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# contextual: Simulating Contextual Multi-Armed Bandit Problems in R

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#### **Abstract**

Over the past decade, contextual bandit algorithms have been gaining in popularity due to their effectiveness and flexibility in solving sequential decision problems—from online advertising and finance to clinical trial design and personalized medicine. At the same time, there are, as of yet, surprisingly few options that enable researchers and practitioners to simulate and compare the wealth of new and existing bandit algorithms in a standardized way. To help close this gap between analytical research and practical evaluation the current paper introduces the object-oriented R package **contextual**: a user-friendly and, through its object-oriented structure, easily extensible framework that facilitates parallelized comparison of contextual and context-free bandit policies through both simulation and offline analysis.

Keywords: contextual multi-armed bandits, simulation, sequential experimentation, R.

#### 1. Introduction

There are many real-world situations in which we have to decide between multiple options, yet are only able to learn the best course of action by testing each option sequentially. In such situations, the underlying concept remains the same for each and every renewed decision: Do you stick to what you know and receive an expected result ("exploit") or choose an option you do not know all that much about and potentially learn something new ("explore")? As we all encounter such dilemma's on a daily basis (Wilson, Geana, White, Ludvig, and Cohen 2014), it is easy to come up with examples for instance:

- When going out to dinner, do you explore new restaurants, or choose a favorite?
- As a website editor, do you place popular or new articles at the top of your frontpage?
- As a doctor, do you prescribe tried and tested medication, or do you also provide promising experimental drugs?

• When visiting a casino, do you stay with the slot machine that just paid out, or do you try some of the other slot machines?

Although people seem to navigate such explore-exploit problems with relative ease, this type of decision problem has proven surprisingly difficult to solve analytically and has been studied extensively since the 1930s (Robbins 1952; Bubeck, Cesa-Bianchi *et al.* 2012) under the umbrella of the "multi-armed bandit" (MAB) problem. The origin of the name can be traced back to the casino example: a one armed bandit is the original name for a slot machine in a casino, as they used to have one arm and tended to steal your money. A multi-armed bandit can then be understood as a set of one-armed bandit slot machines in a casino—in that respect, "many one-armed bandits problem" might have been a better fit (Gelman 2018). Just like in the casino example, the crux of a multi-armed bandit problem is that you only receive a reward for the arm you pull—you remain in the dark about what rewards the other arms might have offered. Consequently, you need some strategy or "policy" that helps you balance the exploration and exploitation of arms to optimize your rewards over repeated pulls. One option would, for instance, be to pull every available arm once and from then on exploit the arm that offered you the highest reward. This reward might, however, be nothing more than a lucky fluke. On the other hand, if you decide to keep exploring other arms, you may lose out on the winnings you might have received from the arm that had been doing so well.

This active exploration of information gathered one step at a time makes multi-armed bandit problems a subset of reinforcement learning type problems —together with supervised and unsupervised learning one of three main classes of machine learning. Where supervised algorithms learn mappings from input values to fully specified class labels and unsupervised learning looks for patterns in data without any such labels, reinforcement learning policies live somewhere in between: bandit policies are able to make use of labels or "rewards" to minimize their loss—but in contast to their supervised siblings, this information has to be actively acquired (Jordan and Mitchell 2015). Bandit policies are then that subset of reinforcement learning algorithms that either do not take further contextual information into account or, otherwise, assume that their choices do not affect this context (Steenwinckel, De Backere, Nelis, Ongenae, and De Turck 2018; Sutton and Barto 1998).

Where the latter brings us to a recent MAB generalization generally known as the *contextual* multi-armed bandit (CMAB) problem. CMAB problems extend on basic "context-free" MABs by adding one crucial element: contextual information (Langford and Zhang 2008). Contextual multi-armed bandits are known by many different names in about as many different fields of research (Tewari and Murphy 2017)—for example as "bandit problems with side observations" (Wang, Kulkarni, and Poor 2005), "bandit problems with side information" (Lu, Pál, and Pál 2010), "associative reinforcement learning" (Kaelbling, Littman, and Moore 1996), "reinforcement learning with immediate reward" (Abe, Biermann, and Long 2003), "associative bandit problems" (Strehl, Mesterharm, Littman, and Hirsh 2006b), or "bandit problems with covariates" (Sarkar 1991). However, the term "contextual multi-armed bandit," as conceived by Langford and Zhang (2008), is the most used—so that is the term we will use in the current paper.

