# On Kernelized Multi-armed Bandits 

Sayak Ray Chowdhury Aditya Gopalan<br>Department of Electrical Communication Engineering Indian Institute of Science

ICML
August 7, 2017

## Overview

Problem Formulation

Algorithms

Regret Bounds

Numerical Results

Conclusion

## Problem Statement

Sequentially Maximize $f: D \rightarrow \mathbb{R}$


- $f$ unknown, $D \subset \mathbb{R}^{d}$


## Problem Statement

Sequentially Maximize $f: D \rightarrow \mathbb{R}$


- $f$ unknown, $D \subset \mathbb{R}^{d}$
- $x^{\star}=\operatorname{argmax} f(x)$ $x \in D$


## Problem Statement

Sequentially Maximize $f: D \rightarrow \mathbb{R}$


- $f$ unknown, $D \subset \mathbb{R}^{d}$
- $x^{\star}=\operatorname{argmax} f(x)$

$$
x \in D
$$

- At each round $t$ :
- Learner chooses $x_{t} \in D$ based on past
- Observes noisy reward $y_{t}=f\left(x_{t}\right)+\varepsilon_{t}$


## Problem Statement

Sequentially Maximize $f: D \rightarrow \mathbb{R}$


- $f$ unknown, $D \subset \mathbb{R}^{d}$
- $x^{\star}=\operatorname{argmax} f(x)$

$$
x \in D
$$

- At each round $t$ :
- Learner chooses $x_{t} \in D$ based on past
- Observes noisy reward $y_{t}=f\left(x_{t}\right)+\varepsilon_{t}$

Performance Metric

- Regret $r_{t}=f\left(x^{*}\right)-f\left(x_{t}\right)$
- Goal: Minimize cumulative regret $\sum_{t=1}^{T} r_{t}$


## Assumptions

- Noise $\varepsilon_{t}$ is $R$-sub-Gaussian


## Assumptions

- Noise $\varepsilon_{t}$ is $R$-sub-Gaussian
- $f$ lies in RKHS of functions: $D \rightarrow \mathbb{R}$
- Positive semi-definite kernel function $k: D \times D \rightarrow \mathbb{R}$ (known)
- Reproducing property: $f(x)=\langle f, k(x, \cdot)\rangle_{k}$
- Induces smoothness: $|f(x)-f(y)| \leq\|f\|_{k}\|k(x, \cdot)-k(y, \cdot)\|_{k}$


## Assumptions

- Noise $\varepsilon_{t}$ is $R$-sub-Gaussian
- $f$ lies in RKHS of functions: $D \rightarrow \mathbb{R}$
- Positive semi-definite kernel function $k: D \times D \rightarrow \mathbb{R}$ (known)
- Reproducing property: $f(x)=\langle f, k(x, \cdot)\rangle_{k}$
- Induces smoothness: $|f(x)-f(y)| \leq\|f\|_{k}\|k(x, \cdot)-k(y, \cdot)\|_{k}$
- $D$ is compact, $\|f\|_{k} \leq B$ known


## Assumptions

- Noise $\varepsilon_{t}$ is $R$-sub-Gaussian
- $f$ lies in RKHS of functions: $D \rightarrow \mathbb{R}$
- Positive semi-definite kernel function $k: D \times D \rightarrow \mathbb{R}$ (known)
- Reproducing property: $f(x)=\langle f, k(x, \cdot)\rangle_{k}$
- Induces smoothness: $|f(x)-f(y)| \leq\|f\|_{k}\|k(x, \cdot)-k(y, \cdot)\|_{k}$
- $D$ is compact, $\|f\|_{k} \leq B$ known
- Bounded variance: $k(x, x) \leq 1$, for all $x \in D$


## Example Kernels

- Squared Exponential kernel: $k(x, y)=\exp \left(\frac{-\|x-y\|_{2}^{2}}{2 / 2}\right)$
- Matérn kernel: $k(x, y)=\frac{2^{1-\nu}}{\Gamma(\nu)}\left(\frac{\|x-y\|_{2} \sqrt{2 \nu}}{l}\right)^{\nu} B_{\nu}\left(\frac{\|x-y\|_{2} \sqrt{2 \nu}}{1}\right)$
- Stationary kernels: $k(x, y) \equiv k(x-y)$


