cluster: A set of users with similar expected rewards.
- ❑ Expected rewards of users are unknown.



➤ **Challenge 2: Can we further reduce the clustering complexity?**

- ❑ Previous works have clustering complexity $O(n)$.
- ❑ n is the number of users.

➤ **Challenge 3: Can we consider and address soft clustering?**

- ❑ Consider overlapping clusters.
- ❑ A user is allowed to belong to multiple clusters.



LOCB: Local Clustering of Linear bandits

➤ Characterizing similar users' behaviors:

- ❑ **Definition (γ -Cluster)**: Given a subset of users $\mathcal{N} \subseteq N$ and a threshold $\gamma > 0$, \mathcal{N} is considered a γ -Cluster if it satisfies: $\forall i, j \in \mathcal{N}, \|\theta^i - \theta^j\| < \gamma$.

➤ Objectives:

- ❑ **Objective #1: Identify clusters** among users, such that the clusters returned by the proposed algorithm are true γ -Clusters with probability at least $1-\delta$.
- ❑ **Objective #2**: Leverage user clusters to improve the quality of recommendation, evaluated by **Regret**.

$$\mathbf{R}_T = \mathbb{E}\left[\sum_{t=1}^T R_t\right] = \sum_{t=1}^T \left(\theta_{i_t}^\top \mathbf{x}_t^* - \theta_{i_t}^\top \mathbf{x}_t \right)$$

Optimal Reward Received Reward

➤ Clustering Module + Pulling Module

➤ **Identify k clusters, given k seeds in each round:**

- ❑ **Seed selection:** Randomly choose k users.
- ❑ **Neighbors:** Two users are neighbors if they belong to the same γ -cluster.
- ❑ **Potential neighbors:** User i is considered as the potential neighbor of seed user s , when:

$$\|\hat{\theta}_{i,t} - \hat{\theta}_{s,t}\| \leq B_{\theta,i}(m_{i,t}, \delta') + B_{\theta,s}(m_{s,t}, \delta').$$

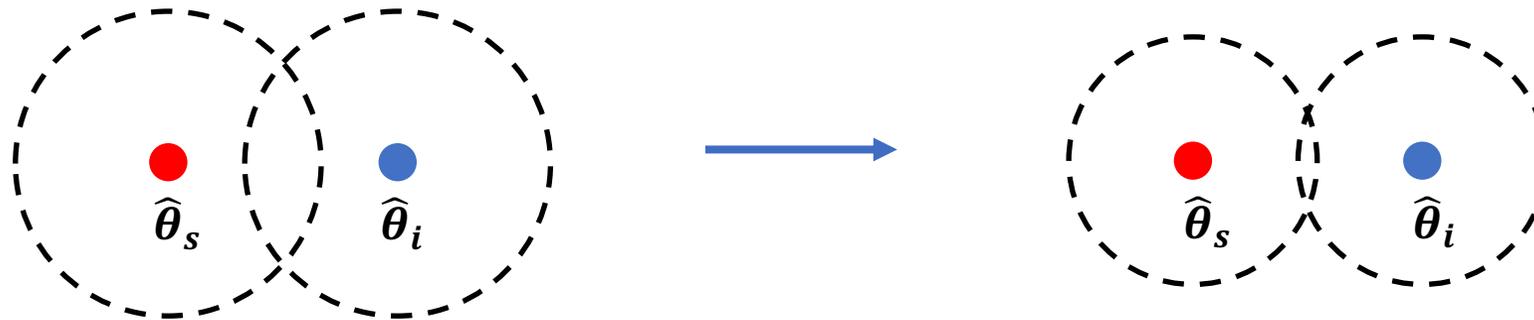
Seed-user parameter
User-specific bound
Seed-specific bound

$$B_{\theta,i}(m_{i,t}, \delta') = \frac{\sigma \sqrt{2d \log t + 2 \log(2/\delta')} + 1}{\sqrt{1 + h(m_{i,t}, H)}},$$

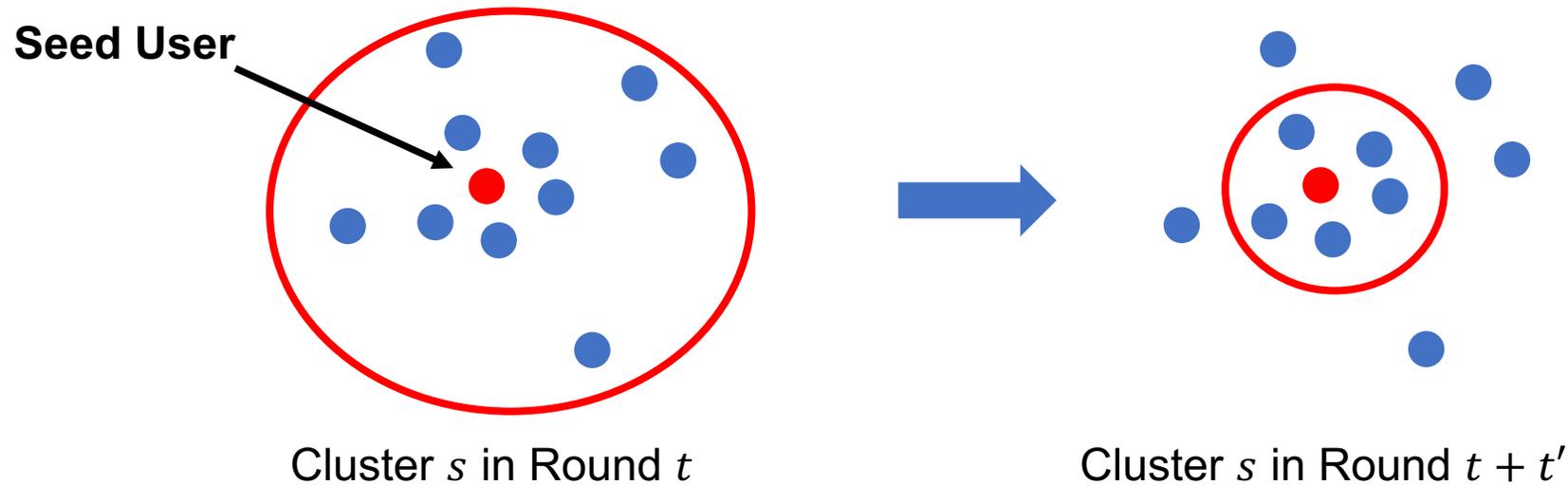
$$h(m_{i,t}, H) = \left(\frac{\lambda m_{i,t}}{4} - 8 \log\left(\frac{m_{i,t} + 3}{H}\right) - 2 \sqrt{m_{i,t} \log\left(\frac{m_{i,t} + 3}{H}\right)} \right)$$

- ❑ **Cluster:** Seed user + Its potential neighbors.

➤ **User specific bound:** with a high probability, $\|\hat{\theta}_{i,t} - \theta_i\| \leq B_{\theta,i}(m_{i,t}, \delta')$



Potential Neighbors



- **Evolution of neighbors:** $\|\hat{\theta}_{i,t} - \hat{\theta}_{s,t}\| \leq B_{\theta,i}(m_{i,t}, \delta') + B_{\theta,s}(m_{s,t}, \delta')$.



User/seed specific bound is shrinking as more rounds are played for these users.

- **Termination criterion**

□ Given cluster $\mathcal{N}_{s,t}$, Clustering Module outputs this cluster when

$$\sup\{B_{\theta,i}(m_{i,t}, \delta') : i \in \mathcal{N}_{s,t}\} < \frac{\gamma}{8}$$



➤ **Individual CB vs. Cluster CB**

❑ Confidence interval for each **cluster**

❑ Confidence interval for each **user**

$$\mathbb{P} \left(\forall t \in [T], |\hat{\theta}_{\mathcal{N}_{s,t}}^\top \mathbf{x}_{a,t} - \theta_{\mathcal{N}_{s,t}}^\top \mathbf{x}_{a,t}| > \boxed{CB_{r,\mathcal{N}_{s,t}}} \right) < \delta' \quad \mathbb{P} \left(\forall t \in [T], |\hat{\theta}_{i,t}^\top \mathbf{x}_{a,t} - \theta_i^\top \mathbf{x}_{a,t}| > \boxed{CB_{r,i}} \right) < \delta'$$

Cluster CB

Individual CB

$$CB_{r,\mathcal{N}_{s,t}} = \frac{1}{|\mathcal{N}_{s,t}|} \sum_{i \in \mathcal{N}_{s,t}} CB_{r,i}$$

➤ **Pulling Module selects one arm by Cluster UCB:**

$$\mathbf{x}_t = \arg \max_{\mathbf{x}_{a,t} \in \mathbf{X}_t} \hat{\theta}_{\mathcal{N}_{s,t}}^\top \mathbf{x}_{a,t} + CB_{r,\mathcal{N}_{s,t}}$$

Cluster-level exploration

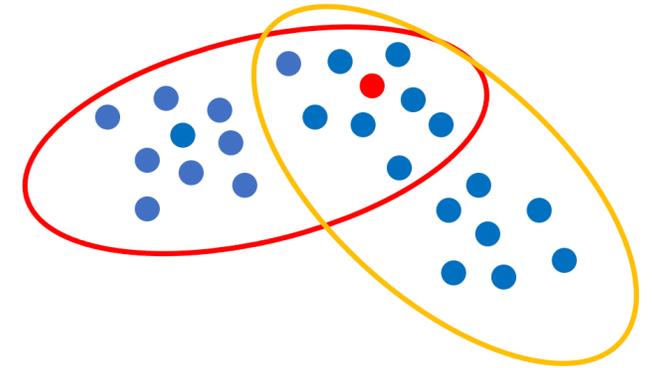
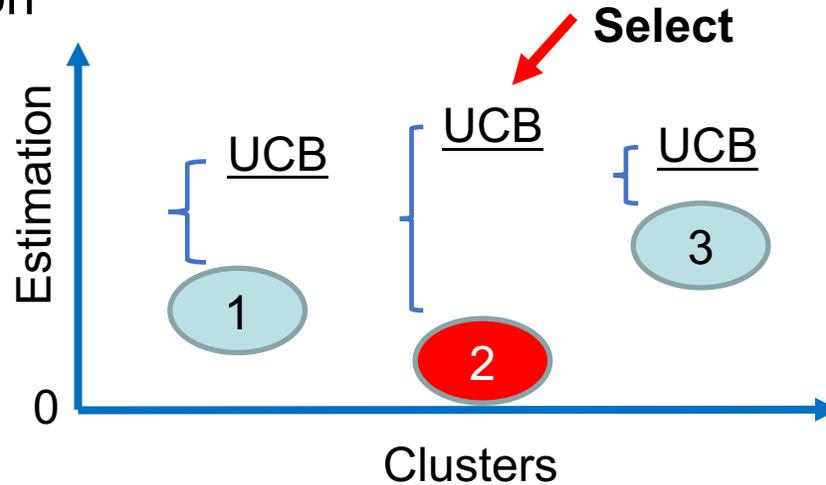
Cluster behavior $\hat{\theta}_{\mathcal{N}_{s,t}} = \frac{1}{|\mathcal{N}_{s,t}|} \sum_{i \in \mathcal{N}_{s,t}} \hat{\theta}_{i,t}$



LOCB: Overlapping Clusters



- A user may belong to multiple overlapping clusters:
 - Cluster selection



- Pulling Module selects the **cluster with the maximum potential**:

$$\mathbf{x}_t = \arg \max_{\mathbf{x}_{a,t} \in \mathbf{X}_t} \max_{s \in \mathcal{S}_t(i_t)} \left(\hat{\boldsymbol{\theta}}_{N_{s,t}}^\top \mathbf{x}_{a,t} + CB_{r, N_{s,t}} \right)$$

Arm set

Cluster set ($O(k)$)

LOCB: Results



➤ Theoretical analysis:

❑ Correctness ✓

THEOREM 5.1 (CORRECTNESS). Given a threshold γ and a set of seeds $S \subseteq N$, for each $s \in S$, let N_s represent the cluster output by LOCB with respect to s . The terminate criterion of Clustering module is defined as:

$$\sup\{B_{\theta,i}(m_{i,t}, \delta') : i \in N_{s,t}\} < \frac{\gamma}{8}.$$

Then, with probability at least $1 - \delta$, after the Clustering module terminates, for each $s \in S$, it has

$$\forall i, j \in N_s, \|\theta_i - \theta_j\| < \gamma.$$

❑ Efficiency ✓

THEOREM 5.2. Suppose each user is evenly served and $m_{i,t} \geq \frac{2 \times 32^2}{\lambda^2} \log\left(\frac{2nd}{\delta'}\right) \log\left(\frac{32^2}{\lambda^2} \log\left(\frac{2nd}{\delta'}\right)\right)$ for any $i \in N$. Then, with probability at least $1 - \delta$, the number of rounds \hat{T} needed for the Clustering module to terminate is upper bounded by

$$\hat{T} < \frac{2nd}{C} \log \frac{nd}{C} + \frac{2n}{C} \left(\log\left(\frac{2^{(d+1)}n}{\delta}\right) - \frac{\gamma^2 - 256}{512\sigma^2} \right) + n.$$

where $C = \frac{\lambda\gamma^2}{16^3\sigma^2}$.

❑ Effectiveness ✓

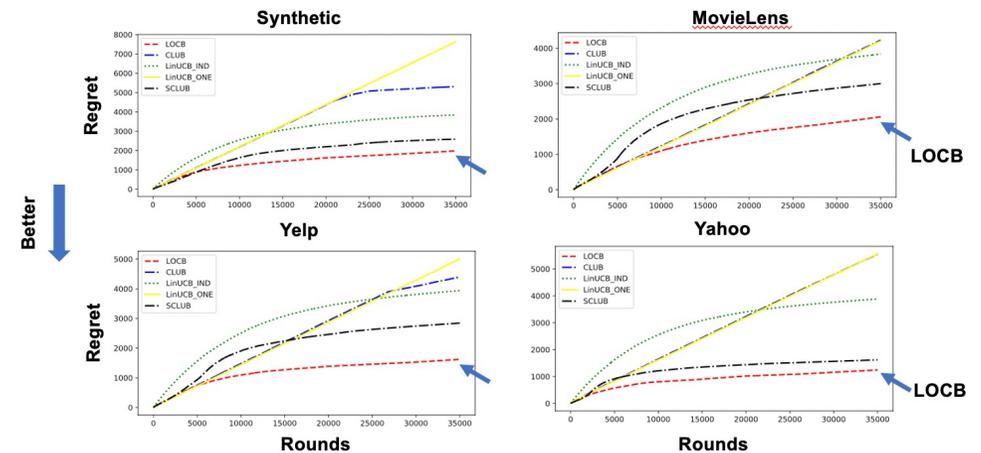
THEOREM 5.3. Suppose that each user is evenly served. Given γ and a set of seeds S , after $T > \hat{T}$ rounds, the accumulated regret of LOCB can be upper bounded as follows:

$$R_T \leq \left[\sqrt{nT} \cdot \sqrt{2d \log(1 + T/dn)} \cdot O\left(\sqrt{d \log(T/\delta)}\right) \right] + (T - O(nd \log nd)) \gamma + O(nd \log nd) \cdot O\left(\sqrt{d \log(Tn/\delta)}\right).$$

➤ Evaluations:

❑ Improve performance up to 12.4%.

	Synthetic			Yelp			MovieLens			Yahoo			
	F1	Pre	Recall	F1	Pre	Recall	F1	Pre	Recall	F1	Pre	Recall	
N-CLUB	0.390	0.246	0.943	0.484	0.334	0.884	N-CLUB	0.417	0.286	0.773	0.454	0.334	0.709
ST-CLUB	0.578	0.549	0.612	0.626	0.593	0.663	ST-CLUB	0.520	0.429	0.663	0.528	0.385	0.841
ST-SCLUB	0.714	0.745	0.687	0.768	0.863	0.693	ST-SCLUB	0.538	0.739	0.424	0.632	0.781	0.532
N-LOCB	0.662	0.618	0.714	0.675	0.620	0.743	N-LOCB	0.472	0.432	0.524	0.615	0.553	0.692
LOCB	0.880	0.913	0.856	0.879	0.908	0.853	LOCB	0.814	0.892	0.749	0.869	0.935	0.813





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➤ **Challenge 1: How to efficiently determining a user's relative group?**

- ❑ User relative group: A set of users with **same expected rewards on a specific item (arm)**.
- ❑ Expected rewards of users are unknown. The mapping function $h(x)$ can be linear or non-linear.