Nevertheless, however named, all CMAB policies differentiate themselves, by definition, from their MAB cousins in that they are able to make use of features that reflect the current state of the world—

<sup>&</sup>lt;sup>1</sup>As Dr. Peter Whittle famously stated "[the problem] was formulated during the [second world] war, and efforts to solve it so sapped the energies and minds of Allied analysts that the suggestion was made that the problem be dropped over Germany, as the ultimate instrument of intellectual sabotage." (Whittle 1979)

features that can then be mapped onto available arms or actions<sup>2</sup>. This access to side information makes CMAB algorithms yet more relevant to many real-life decision problems than their MAB progenitors (Langford and Zhang 2008). To follow up on our previous examples: do you choose the same type of restaurants in your hometown and when on vacation? Do you prescribe the same treatment to male and female patients? Do you place the same news story on the frontpage of your website for both young and old visitors? Probably not—in the real world, it appears no choice exists without at least some contextual information to be mined or mapped. So it may be no surprise that CMAB algorithms have found applications in many different areas: from recommendation engines (Lai and Robbins 1985) to advertising (Tang, Rosales, Singh, and Agarwal 2013) and (personalized) medicine (Katehakis and Derman 1986; Tewari and Murphy 2017), healthcare (Rabbi, Aung, Zhang, and Choudhury 2015), and portfolio choice (Shen, Wang, Jiang, and Zha 2015)—inspiring a multitude of new, often analytically derived bandit algorithms or policies.

However, although CMAB algorithms have found more and more applications, comparisons on both synthetic, and, importantly, real-life, large-scale offline datasets (Li, Chu, Langford, and Wang 2011) have relatively lagged behind<sup>3</sup>. To this end, the current paper introduces the R package **contextual**, to facilitate the development, evaluation, and comparison the of (contextual) multi-armed bandit policies by offering an easily extensible, class-based, modular architecture.

In that respect, **contextual** differentiates itself from several other types of bandit oriented software applications and services, such as:

- 1) Online A/B and basic, out-of-the-box MAB test services such as **Google Analytics** (Google 2018), **Optimizely** (Optimizely 2018), **Mix Panel** (Mixpanel 2018), **AB Tasty** (ABTasty 2018), **Adobe Target** (Adobe 2018), and more.
- 2) More advanced online CMAB test services and software, such as the flexible online evaluation platform **StreamingBandit** (Kruijswijk, Parvinen, van Emden, and Kaptein 2018) and Microsoft's **Custom Decision Service** (Agarwal, Bird, Cozowicz, Hoang, Langford, Lee, Li, Melamed, Oshri, and Ribas 2016).
- 3) Predominantly context-free simulation oriented projects such as **Yelp MOE** (Yelp 2018), which runs sequential A/B tests using Bayesian optimization, and the mainly MAB focused Python packages **Striatum** (NTUCSIE-CLLab 2018) and **SMPyBandits** (Besson 2018).
- 4) Software that facilitates the evaluation of bandit policies on offline data, such as **Vowpal Wab-bit** (Langford, Li, and Strehl 2007), **Jubatus** (Hido, Tokui, and Oda 2013), and **TensorFlow** (Abadi, Barham, Chen, Chen, Davis, Dean, Devin, Ghemawat, Irving, and Isard 2016).

Though each of these applications and services may share certain features with **contextual**, overall, **contextual** clearly distinguishes itself in several respects. First, it focusses on the evaluation of bandit policies on simulated and offline datasets, which discriminates it from the online evaluation oriented packages cited under items 1 and 2. Second, though **contextual** is perfectly capable of simulating

<sup>&</sup>lt;sup>2</sup>That is, before making a choice, the learner receives information on the state of the world or "context" in the form of a d-dimensional feature vector. After making a choice the learner is then able to combine this contextual information with the reward received to make a more informed decision in the next round.