## Example Kernels

- Squared Exponential kernel: $k(x, y)=\exp \left(\frac{-\|x-y\|_{2}^{2}}{2 /^{2}}\right)$
- Matérn kernel: $k(x, y)=\frac{2^{1-\nu}}{\Gamma(\nu)}\left(\frac{\|x-y\|_{2} \sqrt{2 \nu}}{l}\right)^{\nu} B_{\nu}\left(\frac{\|x-y\|_{2} \sqrt{2 \nu}}{1}\right)$
- Stationary kernels: $k(x, y) \equiv k(x-y)$
- Linear Kernel:
- $k(x, y)=x^{\top} y$
- $f(x)=\theta^{T} x, \theta \in \mathbb{R}^{d}$ unknown parameter


## Example Kernels

- Squared Exponential kernel: $k(x, y)=\exp \left(\frac{-\|x-y\|_{2}^{2}}{2 /^{2}}\right)$
- Matérn kernel: $k(x, y)=\frac{2^{1-\nu}}{\Gamma(\nu)}\left(\frac{\|x-y\|_{2} \sqrt{2 \nu}}{l}\right)^{\nu} B_{\nu}\left(\frac{\|x-y\|_{2} \sqrt{2 \nu}}{l}\right)$
- Stationary kernels: $k(x, y) \equiv k(x-y)$
- Linear Kernel:
- $k(x, y)=x^{\top} y$
- $f(x)=\theta^{T} x, \theta \in \mathbb{R}^{d}$ unknown parameter
- Reduces to parametric linear bandit problem (Dani et al., COLT 2008, Abbasi-Yadkori et al., NIPS 2011, ...)


## Algorithm Design Philosophy: Gaussian Processes



Assume:

- Gaussian Process Prior of f : $G P\left(0, v^{2} k(x, y)\right)$
- Noise $\varepsilon_{t} \sim \mathcal{N}\left(0, \lambda v^{2}\right)$


## Algorithm Design Philosophy: Gaussian Processes



Assume:

- Gaussian Process Prior of f : $G P\left(0, v^{2} k(x, y)\right)$
- Noise $\varepsilon_{t} \sim \mathcal{N}\left(0, \lambda v^{2}\right)$
- After $t$ rounds, reward vector $y_{1: t} \sim \mathcal{N}\left(0, v^{2}\left(K_{t}+\lambda I\right)\right)$


## Algorithm Design Philosophy: Gaussian Processes



## Assume:

- Gaussian Process Prior of f : $G P\left(0, v^{2} k(x, y)\right)$
- Noise $\varepsilon_{t} \sim \mathcal{N}\left(0, \lambda v^{2}\right)$
- After $t$ rounds, reward vector $y_{1: t} \sim \mathcal{N}\left(0, v^{2}\left(K_{t}+\lambda /\right)\right)$

Posterior of $f$ after $t$ rounds: $G P\left(\mu_{t}(x), v^{2} k_{t}(x, y)\right)$

$$
\begin{aligned}
\mu_{t}(x) & =k_{t}(x)^{T}\left(K_{t}+\lambda I\right)^{-1} y_{1: t} \\
k_{t}(x, y) & =k(x, y)-k_{t}(x)^{T}\left(K_{t}+\lambda I\right)^{-1} k_{t}(y)
\end{aligned}
$$

## Algorithm 1: Improved GP-UCB (IGP-UCB)

Key Idea: Play the arm with highest UCB


## Algorithm 1: Improved GP-UCB (IGP-UCB)

Key Idea: Play the arm with highest UCB


At each round $t$, play:

$$
x_{t}=\underset{x \in D}{\operatorname{argmax}} \mu_{t}(x)+\beta_{t} \sigma_{t}(x)
$$

## Algorithm 1: Improved GP-UCB (IGP-UCB)

Key Idea: Play the arm with highest UCB


At each round $t$, play:

$$
x_{t}=\underset{x \in D}{\operatorname{argmax}} \mu_{t}(x)+\beta_{t} \sigma_{t}(x)
$$

- $\beta_{t}$ trades off $\mathrm{b} / \mathrm{w}$ exploration and exploitation
- Reduced width $\left(\beta_{t}\right)$ of confidence interval compared to GP-UCB (Srinivas et al., ICML 2010)


## Algorithm 2: Gaussian Process Thompson Sampling (GP-TS)

Key Idea: Sample a random function and play its maximizer


## Algorithm 2: Gaussian Process Thompson Sampling (GP-TS)

Key Idea: Sample a random function and play its maximizer


At each round $t$ :