➤ **Challenge 2: Effective parametric representation of dynamic clusters?**

- ❑ Introducing **meta-learner** capable of representing and swiftly adapting to evolving user clusters.
- ❑ Enabling the rapid acquisition of nonlinear cluster representations.

➤ **Challenge 3: Balancing exploitation and exploration?**

- ❑ A novel UCB-type exploration strategy.
- ❑ Taking both user-side and meta-side information into account.





➤ Characterizing user clusters without linear assumptions:

Definition 3.1 (Relative Cluster). In round t , given an arm $\mathbf{x}_{t,i} \in \mathbf{X}_t$, a relative cluster $\mathcal{N}(\mathbf{x}_{t,i}) \subseteq N$ with respect to $\mathbf{x}_{t,i}$ satisfies

- (1) $\forall u, u' \in \mathcal{N}(\mathbf{x}_{t,i}), \mathbb{E}[r_{t,i}|u] = \mathbb{E}[r_{t,i}|u']$
- (2) $\nexists \mathcal{N}' \subseteq N, \text{ s.t. } \mathcal{N}' \text{ satisfies (1) and } \mathcal{N}(\mathbf{x}_{t,i}) \subset \mathcal{N}'.$

Definition 3.2 (γ -gap). Given two different cluster $\mathcal{N}(\mathbf{x}_{t,i}), \mathcal{N}'(\mathbf{x}_{t,i})$, there exists a constant $\gamma > 0$, such that

$$\forall u \in \mathcal{N}(\mathbf{x}_{t,i}), u' \in \mathcal{N}'(\mathbf{x}_{t,i}), |\mathbb{E}[r_{t,i}|u] - \mathbb{E}[r_{t,i}|u']| \geq \gamma.$$

➤ Objectives:

- ❑ **Objective #1:** Identify clusters among users, such that the clusters returned by the proposed algorithm are accurate user clusters.
- ❑ **Objective #2:** Leverage user correlations to improve the quality of recommendation, evaluated by Pseudo Regret.

$$\mathbf{R}_T = \sum_{t=1}^T \mathbb{E}[r_t^* - r_t \mid u_t, \mathbf{X}_t],$$

Optimal Reward

Received Reward

$$\mathbb{E}[r_t^* \mid u_t, \mathbf{X}_t] = \max_{\mathbf{x}_{t,i} \in \mathbf{X}_t} h_{u_t}(\mathbf{x}_{t,i})$$

General reward function



- Identify relative cluster for **target user** $u_t \in N$:
 - ❑ **Arm-specific**: Different arms can induce distinct user clusters.
 - ❑ **User models**: Each user $u \in N$ is assigned with their own user models $f(\cdot; \theta^u)$.
 - ❑ **Potential neighbors**: User u is the potential neighbor of target user u_t , when:

$$\widehat{N}_{u_t}(\mathbf{x}_{t,i}) = \left\{ u \in N \mid \left| f(\mathbf{x}_{t,i}; \theta_{t-1}^u) - f(\mathbf{x}_{t,i}; \theta_{t-1}^{u_t}) \right| \leq \frac{\nu - 1}{\nu} \gamma \right\}.$$

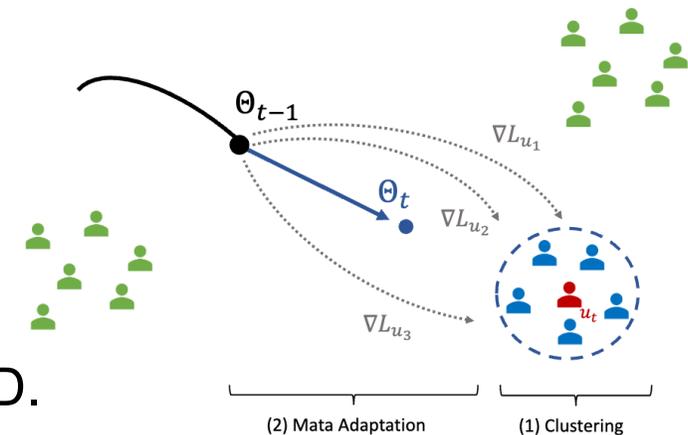
Preference est. for other users

Preference est. for target user

Tunable distance threshold

- **Meta-adaptation**: Adapting to estimated user clusters.

- ❑ Randomly draw a few samples from the historical data of detected cluster $\{\mathcal{T}_{t-1}^u\}_{u \in \widehat{N}_{u_t}(\mathbf{x}_{i,t})}$.
- ❑ The meta-model $f(\cdot; \Theta)$ is adapted through a few steps of SGD.



➤ Informative UCB for reward estimation:

Meta-Model Error

$$\sum_{t=1}^T \mathbb{E}_{r_t | \mathbf{x}_t} \left[|f(\mathbf{x}_t; \Theta_t) - r_t| \mid u_t \right]$$

Gradient Discrepancy between User Model and the Meta-Model

$$\leq \underbrace{\sum_{t=1}^T \frac{O(\|\nabla_{\Theta} f(\mathbf{x}_t; \Theta_t) - \nabla_{\Theta} f(\mathbf{x}_t; \theta_0^{u_t})\|_2)}{m^{1/4}}}_{\text{Meta-side info}} + \sum_{u \in N} \mu_T^u \underbrace{\left[O\left(\sqrt{\frac{S+1}{2\mu_T^u}}\right) + \sqrt{\frac{2 \log(1/\delta)}{\mu_T^u}} \right]}_{\text{User-side info}}$$

User-side Upper Bound based on Service Frequency

➤ Pulling Module selects one arm by Cluster UCB:

$$\mathbf{x}_t = \arg_{\mathbf{x}_{t,i} \in \mathbf{X}_t} \max U_{t,i}$$

$$U_{t,i} = \underbrace{f(\mathbf{x}_{t,i}; \Theta_{t,i})}_{\text{Meta-Model Reward Estimation}} + \underbrace{\frac{\|\nabla_{\Theta} f(\mathbf{x}_{t,i}; \Theta_{t,i}) - \nabla_{\Theta} f(\mathbf{x}_{t,i}; \theta_0^{u_t})\|_2}{m^{1/4}} + \sqrt{\frac{S+1}{2\mu_t^u}} + \sqrt{\frac{2 \log(1/\delta)}{\mu_t^u}}}_{\text{UCB}}$$

M-CNB: Theoretical and Empirical Results

➤ Theoretical analysis from two aspects:

☐ Instance-dependent Regret Bound ✓

Theorem 5.1. Given the number of rounds T and γ , for any $\delta \in (0, 1)$, $R > 0$, suppose $m \geq \tilde{\Omega}(\text{poly}(T, L, R) \cdot Kn \log(1/\delta))$, $\eta_1 = \eta_2 = \frac{R^2}{\sqrt{m}}$, and $\mathbb{E}[|\mathcal{N}_{u_t}(\mathbf{x}_t)|] = \frac{n}{q}$, $t \in [T]$. Then, with probability at least $1 - \delta$ over the initialization, Algorithm 1 achieves the following regret upper bound:

$$R_T \leq \sqrt{qT \cdot S_{TK}^*} + O(1) + O(\sqrt{2qT \log(O(1)/\delta)}).$$

where $S_{TK}^* = \inf_{\theta \in B(\theta_0, R)} \sum_{t=1}^{TK} \mathcal{L}_t(\theta)$.

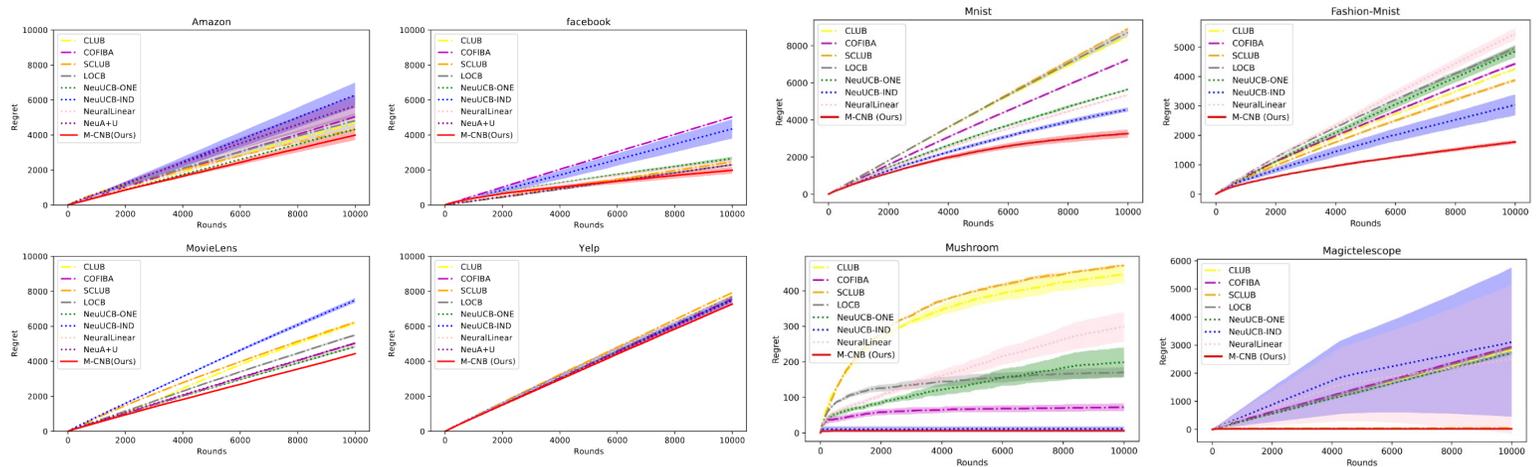
☐ NTK-regression based Regret Bound ✓

Lemma 5.3. Suppose Assumption 5.1 and conditions in Theorem 5.1 holds where $m \geq \tilde{\Omega}(\text{poly}(T, L) \cdot Kn\lambda_0^{-1} \log(1/\delta))$. With probability at least $1 - \delta$ over the initialization, there exists $\theta' \in B(\theta_0, \tilde{\Omega}(T^{3/2}))$, such that

$$\mathbb{E}[S_{TK}^*] \leq \mathbb{E}\left[\sum_{t=1}^{TK} \mathcal{L}_t(\theta')\right] \leq \tilde{O}\left(\sqrt{\tilde{d}} + s\right)^2 \cdot \tilde{d}.$$

➤ Evaluations:

☐ M-CNB (red curve) outperforms baselines, for both recommendation and classification data sets.



□ Motivations: We need to **estimate user correlations on the fly**, during online recommendation.

□ Clustering of Linear Bandits [1, 2, 3, 4, 5, 6]:

- Under **linear** stochastic contextual bandit settings: $r = \langle \theta_u, x \rangle + \eta$.
- User **correlation intensity** between u, u' is measured by $\|\theta_u - \theta_{u'}\|_2$.
- Adopt *combination of linear estimators* for reward estimation & exploration.

□ Clustering of Neural Bandits [7]:

- Under **neural** stochastic contextual bandit settings: $r = h_u(x) + \eta$.
- User clusters with identical preferences ($\forall u, u' \in \mathcal{N}, x \in \mathbb{R}^d: h_u(x) = h_{u'}(x)$).
- Utilizing *gradient-based Meta-Learning* for reward estimation & exploration.

1. Gentile et. al., Online clustering of bandits. ICML 2014.
2. Li et. al., Improved algorithm on online clustering of bandits. IJCAI 2019.
3. Nguyen et. al., Dynamic clustering of contextual multi-armed bandits. CIKM 2014.
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6. Li et. al., Collaborative filtering bandits. SIGIR 2016.
7. Ban et. al., Meta clustering of neural bandits. In submission.

An icon representing an introduction or overview, showing various shopping-related items like a shopping cart, a red shopping bag, a credit card, and a laptop, connected by lines on a grid background.

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An icon representing online clustering, showing a network of people's avatars connected by lines, symbolizing social or data relationships.

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An icon representing graph-based learning, showing a network of nodes and edges with social media icons like LinkedIn, Twitter, and Instagram.

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- Other Scenarios: Bandit Learning with Graph Feedback & Online Graph Classification with Neural Bandit

An icon representing data analysis and recommendation, showing a laptop screen with a bar chart, a magnifying glass over a document, and a calculator.

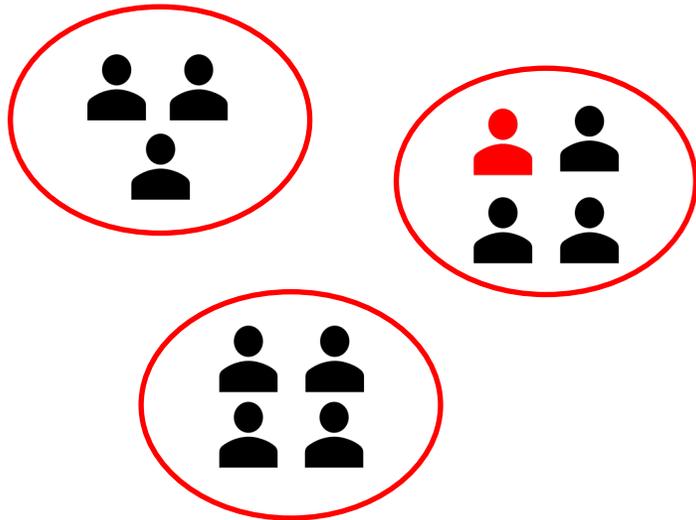
Application in Recommender Systems

- Multi-facet Personalized Recommendation

Clustering of Bandits [1,2]

➤ Coarse-grained user correlations:

- ❑ Users within the same cluster share **identical preferences**.
- ❑ **Contribute equally** to serving user.

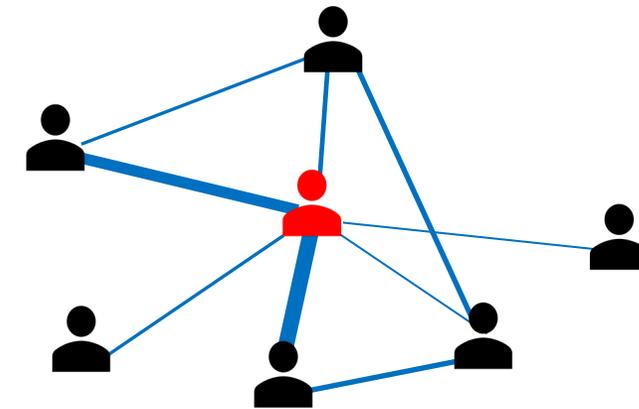


 User (Bandit)

Graph Bandits Learning [3]

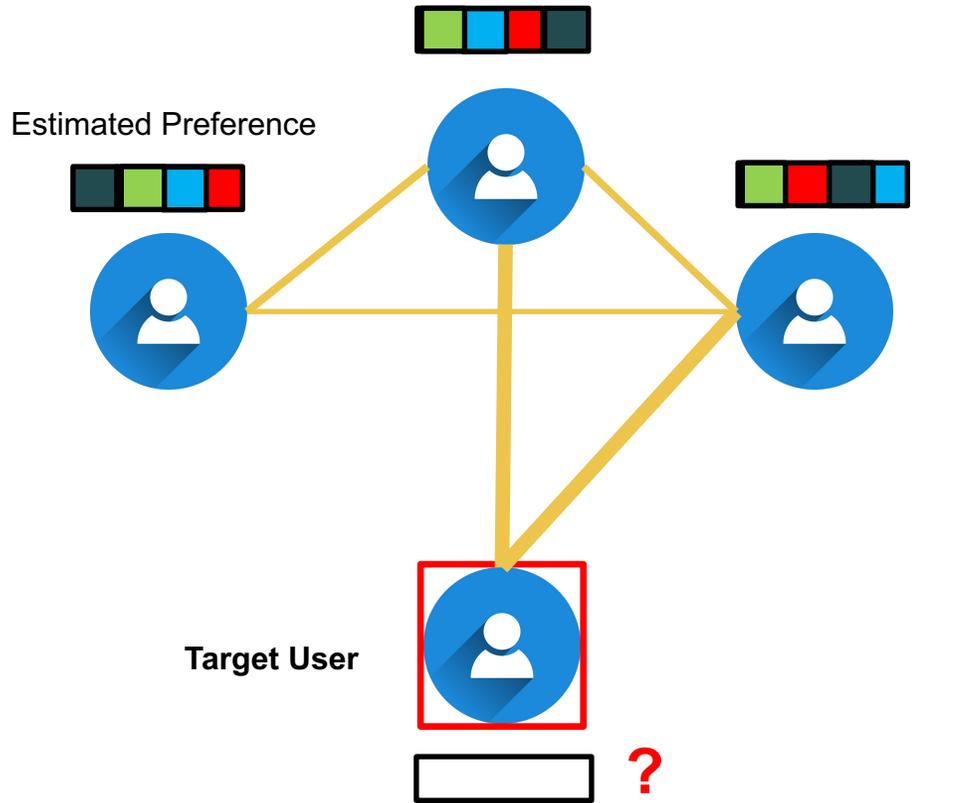
➤ Fine-grained user correlations:

- ❑ Heterogeneity of users is preserved.
- ❑ **Contribute differently** to serving user.