<sup>&</sup>lt;sup>3</sup>Here, a **synthetic** data generator (or Bandit, in **contextual** parlance) compares policies against some simulated environment, usually seeking to model or emulate some online bandit scenario—whereas an **offline** Bandit compares policies against a previous collected data set—generally logged with a completely different policy than the one(s) under evaluation (Li, Chu, Langford, Moon, and Wang 2012).

and comparing context-free MAB policies, its emphasis lies on the simulation of contextual policies, distinguishing it from the projects cited under item 3. Finally, though **contextual** is closely related to the projects cited under item 4, it also, again, differentiates itself in several key respects:

- a) contextual offers a diverse, open and extensible library of common MAB and CMAB policies.
- b) **contextual** is developed in R, opening the door to a lively exchange of code, data, and knowledge between scientists and practitioners trained in R.
- c) **contextual** focusses on ease of conversion of existing and new algorithms into clean, readable and shareable source code.
- d) In building on R's **doParallel** package, **contextual**'s simulations are parallelized by default—and can easily be run on different parallel architectures, from cluster (such as on Microsoft Azure, Amazon ec2 or Hadoop backends) to GPU based.

All in all, though there are some alternatives, there was, as of yet, no extensible and widely applicable R package to analyze and compare, respectively, basic multi-armed, continuum (Agrawal 1995) and contextual multi-armed bandit algorithms on both simulated and offline data. In making the package publicly available, we hope to further the dissemination and evaluation of both existing and new CMAB policies—particularly where such policies were previously only available through single-use scripts or basic, isolated code packages (Gandrud 2016).

In the current paper, we will further introduce **contextual**. Section 2 presents a formal definition of the contextual multi-armed bandit problem, shows how this formalization can be transformed into a clear and concise object-oriented architecture, and describes how to set up a minimal simulation. Section 3 gives an overview of **contextual**'s predefined Bandit and Policy subclasses and demonstrates how to run a very basic Simulation. Section 4 delves a little deeper into the implementation of each of **contextual**'s core superclasses. Section 5 shows how to extend **contextual**'s superclasses to create your own custom Bandit and Policy subclasses. Section 6 demonstrates how to further subclass existing Bandit and Policy implementations. Section 7 focusses on how a Bandit subclass can make use of offline datasets. Section 8 brings all of the previous sections together in a partial replication of a frequently cited contextual bandit paper. In Section 9 we conclude with some comments on the current state of the package and potential future enhancements.

This organization offers the reader several ways to peruse the current paper. If you have a passing knowledge of R and want to run simulations based on **contextual**'s default bandits and policies, the current introduction plus Section 3 should be able to get you up and running. If you are looking for a more formal introduction, read Section 2 as well. If you know your way around R and would like to extend **contextual** to run custom bandits and policies, it is probably best to read the whole paper—with a focus on Sections 4, 5 and 6. Finally, add Sections 8 and possibly 9 if you are seeking to implement your own offline bandits.

## 2. Formalization and implementation

In the current section, we first introduce a more formal definition of the contextual multi-armed bandit problem. Next, we present our concise implementation and demonstrate how to put together a minimal MAB simulation.

#### 2.1. Formalization

On further formalization of the contextual bandit problem, a bandit B can be defined as a set of arms  $k \in \{1, ..., K\}$ , where, for each t, each of the K arms generates rewards according to some reward function dependent on d-dimensional context feature vector  $x_{t,k}$  (Auer, Cesa-Bianchi, and Fischer 2002; Langford and Zhang 2008).

We now define an algorithm or policy  $\pi$ , that seeks to maximize its cumulative reward  $\sum_{t=1}^{T} r_t$  (or minimize its cumulative regret—see equations 1, 2) by sequentually selecting one of bandit B's currently available arms Bubeck *et al.* (2012), here defined as taking action  $a_t$  from  $\mathcal{A}_t \subseteq K$  for every t until a final horizon T.

At each time step t policy  $\pi$  now first observes the current state of the world in relation to bandit B represented by d-dimensional context feature vectors  $x_{t,a}^5$  for each available  $a_t \in \mathcal{A}$ .