- Sample $f_{t}$ from posterior of $f$


## Algorithm 2: Gaussian Process Thompson Sampling (GP-TS)

Key Idea: Sample a random function and play its maximizer


## Regret Bound for IGP-UCB

Result 1
Regret of IGP-UCB is $O\left(\sqrt{T}\left(B \sqrt{\gamma_{T}}+\gamma_{T}\right)\right)$ whp with the choice of confidence width $\beta_{t} \approx B+\sqrt{\gamma_{t}}$ for all $t$

## Regret Bound for IGP-UCB

## Result 1

Regret of IGP-UCB is $O\left(\sqrt{T}\left(B \sqrt{\gamma_{T}}+\gamma_{T}\right)\right)$ whp with the choice of confidence width $\beta_{t} \approx B+\sqrt{\gamma_{t}}$ for all $t$

- $\gamma_{T}$ is Maximum Information Gain after $T$ rounds:

$$
\gamma_{T}=\max _{A \subset D:|A|=T} I\left(y_{A} ; f_{A}\right)
$$

- Mutual Information b/w function values and rewards at set $A$
- Reduction in uncertainty about $f$ after observing rewards
- SE kernel: $\gamma_{T}=O\left((\ln T)^{d+1}\right) \rightarrow$ sublinear regret


## Regret Bound for IGP-UCB

## Result 1

Regret of IGP-UCB is $O\left(\sqrt{T}\left(B \sqrt{\gamma_{T}}+\gamma_{T}\right)\right)$ whp with the choice of confidence width $\beta_{t} \approx B+\sqrt{\gamma_{t}}$ for all $t$

- $\gamma_{T}$ is Maximum Information Gain after $T$ rounds:

$$
\gamma_{T}=\max _{A \subset D:|A|=T} I\left(y_{A} ; f_{A}\right)
$$

- Mutual Information b/w function values and rewards at set $A$
- Reduction in uncertainty about $f$ after observing rewards
- SE kernel: $\gamma_{T}=O\left((\ln T)^{d+1}\right) \rightarrow$ sublinear regret
- Regret of GP-UCB is $O\left(\sqrt{T}\left(B \sqrt{\gamma_{T}}+\gamma_{T} \ln ^{3 / 2} T\right)\right)$ whp and so we improve by $O\left(\ln ^{3 / 2} T\right)$ !


## Regret Bound for GP-TS

## Result 2

- Regret of GP-TS is $O\left(\sqrt{T d \ln (B d T)}\left(B \sqrt{\gamma_{T}}+\gamma_{T}\right)\right)$ whp
- First frequentist regret guarantee of TS in the non-parametric setting of infinite action spaces


## Regret Bound for GP-TS

## Result 2

- Regret of GP-TS is $O\left(\sqrt{T d \ln (B d T)}\left(B \sqrt{\gamma_{T}}+\gamma_{T}\right)\right)$ whp
- First frequentist regret guarantee of TS in the non-parametric setting of infinite action spaces
$\sqrt{d \ln (B d T)} \leftarrow$ Consequence of Discretization


## Regret Bound for GP-TS

## Result 2

- Regret of GP-TS is $O\left(\sqrt{T d \ln (B d T)}\left(B \sqrt{\gamma_{T}}+\gamma_{T}\right)\right)$ whp
- First frequentist regret guarantee of TS in the non-parametric setting of infinite action spaces

$$
\sqrt{d \ln (B d T)} \leftarrow \text { Consequence of Discretization }
$$

Open Question: Can the logarithmic dependency be removed?

## Recovering Regret Bounds for Linear Bandits

## Linear Kernel

- $k(x, y)=x^{\top} y$
- $f(x)=\theta^{T} x, \theta \in \mathbb{R}^{d}$ unknown parameter
- Maximum Information Gain: $\gamma_{T}=O(d \ln T)$
- Regret of IGP-UCB is $\tilde{O}(d \sqrt{T})$ and GP-TS is $\tilde{O}\left(d^{3 / 2} \sqrt{T}\right)$