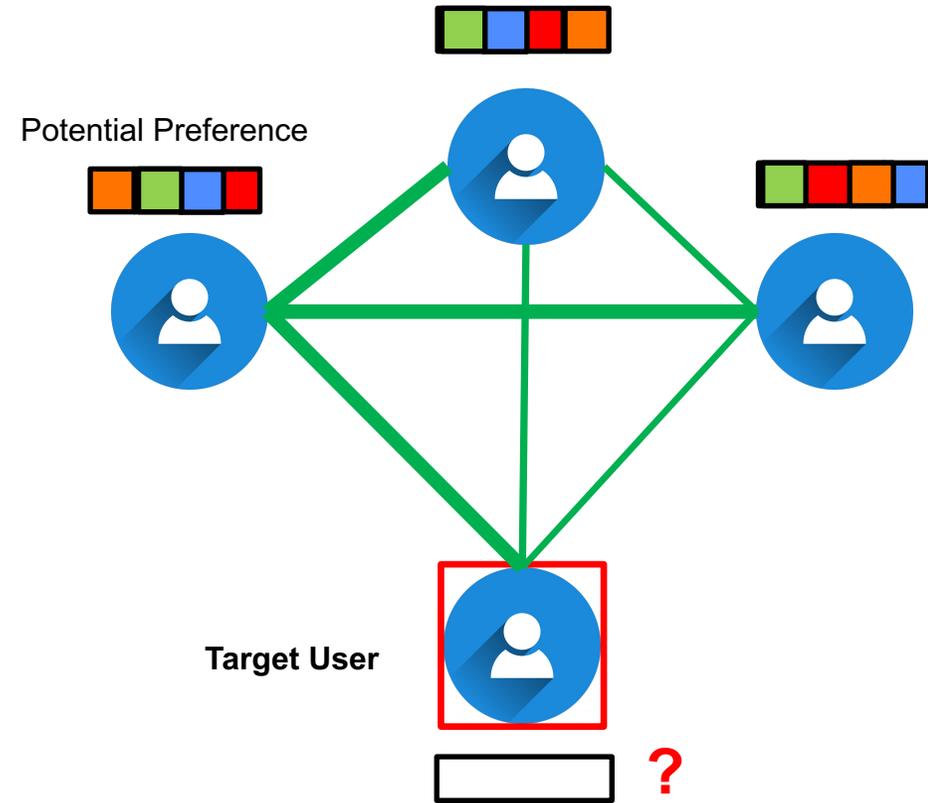
 User correlation with strength
(Unknown)

GNB: Exploitation and Exploration Graphs



User Exploitation Graph

— Correlation w.r.t. **Exploitation**



User Exploration Graph

— Correlation w.r.t. **Exploration**



➤ Definition: User Exploration Graph

□ For arm $x_{i,t}$, unknown user exploration graph

$$\mathcal{G}_{i,t}^{(2),*} = (\mathcal{U}, E, \underline{W_{i,t}^{(2),*}})$$

Set of edge weights

□ For users $u_1, u_2 \in \mathcal{U}$, the corresponding edge weight:

$$w_{i,t}^{(2),*}(u_1, u_2) = \underline{\psi^{(2)}} \left(\mathbb{E}[r_{i,t} | u_1, x_{i,t}] - f_{u_1}^{(1)}(x_{i,t}), \right.$$

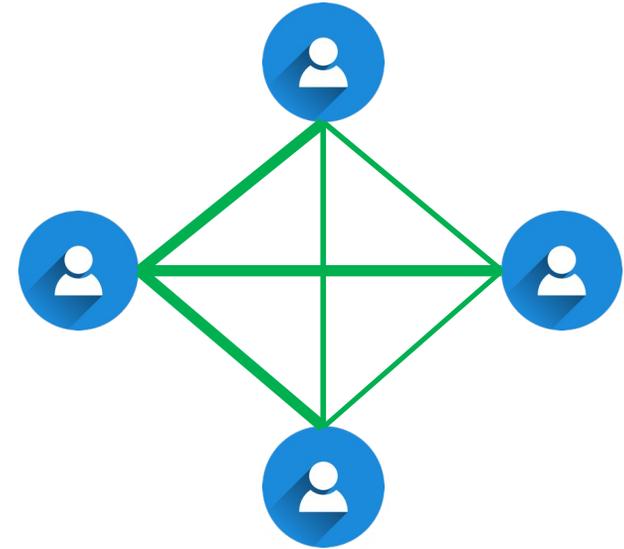
Pre-defined mapping

$$\left. \mathbb{E}[r_{i,t} | u_2, x_{i,t}] - f_{u_2}^{(1)}(x_{i,t}) \right)$$

Potential Gain

Potential Gain:

- $\mathbb{E}[r | u, x] - f_u^{(1)}(x)$
- Measures the **uncertainty** for the reward estimation



User correlations w.r.t. the Potential Gain
(Exploration Graph)

GNB: Problem Definition

- For each round $t \in [T]$:
 - ❑ Receive a target user $u_t \in \mathcal{U}$, and candidate arms \mathcal{X}_t .
 - $\mathcal{X}_t = \{x_{i,t} \in \mathbb{R}^d, \text{ (e.g., } \odot \text{)}\}_{i \in [a]}$
 - ❑ Reward $r_{i,t} = h(g_{i,t}^{(1),*}, u_t, x_{i,t}) + \epsilon_{i,t}$.
 - ❑ Learner **selects** arm $x_t \in \mathcal{X}_t$ as the recommendation.

- **Definition: User Correlation (Exploitation) Graph**
 - ❑ Given arm $x_{i,t}$, **unknown** user exploitation graph
 - $g_{i,t}^{(1),*} = (\mathcal{U}, E, W_{i,t}^{(1),*})$
 - $W_{i,t}^{(1),*}$: set of **edge weights**
 - ❑ For users $u_1, u_2 \in \mathcal{U}$, the corresponding **edge weight**:
 - $w_{i,t}^{(1),*}(u_1, u_2) = \Psi^{(1)}(\mathbb{E}[r_{i,t} | u_1, x_{i,t}], \mathbb{E}[r_{i,t} | u_2, x_{i,t}])$

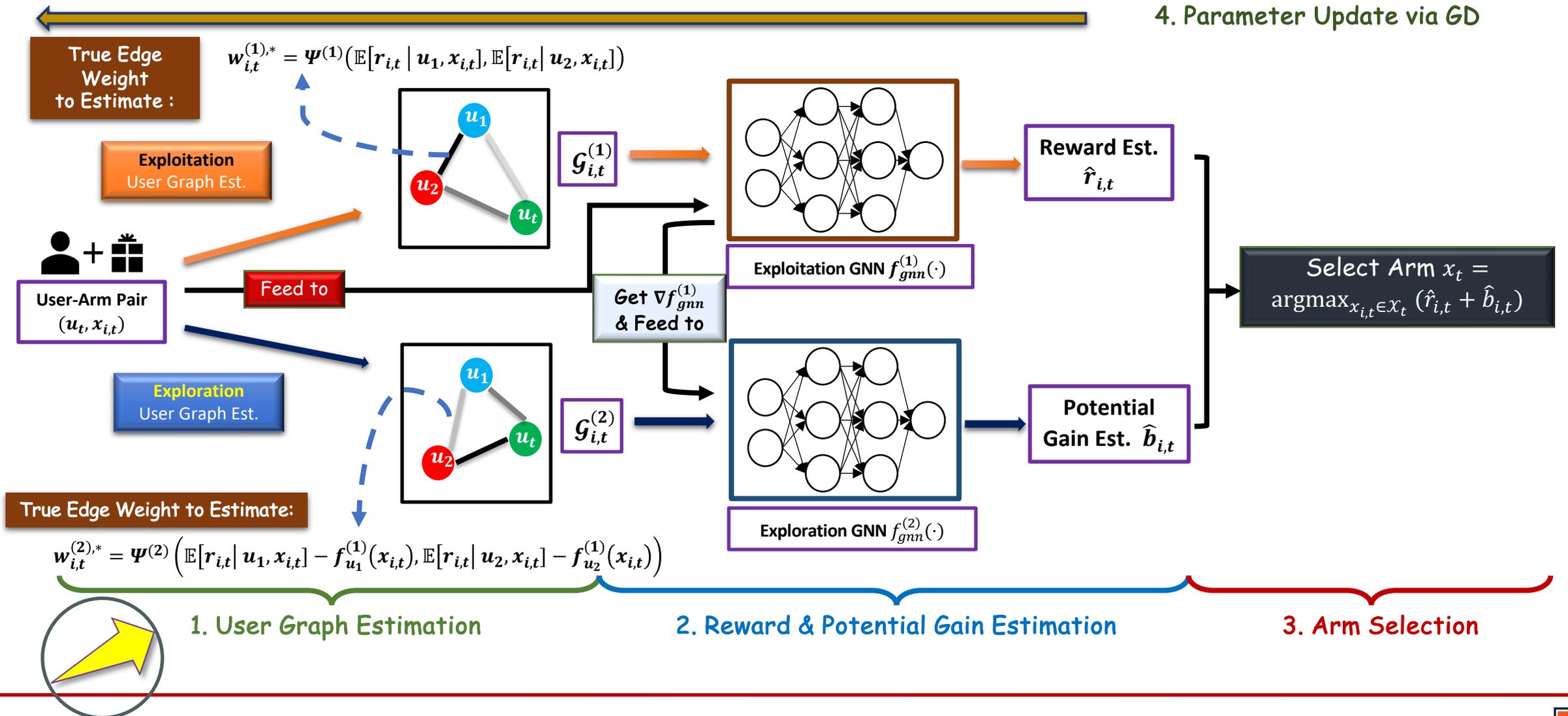
➤ Objective: Minimizing Pseudo Regret

$$R(T) = \sum_{t=1}^T \mathbb{E}[r_t^* - r_t]$$

/ Chosen arm reward
\ Optimal arm reward

$$\mathbb{E}[r_t^*] = \max_{i \in [a]} \mathbb{E}[r_{i,t}]$$

GNB: Framework Overview



User Exploitation Graph Estimation



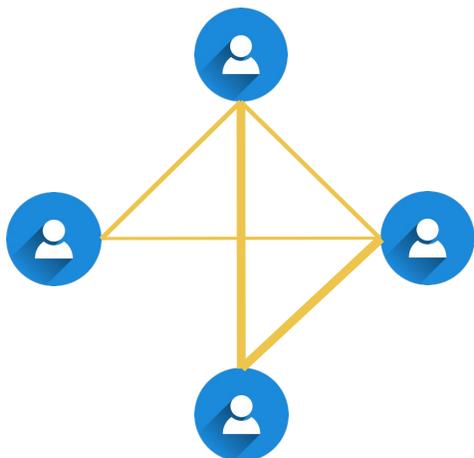
User Preference (expected reward) Estimation:

- Estimated by **user exploitation networks**

$$\{f_u^{(1)}\}_{u \in \mathcal{U}}$$

- Approximating $\mathbb{E}[r \mid \mathbf{u}, \mathbf{x}]$

- **Input:** \mathbf{x} **Label:** r



User correlations w.r.t. the **expected reward**
(**Exploitation Graph**)

➤ User **Exploitation Graph Estimation:**

- Given arm $\mathbf{x}_{i,t}$, **estimated** user exploitation graph

$$\mathcal{G}_{i,t}^{(1)} = (\mathcal{U}, E, W_{i,t}^{(1)})$$

- $W_{i,t}^{(1)}$: set of **estimated edge weights**

- For users $u_1, u_2 \in \mathcal{U}$, **estimated edge weight**

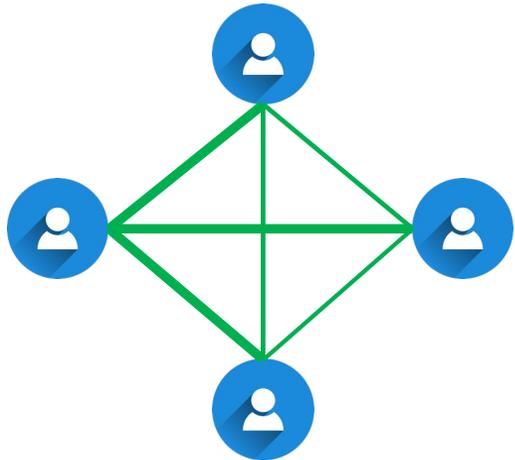
$$\circ w_{i,t}^{(1)}(u_1, u_2) = \underbrace{\Psi^{(1)}(f_{u_1}^{(1)}(\mathbf{x}_{i,t}), f_{u_2}^{(1)}(\mathbf{x}_{i,t}))}_{\text{Estimated User Preference}}$$

Estimated User Preference



Potential Gain:

- Estimated by user **exploration** networks $\{f_u^{(2)}\}_{u \in \mathcal{U}}$
 - **Input:** $\nabla f_u^{(1)}(\mathbf{x})$ -- the **gradients** of $f_u^{(1)}$.
 - **Label:** $r_u - f_u^{(1)}(\mathbf{x})$.