Making use of some arm-selection strategy, policy  $\pi$  then selects one of the available actions in  $\mathcal{A}_t$ . For scalability reasons, policies generally use a limited set of parameters  $\theta_t$  (Kruijswijk *et al.* 2018) to select this action. This set of parameters summarizes all historical interactions  $D_{t'} = (x_{t'}, a_{t'}, r_{t'})$  over  $t = \{1, ..., t'\}$ , ensuring that the dimensionality of  $\theta_{t'} << D_{t'}$ .

As a result of taking action  $a_t$ , policy  $\pi$  receives reward  $r_{a_t,t}$ .

With observation  $(x_{t,a_t}, a_t, r_{t,a_t})$ , the policy now updates its arm-selection strategy. This cycle is then repeated T times.

Schematically, for each round  $t = \{1, ..., T\}$ :

- 1) Policy  $\pi$  observes current context feature vectors  $x_{t,a}$  for  $\forall a \in \mathcal{A}_t$  in bandit B
- 2) Based on all  $x_{t,a}$  and  $\theta_{t-1}$ , policy  $\pi$  now selects an action  $a_t \in \mathcal{A}_t$
- 3) Policy  $\pi$  receives a reward  $r_{t,a_t,x_t}$  from bandit B
- 4) Policy  $\pi$  updates arm-selection strategy parameters  $\theta_t$  with  $(x_{t,a_t}, a_t, r_{t,a_t})$

The goal of the policy  $\pi$  is to optimize its *cumulative reward* over  $t = \{1, ..., T\}$ 

$$R_T = \sum_{t=1}^{T} (r_{t,a_t,x_t}) \tag{1}$$

In practice, the most popular performance measure for bandit policies is *cumulative regret* (Kuleshov and Precup 2014)—defined as the sum of rewards that would have been received by choosing optimal

<sup>&</sup>lt;sup>4</sup>In other words: Every t a policy makes a choice  $a_t$  from a set of  $\mathcal{A}_t$  actions, which is often equal to—but can be a subset of—the set of K arms of bandit B.

<sup>&</sup>lt;sup>5</sup>Some formalizations describe this vector as  $x_t$  (see, for example, Slivkins (2014) or May, Korda, Lee, and Leslie (2012)). This formalization fits bandit scenario's where contextual information at each t is the same for each arm. For instance, a user feature vector  $x_t$  comprising the d features of a visitor to a news site, with articles for arms. Yet when arm-specific features are taken into account as well, formalizations generally describe the feature vector at each t as  $x_{t,a}$  (e.g. Chu, Park, Beaupre, Motgi, Phadke, Chakraborty, and Zachariah (2009), Li, Chu, Langford, and Schapire (2010))—thereby summarizing, for example, information on both a user  $u_t$  and article k. To facilitate both approaches, **contextual** expects its bandits to generate a  $d \times k$  dimensional context feature matrix  $X_t$  at each t.

action a\* at every t subtracted by the sum of rewards awarded to the chosen action a at every t over  $t=\{1,\ldots,T\}$ :

$$\mathbb{E}[R_T] = \mathbb{E}\left[\max_{a*_t=1,\dots,\mathcal{A}_t} \sum_{t=1}^T (r_{t,a*_t,x_t}) - \sum_{t=1}^T (r_{t,a_t,x_t})\right]$$
(2)

Where expectation  $\mathbb{E}[\cdot]$  is taken with respect to random draws of both rewards assigned by a bandit and arms as selected by a policy (Zheng and Hua 2016).

#### 2.2. Implementation

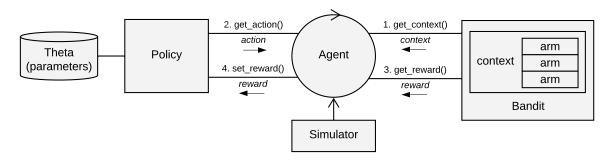


Figure 1: Diagram of **contextual**'s basic structure. The context feature matrix returned by get\_context() is only taken into account by CMAB policies, and may be ignored by MAB policies.