## Recovering Regret Bounds for Linear Bandits

## Linear Kernel

- $k(x, y)=x^{\top} y$
- $f(x)=\theta^{T} x, \theta \in \mathbb{R}^{d}$ unknown parameter
- Maximum Information Gain: $\gamma_{T}=O(d \ln T)$
- Regret of IGP-UCB is $\tilde{O}(d \sqrt{T})$ and GP-TS is $\tilde{O}\left(d^{3 / 2} \sqrt{T}\right)$
- Exactly recovers regrets of OFUL (Abbasi-Yadkori et al., NIPS 2011) and Linear TS (Agrawal and Goyal, ICML 2013)


## Recovering Regret Bounds for Linear Bandits

## Linear Kernel

- $k(x, y)=x^{\top} y$
- $f(x)=\theta^{T} x, \theta \in \mathbb{R}^{d}$ unknown parameter
- Maximum Information Gain: $\gamma_{T}=O(d \ln T)$
- Regret of IGP-UCB is $\tilde{O}(d \sqrt{T})$ and GP-TS is $\tilde{O}\left(d^{3 / 2} \sqrt{T}\right)$
- Exactly recovers regrets of OFUL (Abbasi-Yadkori et al., NIPS 2011) and Linear TS (Agrawal and Goyal, ICML 2013)
- Lower Bound: $\Omega(d \sqrt{T})$ (Dani et al., COLT 2008)


## Numerical Results

Algorithms Compared:

1. GP-Expected Improvement (Močkus, 1975)
2. GP-Probabilistic Improvement (Kushner, 1964)
3. GP-UCB (Srinivas et al., 2010)
4. IGP-UCB (this work)
5. GP-TS (this work)

## Numerical Results

## f sampled from RKHS

(Squared Exponential kernel)


## Numerical Results

$f$ sampled from RKHS
(Squared Exponential kernel)


- IGP-UCB improves over GP-UCB © ©
- GP-TS fares reasonably well ©


## Numerical Results

$f$ sampled from RKHS
(Squared Exponential kernel)


Temperature Sensor Data
(Intel Berkeley Research lab)


- IGP-UCB improves over GP-UCB © - ©
- GP-TS fares reasonably well ©


## Numerical Results

$f$ sampled from RKHS
(Squared Exponential kernel)


- IGP-UCB improves over GP-UCB © © -
- GP-TS fares reasonably well ©

$$
\begin{aligned}
& \text { Temperature Sensor Data } \\
& \text { (Intel Berkeley Research lab) }
\end{aligned}
$$



- IGP-UCB performs similar to GP-UCB $\checkmark$
- GP-TS performs the best ©


## Key Tool: New Concentration Inequality

Setup:

- Feature map $\varphi: D \rightarrow$ RKHS
- $S_{t}=\sum_{s=1}^{t} \varepsilon_{s} \varphi\left(x_{s}\right) \leftarrow$ RKHS-valued Martingale
- $V_{t}=I+\sum_{s=1}^{t} \varphi\left(x_{s}\right) \varphi\left(x_{s}\right)^{T} \leftarrow$ possibly of infinite dimension


## Key Tool: New Concentration Inequality

Setup:

- Feature map $\varphi: D \rightarrow$ RKHS
- $S_{t}=\sum_{s=1}^{t} \varepsilon_{s} \varphi\left(x_{s}\right) \leftarrow$ RKHS-valued Martingale
- $V_{t}=I+\sum_{s=1}^{t} \varphi\left(x_{s}\right) \varphi\left(x_{s}\right)^{T} \leftarrow$ possibly of infinite dimension


## Result 3: Self-Normalized CI for RKHS-valued Martingales

- For all $t:\left\|S_{t}\right\|_{V_{t}^{-1}}^{2} \leq 2 R^{2} \ln \left(\frac{\sqrt{\operatorname{det}\left(K_{t}+l\right)}}{\delta}\right)$ with probability at least $1-\delta$ if $K_{t}$ is positive-definite
- Generalizes finite-dimensional Inequality for vector-valued Martingales (Abbasi-Yadkori et al., NIPS 2011)
- Curse of Dimensionality $\rightarrow$ Mixing over Gaussian Processes


## Summary

For Non-parametric Bandits :

- Improved existing UCB based algorithm
- Introduced new Thompson Sampling based algorithm
- Developed new self-normalized concentration inequality for RKHS-valued martingales


## Summary

For Non-parametric Bandits :

- Improved existing UCB based algorithm
- Introduced new Thompson Sampling based algorithm
- Developed new self-normalized concentration inequality for RKHS-valued martingales

Future Work:

- Kernel function not known to the learner
- Time varying functions from RKHS

Thank You

Poster Tonight