User correlations w.r.t. the Potential Gain
(**Exploration Graph**)

➤ User **Exploration Graph Estimation:**

- Given arm $x_{i,t}$, **estimated** user exploration graph

$$\mathcal{G}_{i,t}^{(2)} = (\mathcal{U}, E, \underline{W}_{i,t}^{(2)})$$

Edge weight **estimations**

- For users $u_1, u_2 \in \mathcal{U}$, **estimated** edge weight

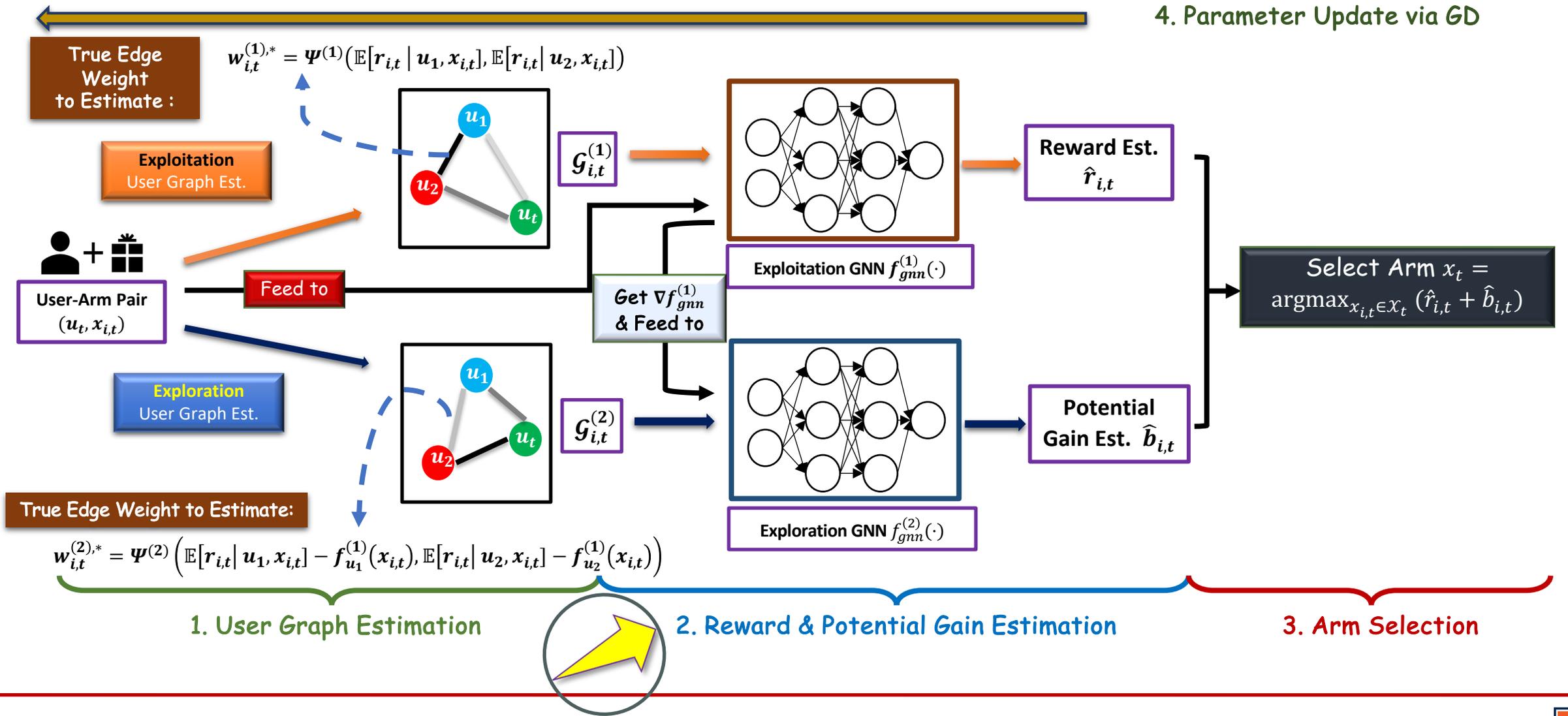
$$w_{i,t}^{(2)}(u_1, u_2) = \Psi^{(2)} \left(\underbrace{f_{u_1}^{(2)}(\nabla f_{u_1}^{(1)}(\mathbf{x}_{i,t})), f_{u_2}^{(2)}(\nabla f_{u_2}^{(1)}(\mathbf{x}_{i,t}))}_{\text{Estimated Potential Gain}} \right)$$

Estimated Potential Gain

1. Yunzhe Qi*, Yikun Ban*, and Jingrui He. Graph neural bandits. KDD 2023.

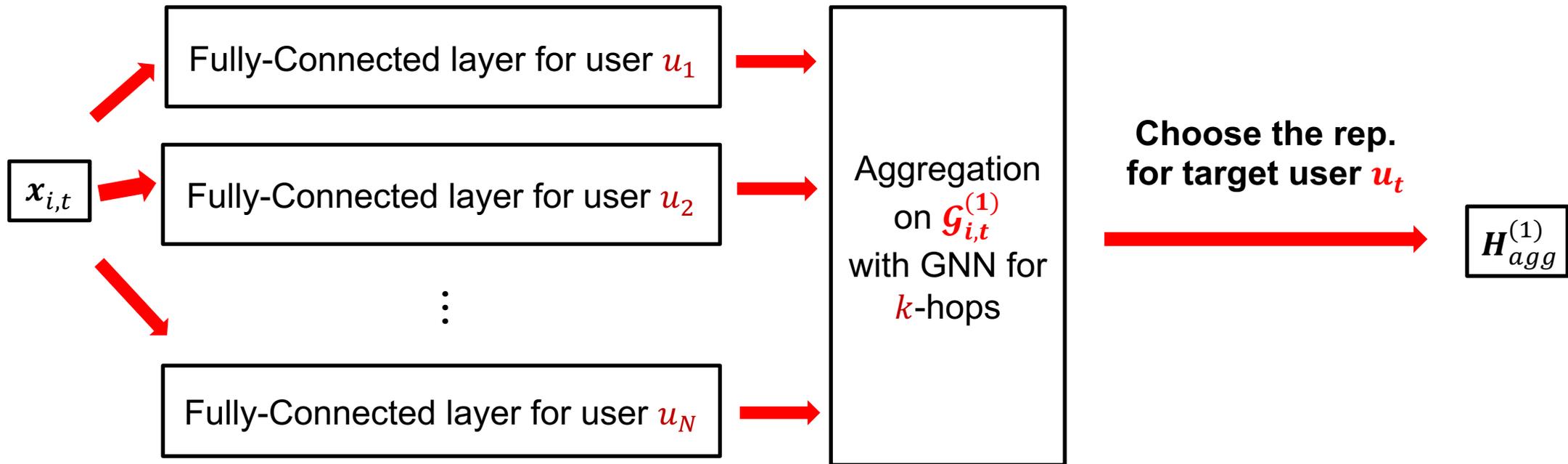
2. Yikun Ban, et al. EE-Net: Exploitation-Exploration Neural Networks in Contextual Bandits. In ICLR 2022.

GNB: Framework Overview



GNB: Aggregation on User Exploitation Graph

- For each arm $x_{i,t} \in \mathcal{X}_t$, reward estimation with estimated **user exploitation graph** $\mathcal{G}_{i,t}^{(1)}$.
- Given target user u_t , obtain **User-specific Arm Representation** H_{agg} :

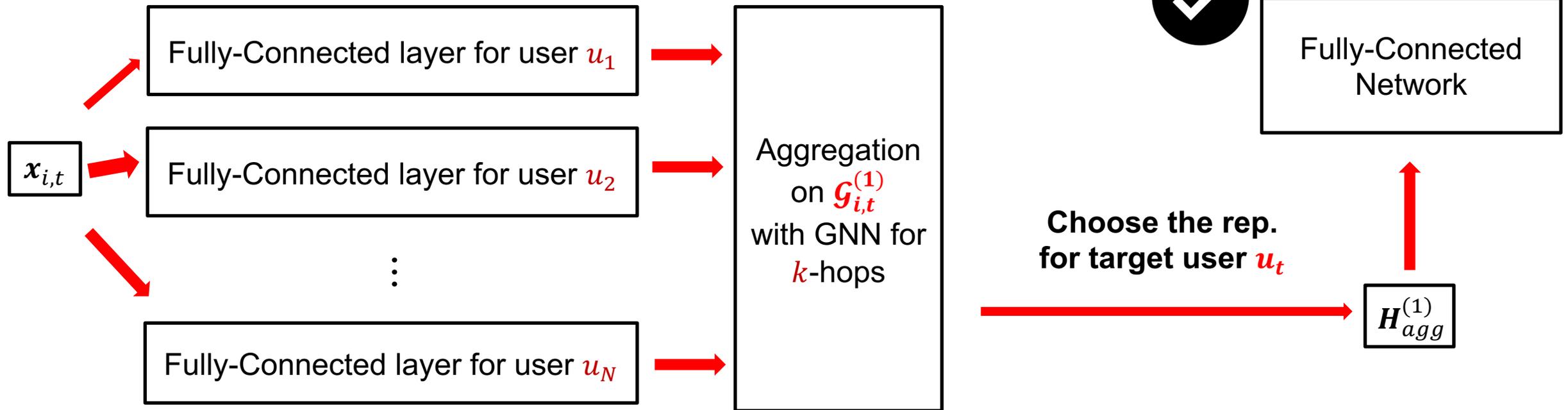


GNB: Arm Reward Estimation



- For each arm $x_{i,t} \in \mathcal{X}_t$, reward estimation with estimated user exploitation graph $\mathcal{G}_{i,t}^{(1)}$.
- Point reward estimation for each arm $x_{i,t} \in \mathcal{X}_t$:

$$\hat{r}_{i,t} = f_{gnn}^{(1)} \left(x_{i,t}, \mathcal{G}_{i,t}^{(1)}; [\Theta_{gnn}^{(1)}]_{t-1} \right)$$



GNB: Potential Gain Estimation



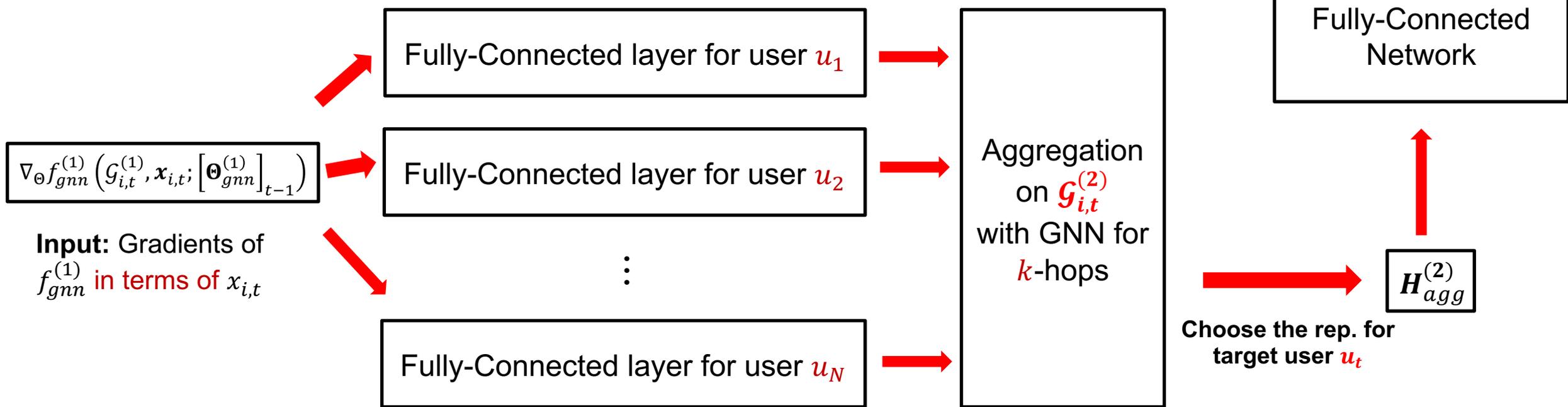
□ For each arm $x_{i,t} \in \mathcal{X}_t$, reward estimation with estimated **user exploration graph** $\mathcal{G}_{i,t}^{(2)}$.

➤ Potential gain estimation for each arm $x_{i,t} \in \mathcal{X}_t$:

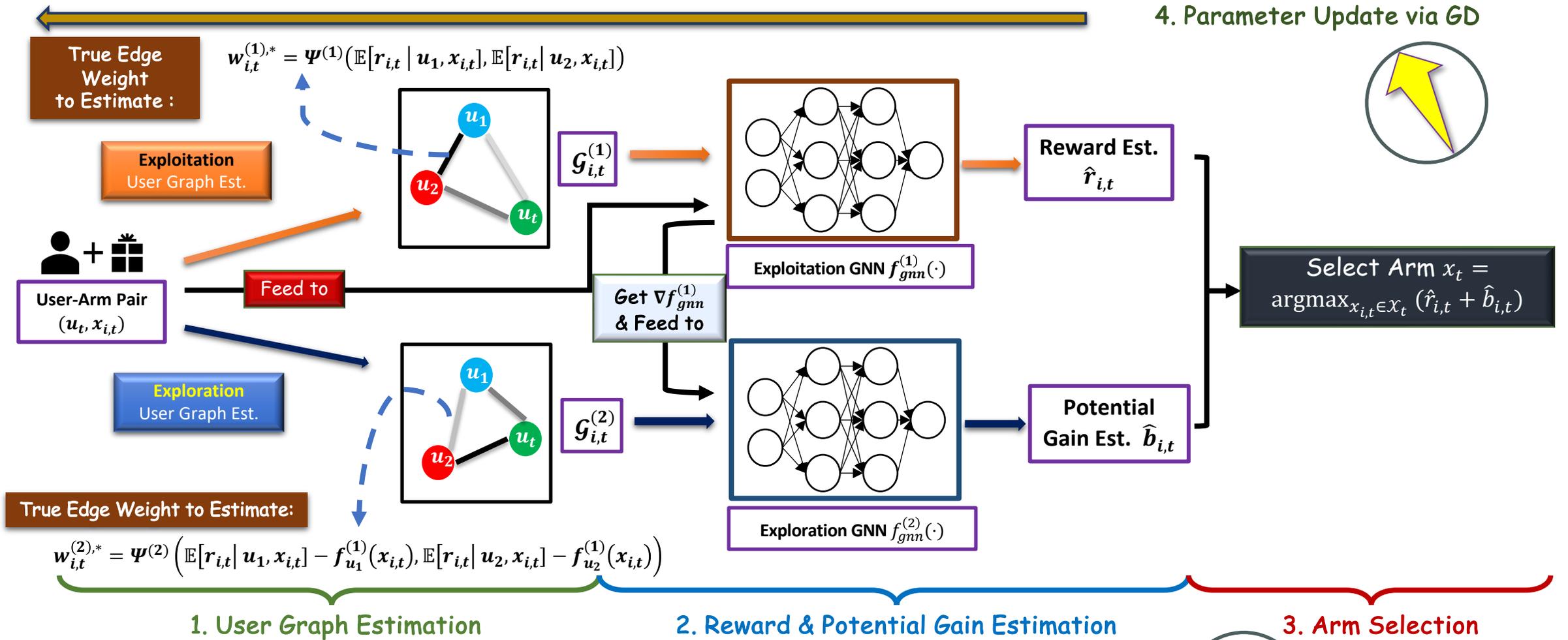


Estimated Potential Gain

$$\hat{b}_{i,t} = f_{gnn}^{(2)} \left(\nabla_{\Theta} f_{gnn}^{(1)}, \mathcal{G}_{i,t}^{(2)}; \left[\Theta_{gnn}^{(2)} \right]_{t-1} \right)$$



GNB: Framework Overview





GNN + User Exploitation Graph

GNN + User Exploration Graph

➤ Arm Selection Strategy:

❑ Select arm $x_t = \operatorname{argmax}_{x_{i,t} \in \mathcal{X}_t} (\hat{r}_{i,t} + \hat{b}_{i,t})$.

Estimated Reward

Estimated Potential Gain

❑ Receive the corresponding true reward r_t .

➤ Train the model parameters (User models + GNN models) with **Gradient Descent (GD)**.

➤ Update user graphs.





➤ **Pseudo regret for T rounds:**

$$R(T) = \sum_{t=1}^T \mathbb{E}[(r_t^* - r_t)]$$

➤ **Given sufficiently large network width m (over-parameterization), under mild assumptions, with the probability at least $1 - \delta$:**

$$R(T) \leq \sqrt{T} \cdot (O(L\xi_L) \cdot \sqrt{2 \log(\frac{Tn \cdot a}{\delta})}) + \sqrt{T} \cdot O(L) + O(\xi_L) + O(1).$$

where n is the number of users, a is the number of arms in each round, and T is the number of rounds.