Our class structure builds on the previous formalization and offers a clean class structure with an easily programmable interface. The following six classes form the backbone of the package (see also Figure 1):

- Bandit: R6 class Bandit is the parent class of all **contextual** Bandit subclasses. It is responsible for the generation of **contexts** and **rewards**.
- Policy: R6 class Policy is the parent class of all **contextual**'s Policy implementations. For each  $t = \{1, ..., T\}$  it has to choose one of a Bandit's k arms, and update its parameters theta in response to the resulting reward.
- Agent: R6 class Agent is responsible for the running of one Bandit/Policy pair. As such, multiple Agents can be run in parallel with each separate Agent keeping track of t for its assigned Policy and Bandit pair. To be able to fairly evaluate and compare each agent's performance, and to make sure that simulations are replicable, seeds are set equally and deterministically for each agent over all horizon times simulations time steps of each agent's simulation.
- Simulator: R6 class Simulator is the entry point of any **contextual** simulation. It encapsulates one or more Agents (running in parallel to each other, by default), creates an Agent clone (each with its own deterministic seed) for each to be repeated simulation, runs the Agents, and saves the log of all Agent interactions to a History object.

- History: R6 class History keeps a log of all Simulator interactions. It allows several ways to interact with the data, provides summaries of the data, and can save and load simulation data in several different (data.table, data.frame and CSV) formats.
- Plot: R6 class Plot generates plots from History logs. It is usually invoked by calling the generic plot(h) function, where h is an History class instance.

#### 2.3. Putting it together: a first MAB simulation

#### Running a simulation

Building on the introduction of **contextual**'s core classes in the previous section, we can now put together the following five line MAB simulation:

```
> library(contextual)
>
> bandit <- BasicBernoulliBandit$new(weights = c(0.9, 0.1, 0.1))
> policy <- EpsilonGreedyPolicy$new(0.1)
> agent <- Agent$new(policy,bandit)
> simulator <- Simulator$new(agents = agent, simulations = 100, horizon = 50)
> history <- simulator$run()</pre>
```

In these lines we start out by instantiating the Bandit subclass BasicBernoulliBandit (covered in Section 5) as bandit, with three Bernoulli arms, each offering a reward of one with reward probability  $\theta$ , and otherwise a reward of zero. For the current simulation, we have set the bandit arm probabilities of reward to respectively 0.9, 0.1 and 0.1 through the policy's weight parameter. In BasicBernoulliBandit, the number of bandit arms equals length of weight vector. That is, the bandit instance's number of arms bandit\$k now equals 3, and, for this context-free bandit, its number of feature dimension bandit\$d remains NULL.

Next, we instantiate the Policy subclass EpsilonGreedyPolicy (covered in Section 5.3) as object policy, with its epsilon parameter set to 0.1.

We then assign both our bandit and our policy to Agent instance agent. This agent is added to a Simulator that is set to one hundred simulations, each with a horizon of fifty—that is, simulator runs one hundred simulations, each with a different (deterministic) random seed, for fifty time steps t.

In anticipation of Section 4: For a policy to be able to initialize its parameters, during initialisation, an agent instance makes bandit\$k (number of arms) and bandit\$d (number of dimensions) available to its policy through calls to policy\$set\_parameters(context\_initial\_params) and policy\$initialize\_theta(context\_initial\_params\$k). On starting the simulation, the (potentially changing) number of arms and features dimension remain available for each time step t through respectively context\$k and context\$d.

Running the Simulator then starts several (by default, the number of CPU cores minus one) worker processes, splitting simulations as efficiently as possible over each parallel worker. For each simulation, for every time step t, agents runs through each of the four function calls that constitute their main loop.

A main loop that relates one on one to the four steps defined in our CMAB formalization from Section 2.1:

- 1) agent calls bandit $\$get\_context(t)$ . The bandit returns a named list that contains the current  $d \times k$  dimensional feature matrix context\$X, the number of arms context\$k and the number of features per arm context\$d.
- 2) agent calls policy\$get\_action(t, context). The policy computes which arm to play based on the current values in named lists theta and context. The policy returns a named list containing action\$choice, which holds the index of the arm to play.
- 3) agent calls bandit\$get\_reward(t, context, action). The bandit returns a named list containing the reward for the action chosen in [2] and, optionally, an optimal\_reward—when computable.
- 4) agent calls policy\$set\_reward(t, context, action, reward). The policy uses the action taken, the reward received, and the current context to update its set of parameter values in theta.