Remarks:

- ❑ Achieves the regret bound of $\mathcal{O}(\sqrt{T \log(nT)})$.
 - Existing works with **user clustering** need $\mathcal{O}(\sqrt{nT \log(T)})$ for user collaboration modeling.
- ❑ Free of the terms d
 - d (arm context dimension, common in **linear bandit** works)

Experiments: Real Data Sets

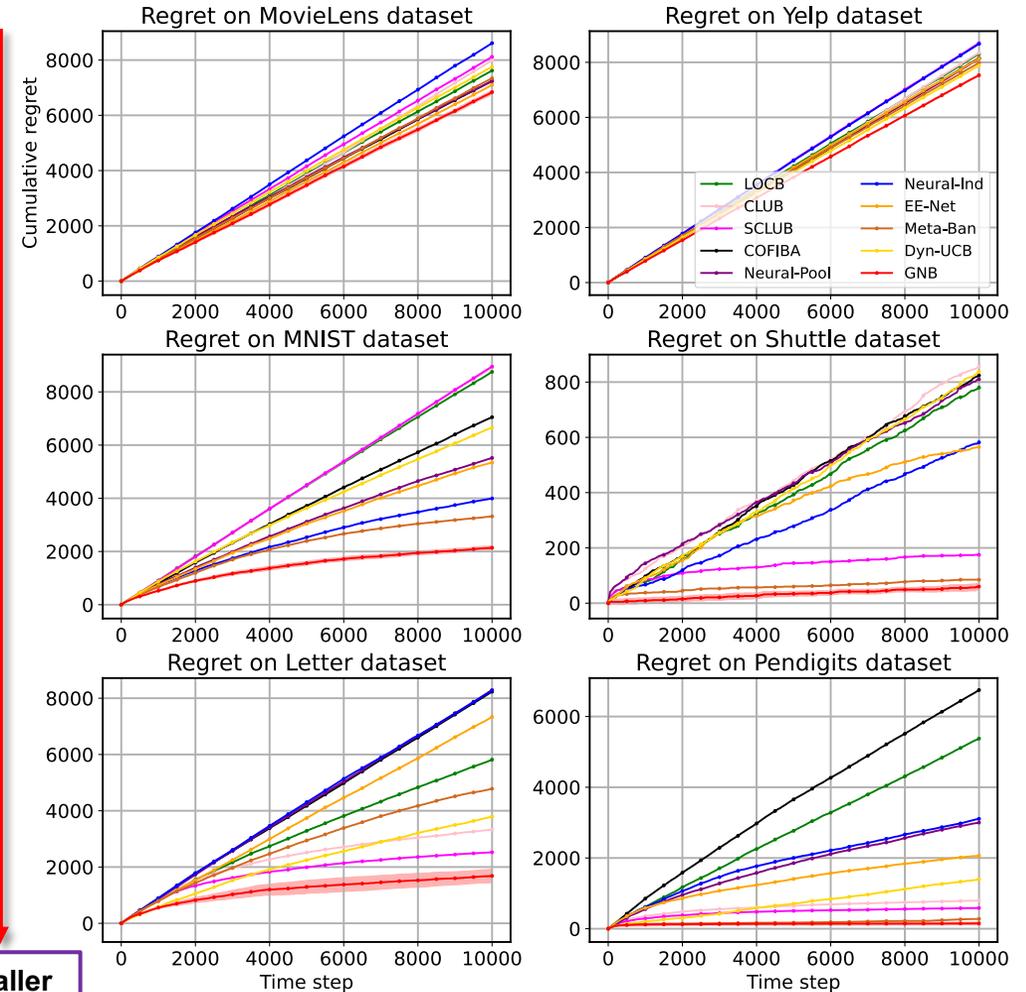


➤ Experiment settings:

- ❑ Under **online recommendation** settings, we evaluate the proposed GNB framework on **six** real data sets with different specifications.
- ❑ We include **nine** state-of-the-art related algorithms as the baselines, including both linear and neural algorithms.

➤ Summary of experiment results:

- ❑ **Neural algorithms** generally perform better than **linear ones**, with the representation power of neural networks.
- ❑ GNB can generally achieve the **best performance** against the strong baselines.



Smaller
= Better



An icon representing an introduction or overview, showing various shopping-related items like a shopping cart, a red shopping bag, a credit card, and a laptop, connected by lines on a grid background.

Introduction

- Background & Motivations
- Challenges

An icon representing online clustering, showing a network of people's faces connected by lines, symbolizing social networks or data clusters.

Online Clustering of Bandits

- Clustering of Linear Bandits
- Clustering of Neural Bandits

An icon representing graph-based learning, showing a network of nodes with social media logos like LinkedIn, Instagram, and Twitter, connected by lines.

Graph Bandit Learning with Collaboration

- User side: Graph Neural Bandits
- Arm side: Neural Bandit with Arm Group Graph
- Other Scenarios: Bandit Learning with Graph Feedback & Online Graph Classification with Neural Bandit

An icon representing data analysis and recommendation, showing a laptop screen with a bar chart, a magnifying glass over a document, and a calculator.

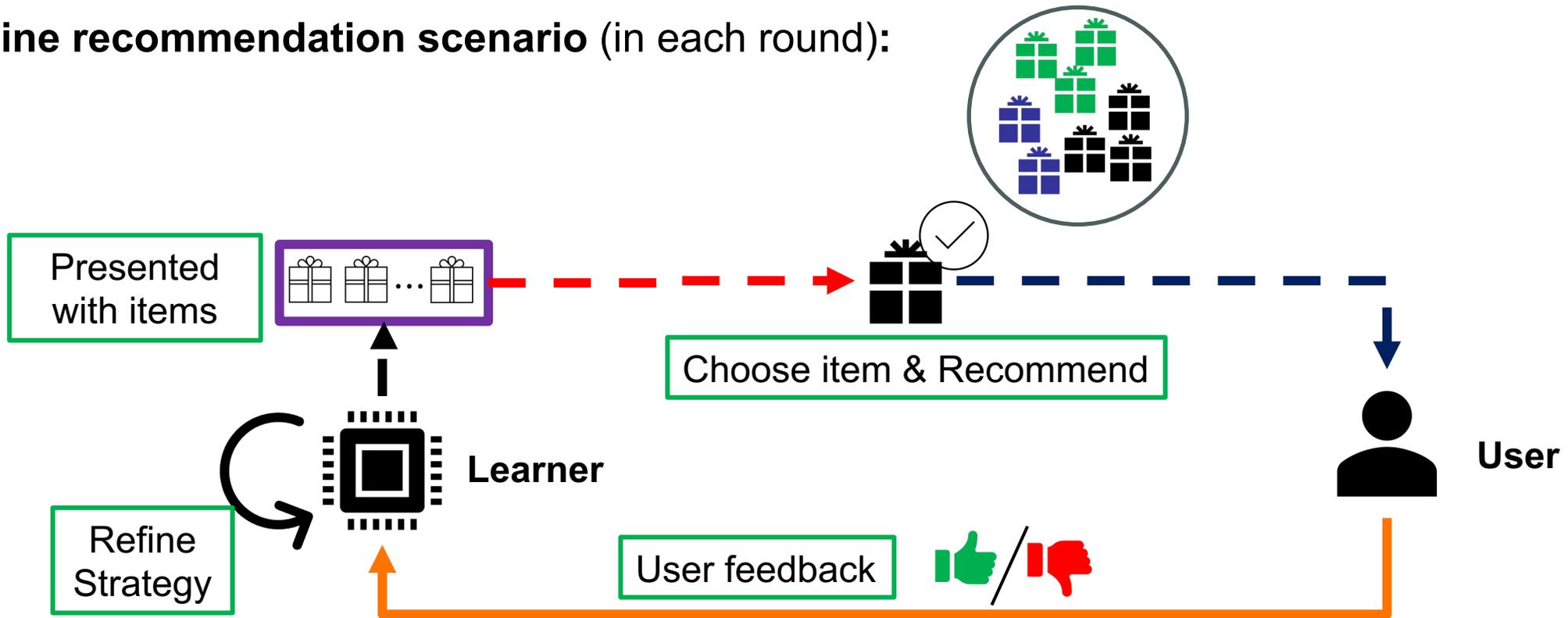
Bandits for Combo Recommendation

- Multi-facet Contextual Bandits

Online Recommendation with Arm Group Information



- Online recommendation scenario (in each round):



Leverage the **available arm group information** can help improve recommendation quality.



➤ The **group (category) information** for arms (items) is commonly accessible:

❑ **Media contents:**

- Music, Movies (grouped by **genres**)

❑ **Text contents:**

- Articles (grouped by **literary styles**)

❑ **E-commerce:**

- Restaurants (grouped by **cuisine types**)

❑ Etc.

No existing **MAB** method trying to directly leverage the **available arm group information**.



Formal Problem Definition

- **Arm Groups:**
 - Assume a fixed pool \mathcal{C} of $|\mathcal{C}| = N_c$ **arm groups**.
 - Each **arm group** $c \in \mathcal{C}$ (e.g., movie genre) relates to an arm distribution \mathcal{D}_c .
- **For each round $t \in [T]$:**
 - Receive a set of arms \mathcal{X}_t , and the corresponding set of **arm groups** $\mathcal{C}_t \subseteq \mathcal{C}$.
 - $\mathcal{X}_t = \left\{ \mathbf{x}_{c,t}^{(i)} \in \mathbb{R}^{d_x}, \text{ (e.g., } \begin{matrix} \text{[]} \\ \text{[]} \\ \text{[]} \end{matrix} \text{)} \right\}_{c \in \mathcal{C}_t, i \in [n_{c,t}]}$
 - $\mathbf{x}_{c,t}^{(i)} \sim \mathcal{D}_c$
 - Reward $r_{c,t}^{(i)} = h(W^*, \mathbf{x}_{c,t}^{(i)}) + \epsilon_{c,t}^{(i)}$.
 - Unknown affinity matrix for arm groups:
 $W^* \in \mathbb{R}^{N_c \times N_c}$
 - Learner **chooses** arm $x_t \in \mathcal{X}_t$.

➤ Objective: Minimizing Pseudo Regret

$$\begin{aligned}
 R(T) &= \sum_{t=1}^T \mathbb{E}[(r_t^* - r_t)] \\
 &= \sum_{t=1}^T \underbrace{|h(W^*, \mathbf{x}_t^*)|}_{\text{Optimal arm}} - \underbrace{|h(W^*, \mathbf{x}_t)|}_{\text{Chosen arm}}
 \end{aligned}$$



Modeling with Arm Group Graph (AGG)

➤ Apply Arm Group Graph (AGG) to model **arm group correlations**:

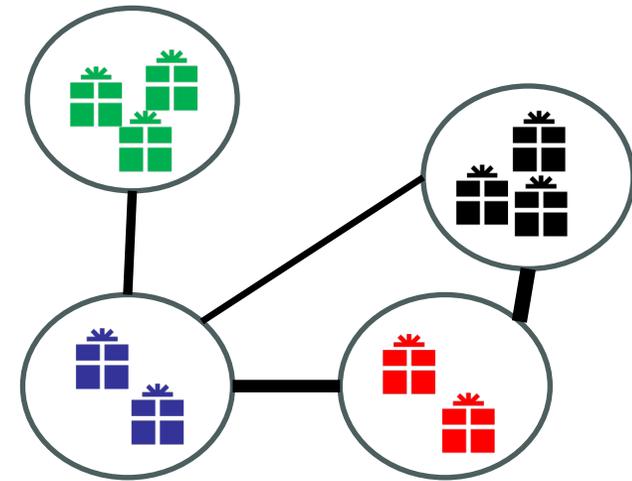
➤ In round $t \in [T]$:

- Undirected graph $\mathcal{G}_t = (V, E, W_t)$
 - V : set of nodes
 - **Each node is an arm group** $c \in \mathcal{C}$, N_c nodes in total
 - $E = \{e(c, c')\}_{c, c' \in \mathcal{C}}$: set of edges
 - W_t : Set of **edge weights**

- **Arm group correlations** are modeled by the edge weights from set W_t .

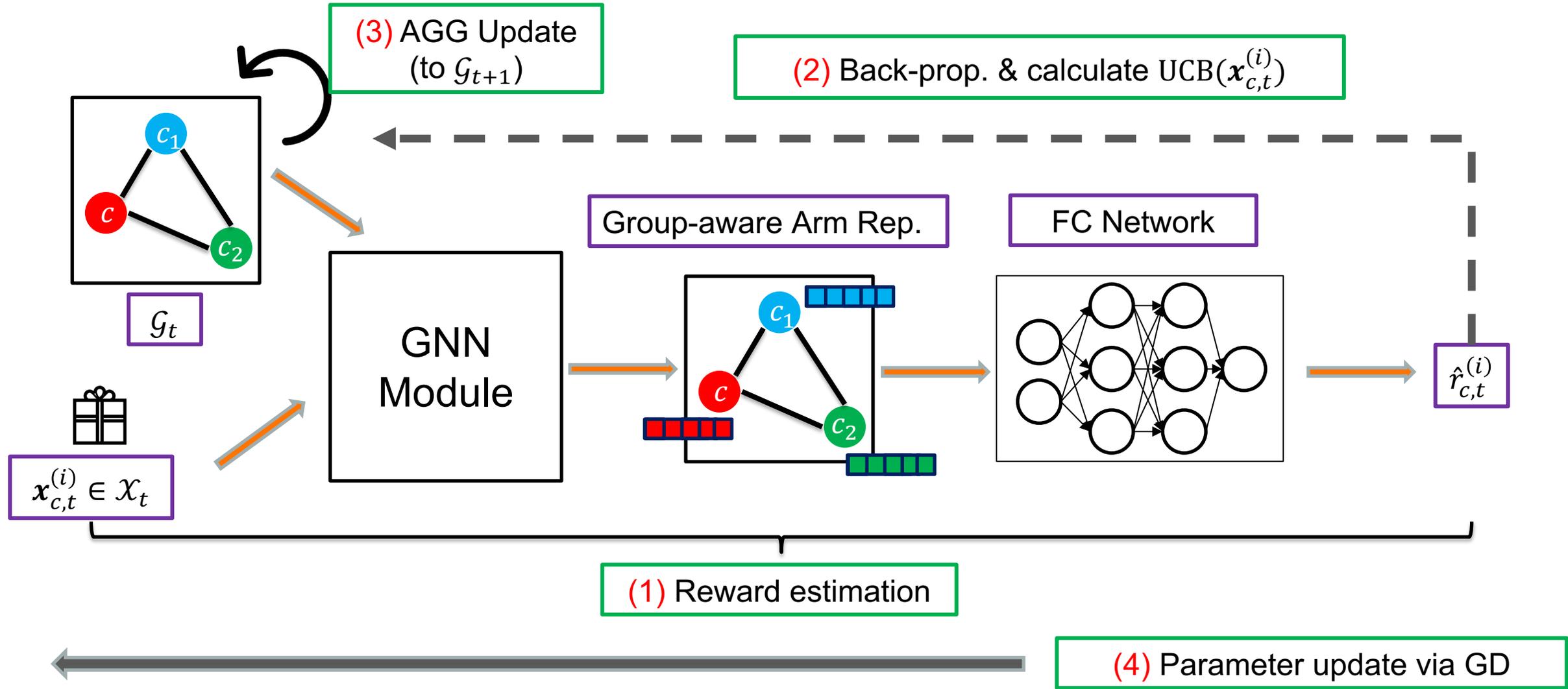
➤ True reward: $r_{c,t}^{(i)} = h(\mathcal{G}^*, x_{c,t}^{(i)}) + \epsilon_{c,t}^{(i)}$.

- **Unknown true graph:** \mathcal{G}^*
- **Unknown affinity matrix:** $W^* \in \mathbb{R}^{N_c \times N_c}$



Arm Group Graph

Proposed Framework: AGG-UCB





- **Recall for Arm Groups:**

- Assume a fix pool \mathcal{C} of $|\mathcal{C}| = N_c$ arm groups.
- Each group $c \in \mathcal{C}$ has a context distribution \mathcal{D}_c .

- **Definition: True edge weights**

□ For $c, c' \in \mathcal{C}$, **true** edge weight in \mathcal{G}^* :

- $w^*(c, c') = \exp\left(\frac{-\left\|\mathbb{E}_{x \sim \mathcal{D}_c}[\phi(x)] - \mathbb{E}_{x' \sim \mathcal{D}_{c'}}[\phi(x')]\right\|^2}{\sigma_s}\right)$

- $\phi(\cdot)$: kernel mapping function

- **Arm Group Graph estimation:**

□ Estimated edge weight in round $t \in [T]$:

- $w_t(c, c') = \exp\left(\frac{-\|\Psi_t(\mathcal{D}_c) - \Psi_t(\mathcal{D}_{c'})\|^2}{\sigma_s}\right)$

- **Kernel Mean Embedding** ^[1]: $\Psi_t(\mathcal{D}_c)$

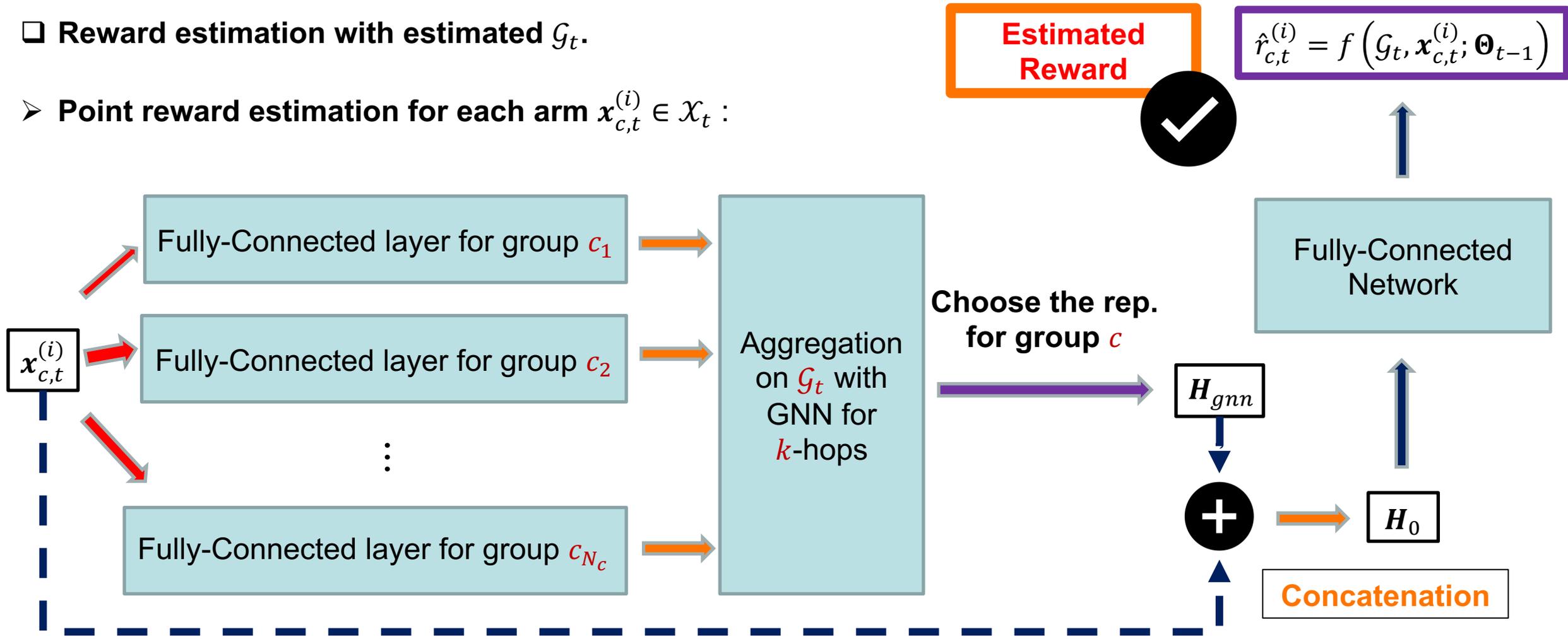
□ $w_t(c, c') \in W_t$: **weight** for edge $e(c, c') \in E$ in graph \mathcal{G}_t



AGG-UCB: Arm Reward Estimation

□ Reward estimation with estimated \mathcal{G}_t .

➤ Point reward estimation for each arm $x_{c,t}^{(i)} \in \mathcal{X}_t$:





➤ **Exploration** with Upper Confidence Bound (UCB):

□ The **UCB**(·) satisfies :

$$\mathbb{P} \left(\left| \underbrace{f \left(\mathcal{G}_t, \mathbf{x}_{c,t}^{(i)}; \Theta_{t-1} \right)}_{\text{Reward Est.}} - \underbrace{h \left(\mathcal{G}^*, \mathbf{x}_{c,t}^{(i)} \right)}_{\text{Exp. Reward}} \right| > \mathbf{UCB} \left(\mathbf{x}_{c,t}^{(i)} \right) \right) \leq \delta$$

➤ **Arm Selection Strategy**:

□ Select arm $\mathbf{x}_t = \operatorname{argmax}_{\mathbf{x}_{c,t}^{(i)} \in \mathcal{X}_t} \left(\hat{r}_{c,t}^{(i)} + \gamma \cdot \mathbf{UCB} \left(\mathbf{x}_{c,t}^{(i)} \right) \right)$

□ Receive the corresponding **true reward** r_t



Theoretical and Empirical Results

□ **Theoretical:** Given **sufficiently large network width** m , with the probability at least $1 - \delta$:

$$R(T) \leq 2 \cdot (2B_4\sqrt{T} + 2 - B_4) + 2\sqrt{2\tilde{d}T \log(1 + T/\lambda)} + 2T \cdot (\sqrt{\lambda}S + \sqrt{1 - 2\log(\delta/2)} + (\tilde{d} \log(1 + T/\lambda)))$$

Achieves the regret bound of $\mathcal{O}(\tilde{d}\sqrt{T\log^2(T)} \cdot \log(N_c))$

□ **Empirical:** Leveraging arm group information with **AGG-UCB** can improve good performances.

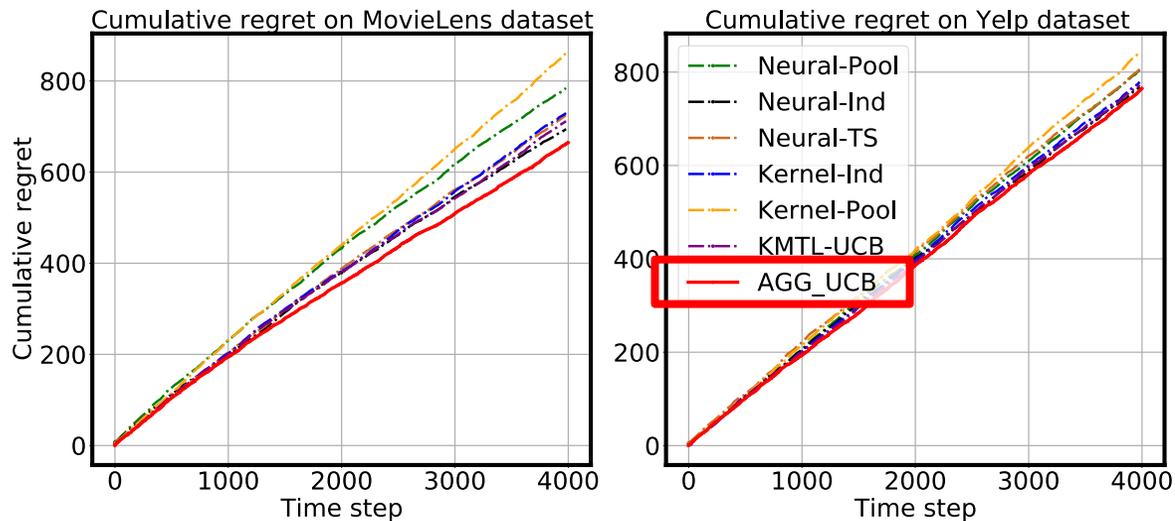


Figure 1: Cumulative regrets on recommendation data sets

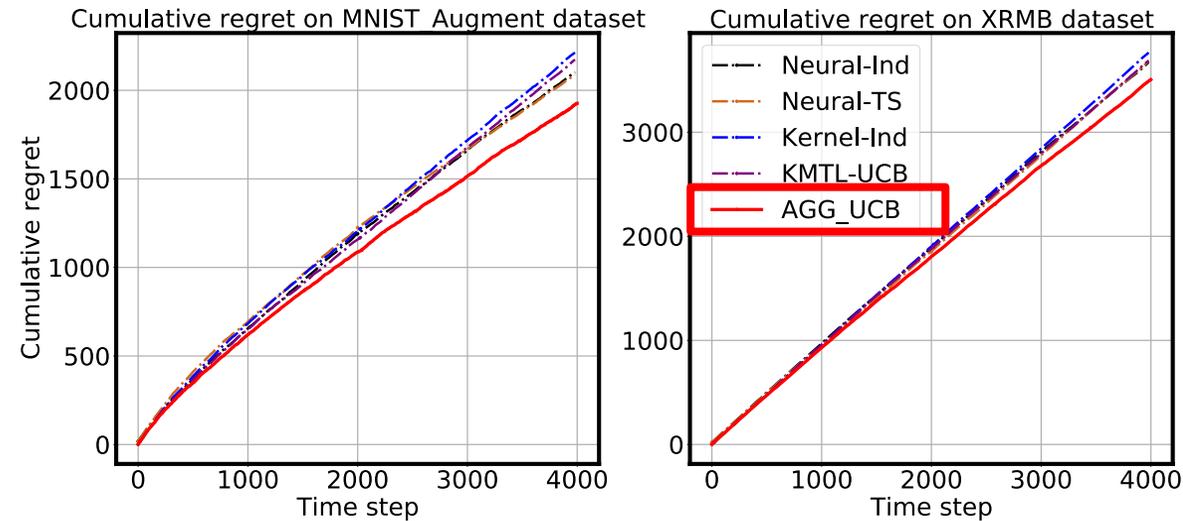


Figure 2: Cumulative regrets on Classification data sets



1. Bandit Learning with Graph Feedback [1]:

- ❑ Arms are nodes on a graph $G = (V, E)$. In each round $t \in [T]$, the learner chooses one node $I_t \in V$.
- ❑ Learner observes **reward for chosen arm** I_t , and **neighbor rewards** (e.g., out-neighbors in a directed graph).
- ❑ **Objective**: minimizing the cumulative pseudo regret over T rounds.

2. Optimal Graph Search with Bandit [2]:

- ❑ In each round $t \in [T]$, the learner aims to choose **one graph** $G_t \in \mathcal{G}$, from a **fixed** graph domain \mathcal{G} .
Reward generated by $r_t = h(G_t) + \epsilon_t$.
- ❑ **Objective**: minimizing the cumulative pseudo regret over T rounds.
- ❑ **Application example**: material designing, drug search.





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Bandits for Combo Recommendation

- Multi-facet Contextual Bandits

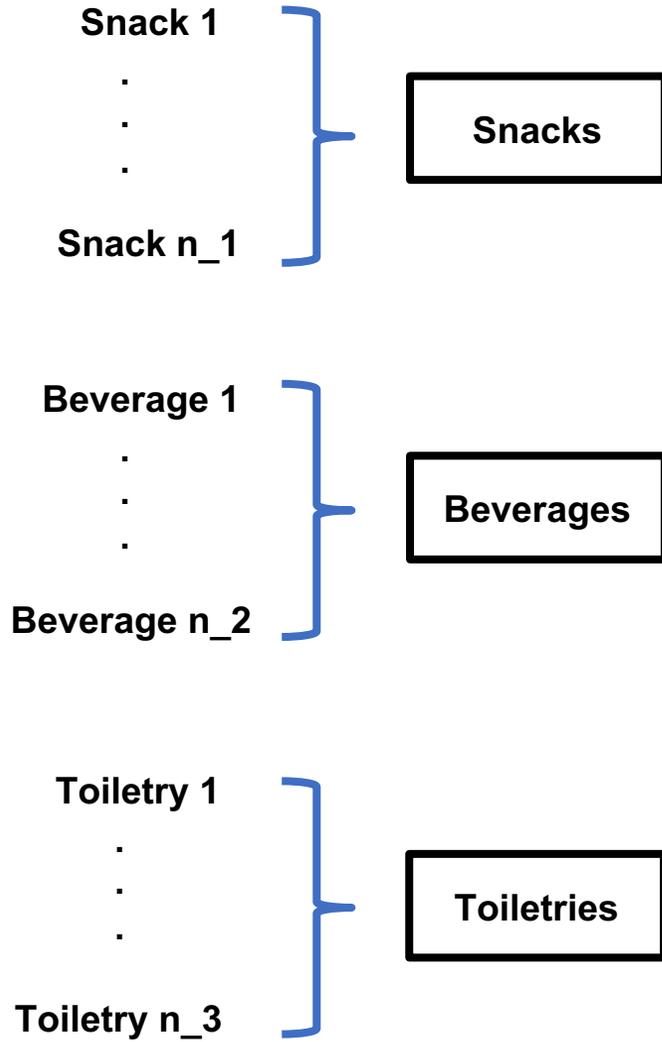


Motivated Case: Promotion Campaign

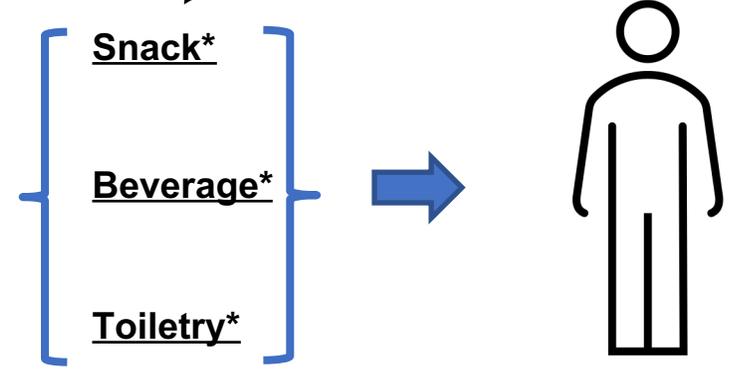


E-commerce

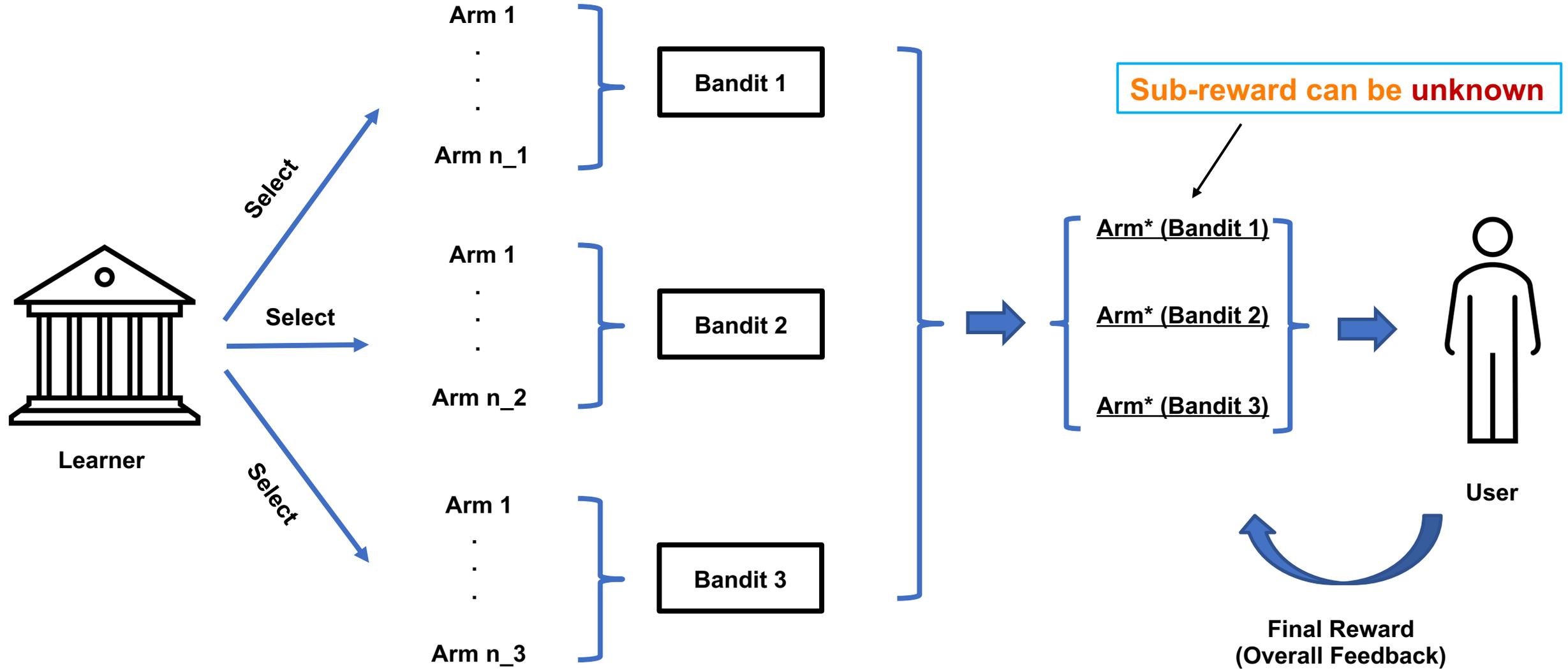
Which to pick?



Sub-reward can be unknown



Application: Multi-facet Recommendation with Neural Bandits



Formal Definition of Multi-facet Contextual Bandit : In Round t



- **Sub-reward Functions** (unknown):

$$r_t^1 = h_1(x_t^1) \quad (\text{Linear or Non-linear})$$

$$r_t^2 = h_2(x_t^2)$$

⋮

$$r_t^K = h_K(x_t^K)$$

Assumption1: $h_k(0) = 0, \forall k$

- **Final Reward Function** (unknown):

$$R_t = H(r_t^1, r_t^2, \dots, r_t^K) + \boxed{\epsilon_t} \quad \leftarrow \text{Noise}$$

Expectation: $H(X_t) = E[R_t | X_t] = H(r_t^1, r_t^2, \dots, r_t^K)$

Assumption2: H is \bar{C} - Lipschitz continuous.