#### Results of the simulation

On completion of all of its agents' simulation runs, Simulator returns a history object which contains a complete log of all interactions. This history log can then, for example, be summarized and plotted:

```
> summary(history)
```

#### Agents:

**EpsilonGreedy** 

## Cumulative regret:

```
agent t sims cum_regret cum_regret_var cum_regret_sd EpsilonGreedy 50 100 7.94 87.59232 9.359077
```

#### Cumulative reward:

```
agent t sims cum_reward cum_reward_var cum_reward_sd EpsilonGreedy 50 100 37.84 91.04485 9.541742
```

#### Cumulative reward rate:

```
agent t sims cur_reward cur_reward_var cur_reward_sd EpsilonGreedy 50 100 0.7568 1.820897 0.1908348
```

> plot(history, type = "arms", interval = 50)

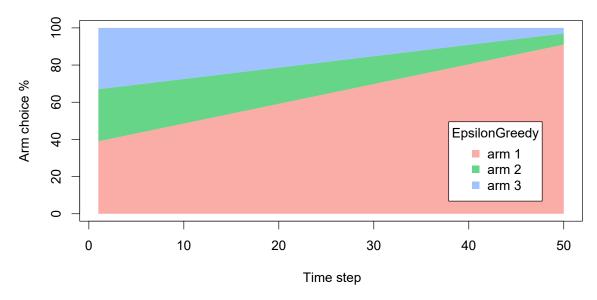


Figure 2: The percentage each of the three arms of the bandit was chosen by the policy overall simulations per time step *t*. Plotted with both an interval and a horizon of fifty, the plot represents the progression of this percentage from time step 1 to step 50 without plotting intervening steps.

## 3. Basic usage

The current section offers an overview of **contextual**'s predefined bandits and policies and further demonstrates how to run them.

#### 3.1. Implemented policies and bandits

Though contextual was designed to make it easy to develop custom bandit and policy classes, as demonstrated in the previous section, it is also possible to run basic simulations with just its built-in bandits and policies. See Table 1 for an overview of all available policies and Table 2 for an overview of all currently implemented bandits—where possible referencing their original papers.

	$\epsilon$ -Greedy	UCB	<b>Thomspon Sampling</b>	Other	Special	
MAB	$\epsilon$ -Greedy <sup>1</sup> $\epsilon$ -First	UCB1 <sup>2</sup> UCB-tuned <sup>3</sup>	Thompson Sampling <sup>4</sup> BootstrapTS <sup>5</sup>	Softmax <sup>6</sup> Gittins <sup>7</sup>	Random Oracle	
CMAB	Epoch-Greedy <sup>9</sup>	LinUCB <sup>10</sup> COFIBA <sup>11</sup>	LinTS <sup>12</sup> LogitBTS <sup>13</sup>		LiF <sup>8</sup>	

Table 1: An overview of **contextual**'s predefined contextual and context-free policy classes.

<sup>&</sup>lt;sup>1</sup> Sutton and Barto (1998) <sup>2</sup> Auer *et al.* (2002) <sup>3</sup> Auer *et al.* (2002) <sup>4</sup> Agrawal and Goyal (2011) <sup>5</sup> Eckles and Kaptein (2014) <sup>6</sup> Vermorel and Mohri (2005) <sup>7</sup> Brezzi and Lai (2002) <sup>8</sup> Kaptein *et al.* (2016) <sup>9</sup> Langford and Zhang (2008) <sup>10</sup> Li *et al.* (2010) <sup>11</sup> Li (2016) <sup>12</sup> Agrawal and Goyal (2012) <sup>13</sup> Eckles and Kaptein (2014)

MAB	CMAB	Offline	Continuous
BasicBernoulliBandit BasicGaussianBandit	ContextualBernoulli ContextualLogit ContextualHybrid ContextualLinear ContextualWheel <sup>1</sup>	OfflinePolicyEvaluator <sup>2</sup> DoublyRobust <sup>3</sup>	ContinuumBandit

Table 2: An overview of **contextual**'s predefined synthetic and offline bandit classes.

#### 3.2. Running basic simulations

In the current subsection we demonstrate how to run simulations with **contextual**'s predefined Bandit and Policy subclasses on the basis of a familiar bandit scenario.

#### The scenario

Since online advertising is one of the areas where bandit policies have found widespread application, we will use it as the setting for our basic bandit tutorial. Generally, the goal in online advertising is to determine which out of several ads to serve a visitor to a particular web page. Translated to a bandit setting, in online advertising:

- The context is usually determined by visitor and web page characteristics.
- Arms are represented by the pool of available ads.
- An action equals a shown ad.
- Rewards are determined by a visitor clicking (a reward of 1) or not clicking (a reward of 0) on the shown ad.

For the current tutorial, we limit the number of advertisements we want to evaluate to three, and set ourselves the objective of finding which policy would offer us the highest total click-through rate<sup>6</sup> over four hundred impressions.

#### Comparing context-free policies

Before we are able to evaluate any policies, we first need to model our three ads—each with a different probability of generating a click—as the arms of a bandit. For our current simulation we choose to model the ads with the weight-based ContextualBernoulliBandit, as this allows us to set weights determining the average reward probability of each arm. As can be observed in the source code below, for the current simulation, we set the weights of the arms to respectively  $\theta_1 = 0.8$ ,  $\theta_2 = 0.4$  and  $\theta_3 = 0.2$ .

We also choose two context-free policies to evaluate and compare:

<sup>&</sup>lt;sup>1</sup> Riquelme *et al.* (2018) <sup>2</sup> Li *et al.* (2011) <sup>3</sup> Dudík *et al.* (2011)

<sup>&</sup>lt;sup>6</sup>Click-through rate (CTR) is the ratio of users who click on a specific link or ad to the number of total users who view it (Briggs and Hollis 1997).

- EpsilonFirstPolicy: explores the three ads uniformly at random for a preset period and from thereon exploits the ad with the best click-through rate<sup>7</sup>. For our current scenario, we set the exploration period to one hundred impressions. A formal definition and implementation of the algorithm can be found in Section 5.2.
- EpsilonGreedyPolicy: explores one of the ads uniformly at random  $\epsilon$  of the time and exploits the ad with the best current click-through rate  $1 \epsilon$  of the time. For our current scenario, we set  $\epsilon = 0.4$ . For a formal definition and implementation see Section 5.3.

Next, we assign the bandit and our two policy instances to two agents. Finally, we assign a list holding both agents to a Simulator instance, set the simulator's horizon to four hundred and the number of repeats to ten thousand, run the simulation, and plot() its results:

```
# Load and attach the contextual package.
library(contextual)
# Define for how long the simulation will run.
horizon <- 400
# Define how many times to repeat the simulation.
simulations <- 10000
# Define the probability that each ad will be clicked.
click_probabilities <- c(0.8, 0.4, 0.2)
# Initialize a ContextualBernoulliBandit
bandit <- ContextualBernoulliBandit$new(weights = click_probabilities)</pre>
# Initialize an EpsilonGreedyPolicy with a 40% exploiration rate.
eg_policy <- EpsilonGreedyPolicy$new(epsilon = 0.4)</pre>
# Initialize an EpsilonFirstPolicy with a 100 step exploration period.
ef_policy <- EpsilonFirstPolicy$new(first = 100)</pre>
# Initialize two Agents, binding each policy to a bandit.
ef_agent <- Agent$new(ef_policy, bandit)</pre>
eg_agent <- Agent$new(eg_policy, bandit)</pre>
# Assign both agents to a list.
agents <- list(ef_agent, eg_agent)</pre>
# Initialize Simulator with agent list, horizon, and nr of simulations.
simulator <- Simulator$new(agents, horizon, simulations)</pre>
# Now run the simulator.
history <- simulator$run()</pre>
# Finally, plot the average reward per time step t
plot(history, type = "average", regret = FALSE, lwd = 2)
# And the cumulative reward rate, which equals the Click Through Rate)
plot(history, type = "cumulative", regret = FALSE, rate = TRUE, lwd = 2)
```

<sup>&</sup>lt;sup>7</sup>A type of policy also known as an A/B test (Kohavi, Henne, and Sommerfield 2007).