- **Evaluation Measure: Regret**

$$\begin{aligned} \text{Reg} &= E \left[\sum_t (R_t^* - R_t) \right] \\ &= \sum_t [\underbrace{H(X_t^*)}_{\text{Optimal Final Reward}} - \underbrace{H(X_t)}_{\text{Received Final Reward}}] \end{aligned}$$

Optimal Final Reward

Received Final Reward

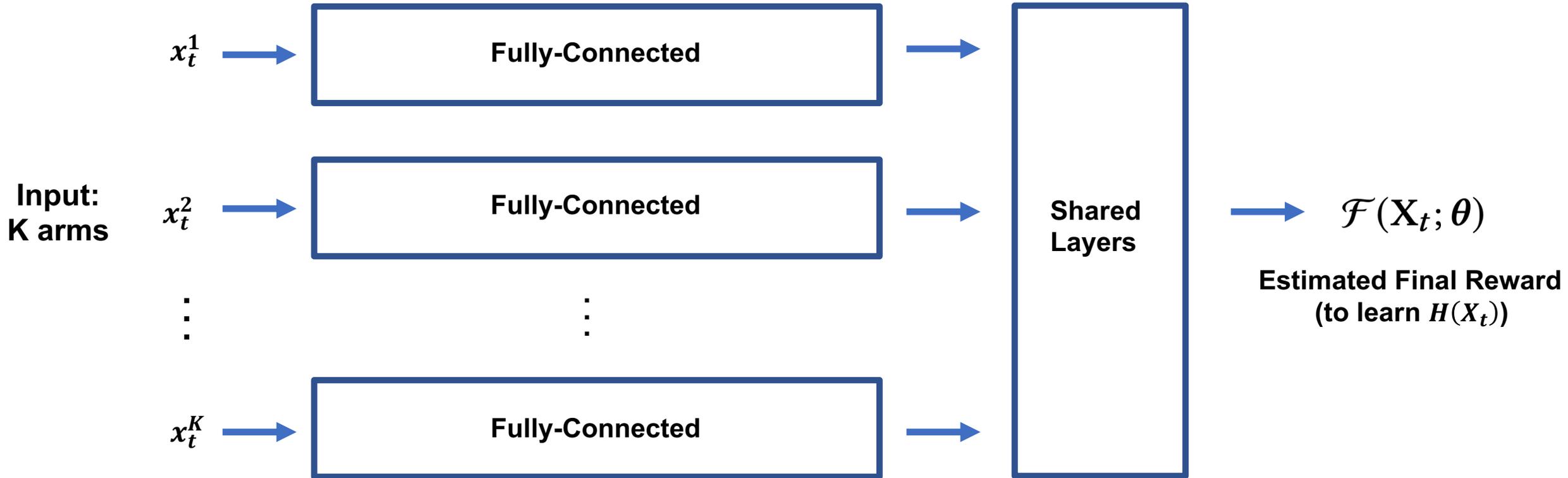
- **Goal: Minimize the regret of T rounds.**



MuFasa: Exploitation (Neural Network Model)



As all bandits serve the same user





➤ **UCB:** $\mathbb{P} (|\mathcal{F}(\mathbf{X}_t; \boldsymbol{\theta}_t) - \mathcal{H}(\mathbf{X}_t)| > \text{UCB}(\mathbf{X}_t)) \leq \delta,$

➤ **K selected arms are determined by:**

$$\mathbf{X}_t = \arg \max_{\mathbf{X}'_t \in \mathcal{S}_t} (\mathcal{F}(\mathbf{X}'_t; \boldsymbol{\theta}_t) + \text{UCB}(\mathbf{X}'_t)).$$

Where

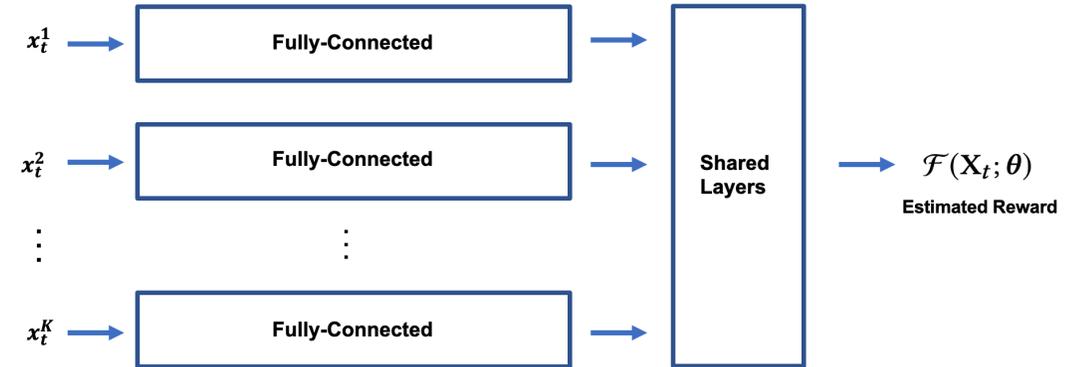
$$\mathcal{S}_t = \{(\mathbf{x}_t^1, \dots, \mathbf{x}_t^k, \dots, \mathbf{x}_t^K) \mid \mathbf{x}_t^k \in \mathbf{X}_t^k, k \in [K]\},$$

(all possible combinations of K arms)

MuFasa: Novel Upper Confidence Bound (UCB)



➤ With the assembled neural framework (MuFasa):



➤ With probability at least $1 - \delta$, the UCB holds

$$|\mathcal{F}(\mathbf{X}_t; \boldsymbol{\theta}_t) - \mathcal{H}(\mathbf{X}_t)| \leq \bar{C} \sum_{k=1}^K \mathcal{B}^k + \mathcal{B}^F = \text{UCB}(\mathbf{X}_t), \text{ where}$$

$$\mathcal{B}^k = \gamma_1 \|g_k(\mathbf{x}_t^k; \boldsymbol{\theta}_t^k) / \sqrt{m_1}\|_{\mathbf{A}_t^{k-1}} + \gamma_2 \left(\frac{\delta}{k+1}\right) \|g_k(\mathbf{x}_t^k; \boldsymbol{\theta}_0^k) / \sqrt{m_1}\|_{\mathbf{A}_t^{k'-1}} + \gamma_1 \gamma_3 + \gamma_4$$

Error of facet-specific networks

$$\mathcal{B}^F = \gamma_1 \|G(\mathbf{f}_t; \boldsymbol{\theta}_t^\Sigma) / \sqrt{m_2}\|_{\mathbf{A}_t^{F-1}} + \gamma_2 \left(\frac{\delta}{k+1}\right) \|G(\mathbf{f}_t; \boldsymbol{\theta}_0^\Sigma) / \sqrt{m_2}\|_{\mathbf{A}_t^{F'-1}} + \gamma_1 \gamma_3 + \gamma_4$$

Error of shared network



$$\begin{aligned} \text{Reg} &= E \left[\sum_t (R_t^* - R_t) \right] \\ &= \sum_t [H(\mathbf{X}_t^*) - H(\mathbf{X}_t)] \end{aligned}$$

- After T rounds, with probability at least $1 - \delta$,

$$\begin{aligned} \text{Reg} &\leq (\bar{C}K + 1) \sqrt{T} 2 \sqrt{\tilde{P} \log(1 + T/\lambda) + 1/\lambda + 1} \\ &\quad \cdot \left(\sqrt{(\tilde{P} - 2) \log \left(\frac{(\lambda + T)(1 + K)}{\lambda \delta} \right)} + 1/\lambda + \lambda^{1/2} S + 2 \right) + 2(\bar{C}K + 1), \end{aligned}$$

- Achieve near-optimal regret bound $\tilde{O}((K + 1)\sqrt{T})$, same as a single linear bandit $\tilde{O}(\sqrt{T})$



All Sub-rewards Available (Different Final Reward Function)

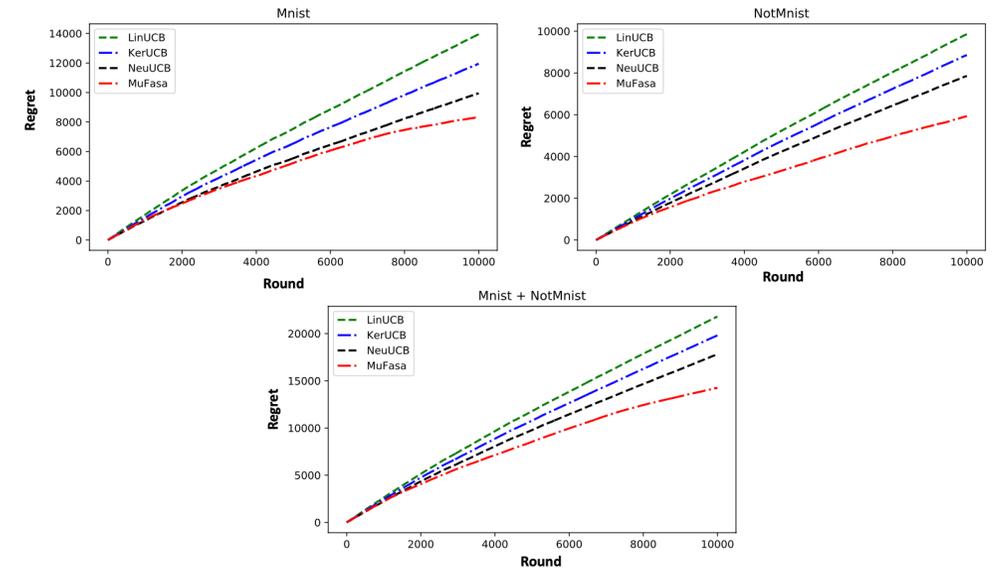
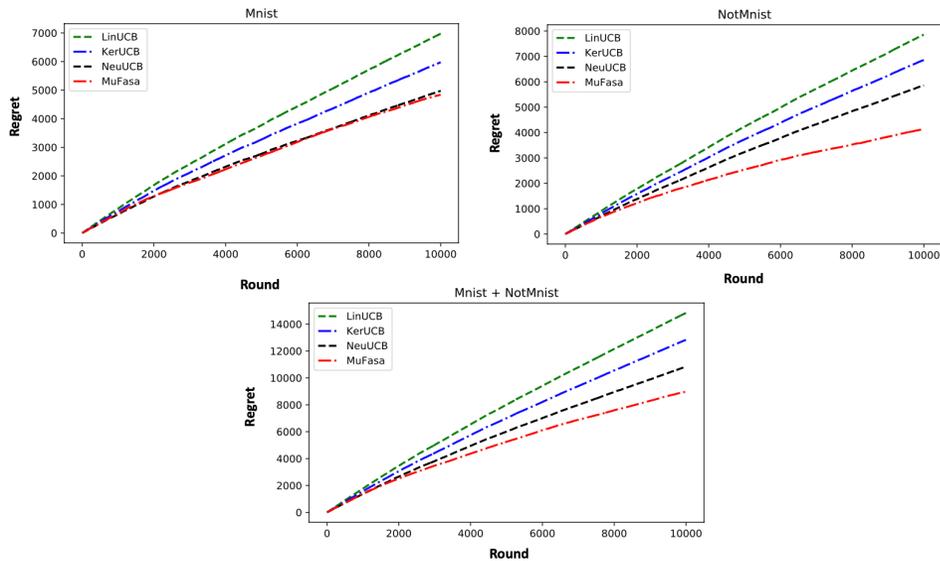


Figure: Regret comparison on Mnist+NotMnist with H_1 .

$$H_1(\text{vec}(\mathbf{r}_t)) = r_t^1 + r_t^2$$

Observation:

- Superiority of MuFasa is slightly higher on H_2 , compared to H_1 .

Figure: Regret comparison on Mnist+NotMnist with H_2 .

$$H_2(\text{vec}(\mathbf{r}_t)) = 2r_t^1 + r_t^2.$$

Insights:

- MuFasa can select arms according to different weights of bandits (Bandit 1 has higher weight in H_2).



Partial Sub-rewards Available

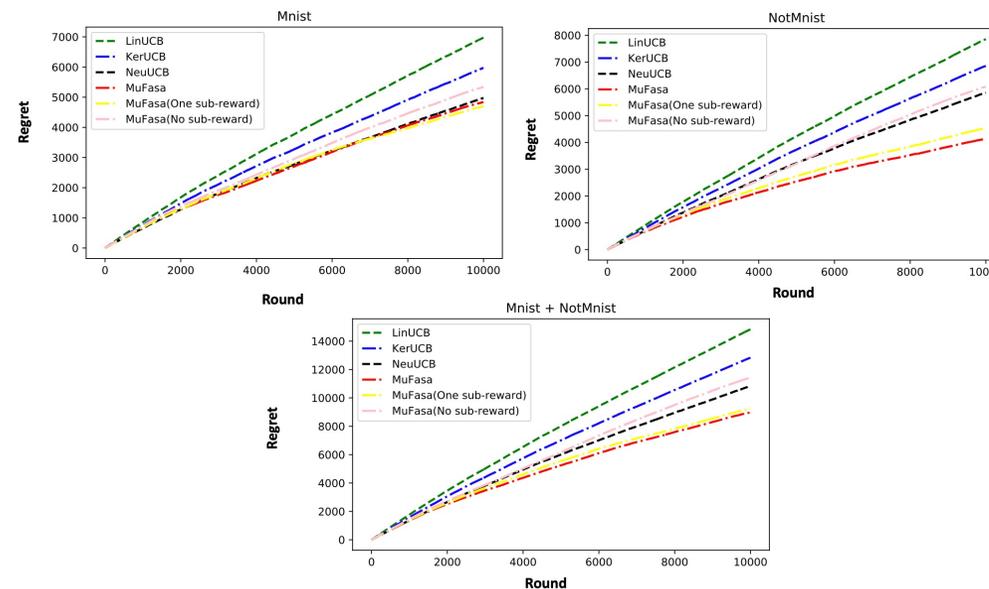
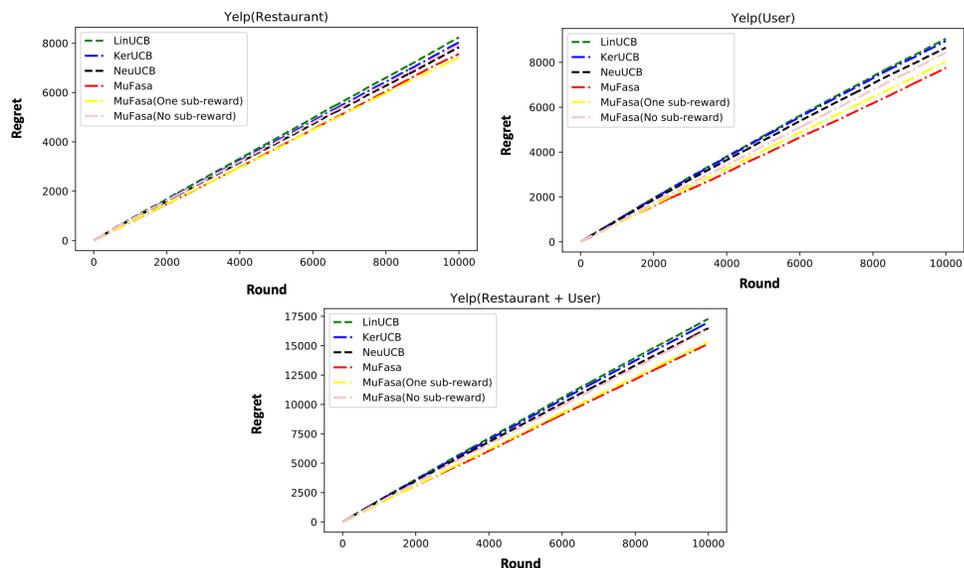


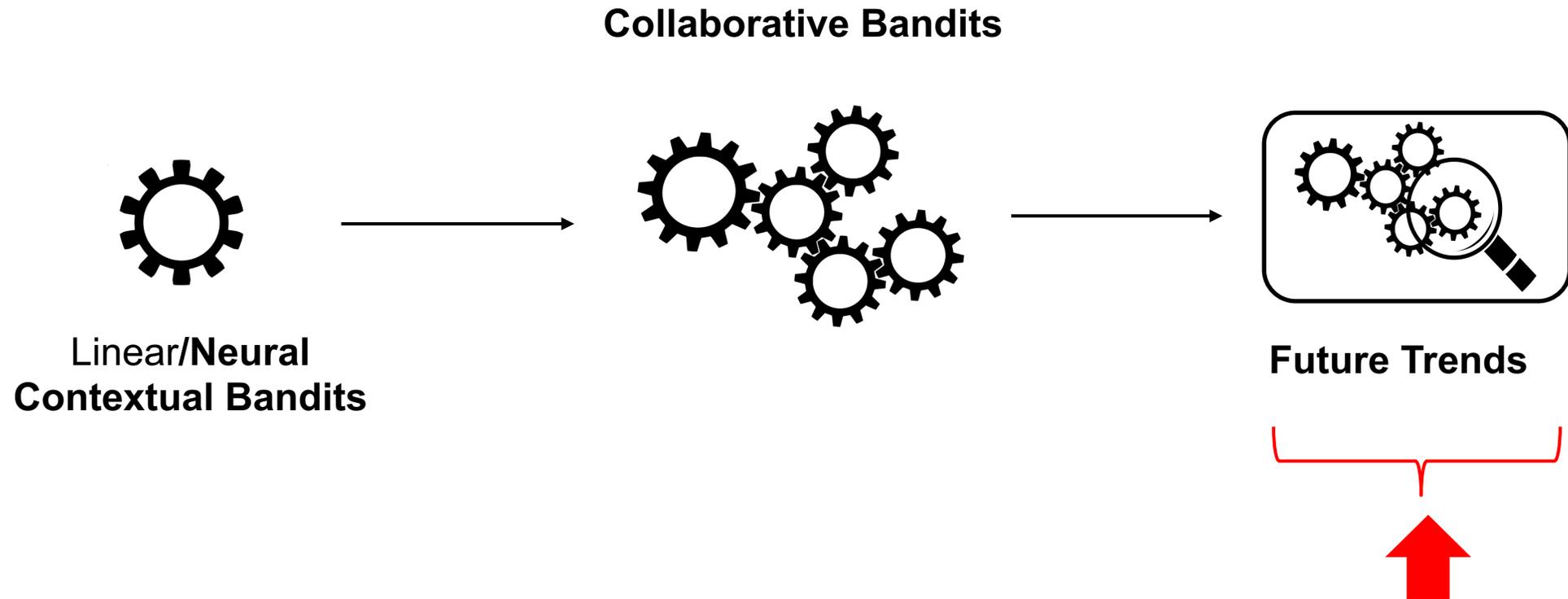
Figure: Regret comparison on Yelp with different reward availability.

Figure: Regret comparison on Mnist+NotMnist with different reward availability.

Observation:

- **With one sub-reward, MuFasa still outperforms all baselines.**
- **Without any sub-reward, MuFasa's performance is close to the best baseline.**

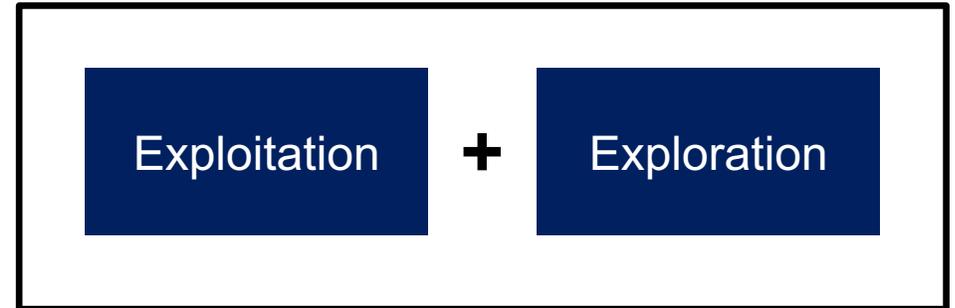




Trustworthy Exploration: Transparency



Q: Can we have a **transparent** exploration with clear rationales and explanations?



➤ Challenges:

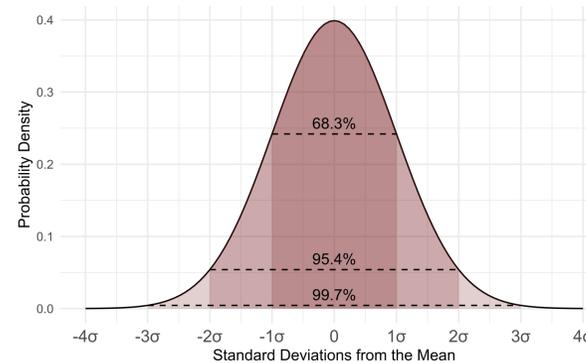
- ❑ More exploration models based on neural networks (**Black Box**).

Black Box !

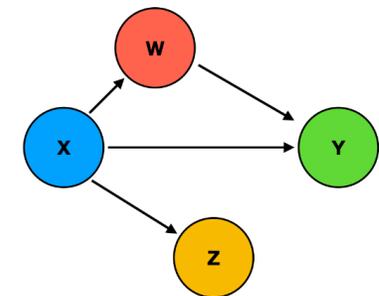
E.g. [Ban et al. ICLR 2022]

➤ Future Directions:

- ❑ Bayesian Bandits/RL.
- ❑ Causal Bandits/RL.



Statistics



Causal Inference

Trustworthy Exploration: Fairness



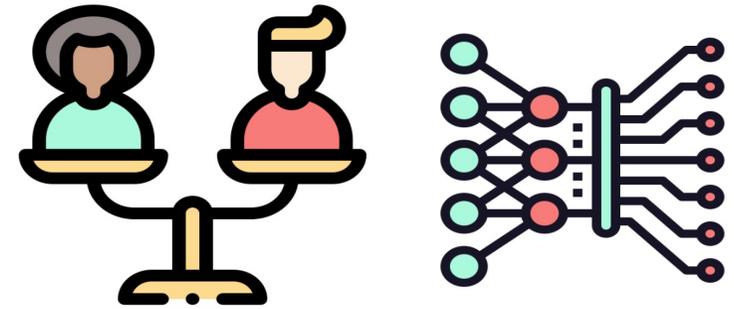
Q: How to ensure **fairness** in the context of exploration?

➤ **Challenges:**

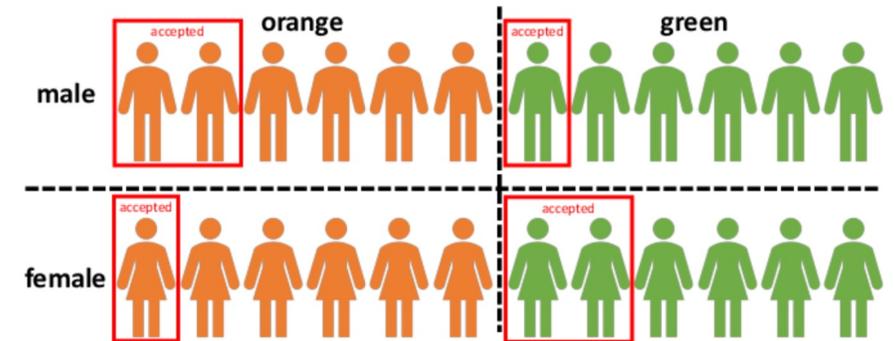
- ❑ **Non-IID** data.
- ❑ balance required between **exploration power** and **fairness**.

➤ **Future Directions:**

- ❑ Derive fairness confidence interval for exploration.
- ❑ Fairness Regularization.



Group Fairness



Group Fairness [1]

Trustworthy Exploration: Privacy



Q: Can we have an exploration strategy preserving privacy?

➤ **Challenges:**

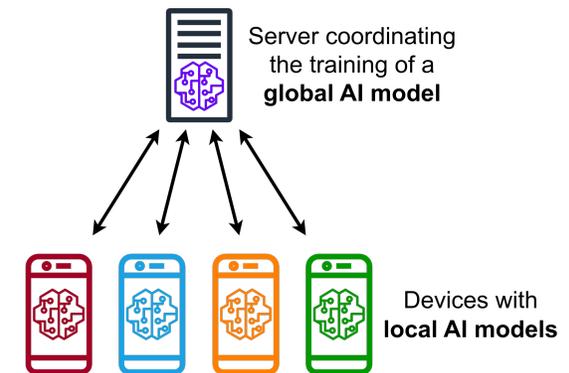
- ❑ Privacy-preserving exploration methods.

➤ **Future Directions:**

- ❑ Federated Bandits/RL.



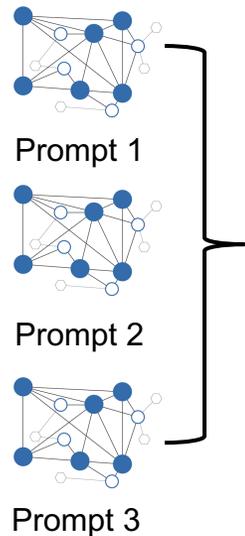
User Privacy



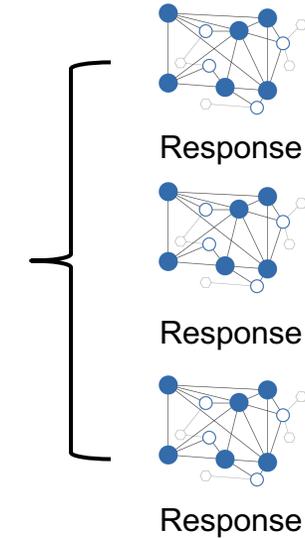
Federated Learning



Customized Exploration: Large Language Model



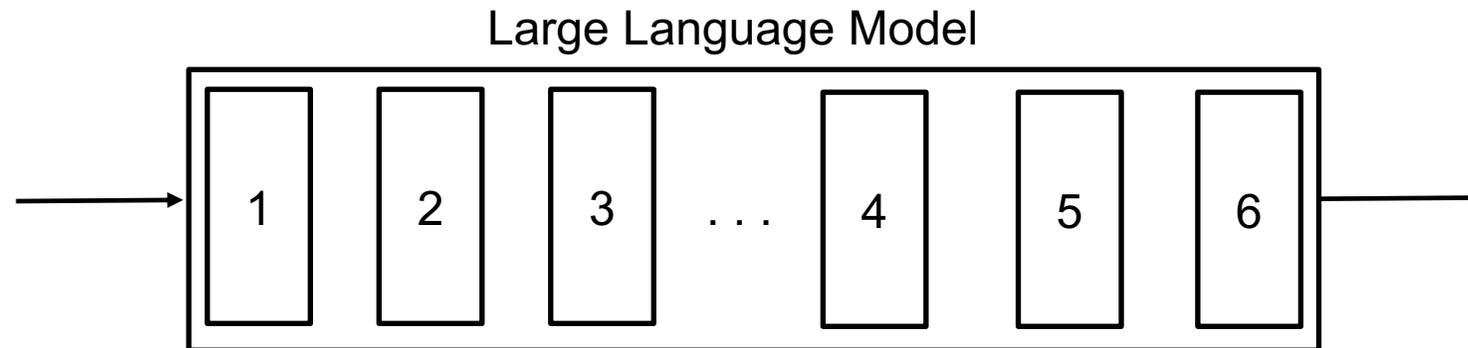
Exploit
?
Explore



Exploit
?
Explore

(1) Prompting with Exploration

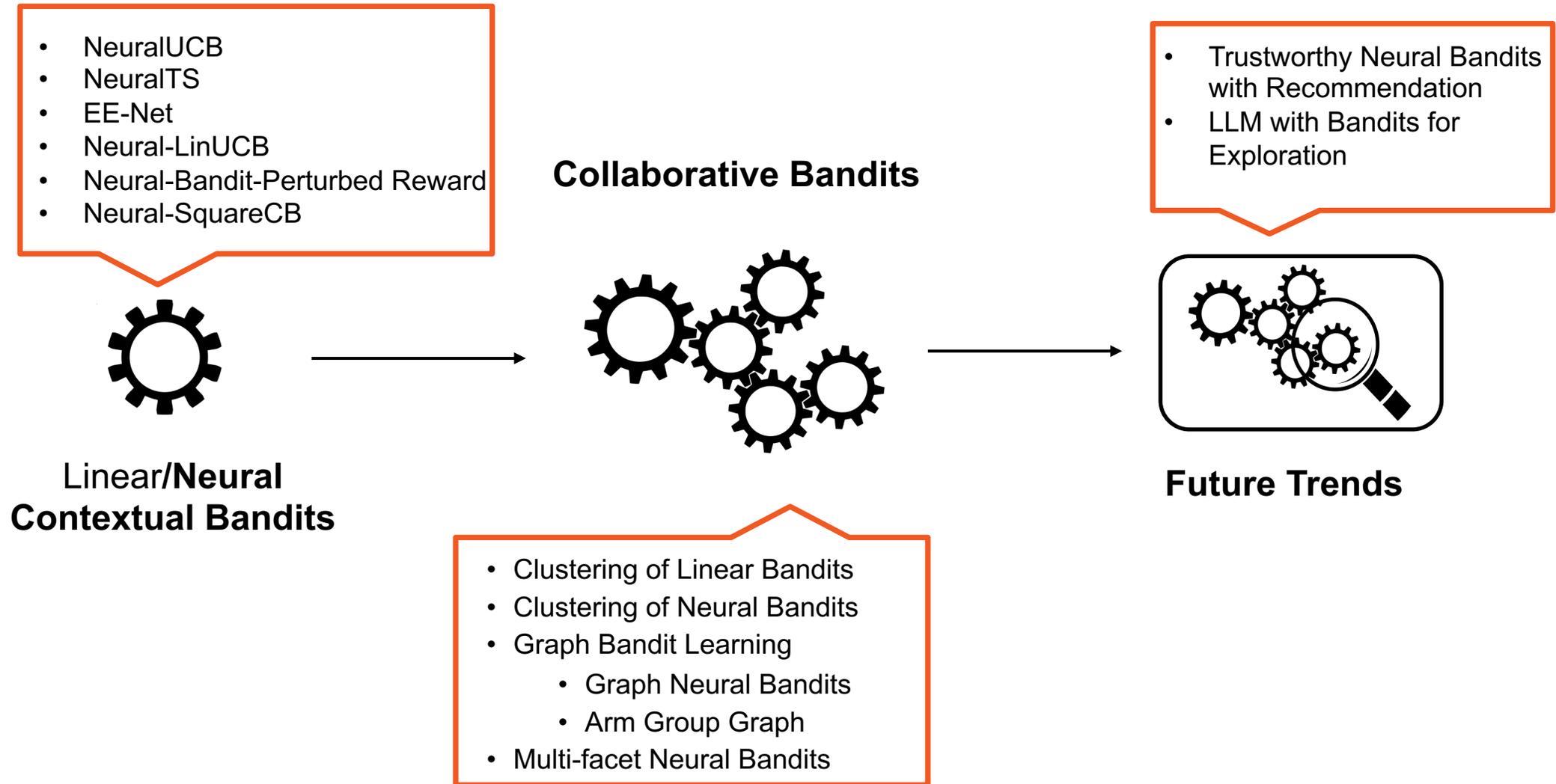
(2) Answering with User-specific Exploration



(3) Fine-tuning with Exploration

1. Lin, Xiaoqiang, et al. "Use your INSTINCT: instruction optimization using neural bandits coupled with transformers." ICML 2024.
2. Chen, Zekai, et al. "Online Personalizing White-box LLMs Generation with Neural Bandits." *arXiv preprint arXiv:2404.16115* (2024).
3. Köpf, Andreas, et al. "Openassistant conversations-democratizing large language model alignment." NeurIPS 2023.
4. Rafailov, Rafael, et al. "Direct preference optimization: Your language model is secretly a reward model." NeurIPS 2023.
5. Zhang, Qingru, et al. "Platon: Pruning large transformer models with upper confidence bound of weight importance." ICML 2022.





Neural Contextual Bandits for Personalized Recommendation



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Time: 9:00 AM – 12:30 PM, 13 May 2024

Location: Virgo 1, Resorts World Sentosa Convention Centre, Singapore

Website: www.banyikun.com/wwwtutorial/