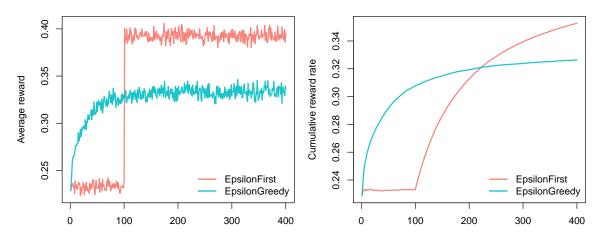


Figure 3: Average reward (left) and cumulative reward rate (equaling click-through rate, right) of  $\epsilon$ -first and  $\epsilon$ -greedy policies.

As can be observed in Figure 3, within our horizon of T=400, EpsilonFirstPolicy has accumulated more rewards than EpsilonGreedytPolicy. It is easy to see why: The winning arm is better than the other two—by a margin. So EpsilonFirstPolicy has no difficulty in finding the optimal arm within its exploration period of one hundred impressions. Up to that point, EpsilonGreedyPolicy had the advantage of a headstart, as it was already able to exploit for  $1-\epsilon$  or sixty percent of the time. But from one hundred impressions on, EpsilonFirstPolicy switches from full exploration to full exploitation mode. In contrast to EpsilonGreedyPolicy, it is now able to exploit the arm that proved best during exploration all of the time. As a result, it catch up with (and then surpass) the rewards accumulated by EpsilonGreedyPolicy within less than one hundred and fifty impressions.

#### Adding context

If that is all we know of our visitors, we expect the results to be stationary over time, and these are the only policies available, the choice is clear: for this scenario, you would pick EpsilonFirstPolicy<sup>8</sup>. However, if we have contextual information on our visitors—for instance, their age—we might be able to do better. Let us suggest that we expect that some of our ads are more effective for older visitors, and other ads more effective for younger visitors.

To incorporate this expectation in our simulation, we need to change the way our bandit generates its rewards. Fortunately, in the case of our ContextualBernoulliBandit, the introduction of two contextual features only requires the addition of a single row to its weight matrix—as ContextualBernoulliBandit parses each of the d rows of its weight matrix as a binary contextual feature randomly selected or sampled 1/d of the time.

We took care to set the combined weight per arm such that each arm generates the same average rewards as previously. So we do not expect a substantial difference with the last simulation's outcome for our context-free policies EpsilonFirstPolicy and EpsilonGreedyPolicy.

We therefore now also include the contextual LinUCBDisjointPolicy (Li *et al.* 2010), which, in assuming its reward function is a linear function of the context, should be able to incorporate our new contextual information into its decision-making process. See 5.4 for a detailed description and

<sup>&</sup>lt;sup>8</sup>Also: if our bandit represents our visitors' click behavior realistically, if our policies' parameters are optimal, etcetera.

implementation details of this policy. Now let us rerun the simulation:

```
#
                                                   -----> ads: k = 3
click_probs
                    <- matrix(c(
                                   0.2,
                                         0.3, 0.1,
                                                        # --> d1: old
                                                       # --> d2: young (p=.5)
                                   0.6.
                                         0.1, 0.1
                                                    ),
                                                              features: d = 2
                                   nrow = 2, ncol = 3, byrow = TRUE)
# Initialize a ContextualBernoulliBandit with contextual weights
                    <- ContextualBernoulliBandit$new(weights = click_probs)</pre>
context_bandit
# Initialize LinUCBDisjointPolicy
                    <- LinUCBDisjointPolicy$new(0.6)
lucb_policy
# Initialize three Agents, binding each policy to a bandit.
                    <- Agent$new(ef_policy, context_bandit)
ef_agent
eg_agent
                    <- Agent$new(eg_policy, context_bandit)
                    <- Agent$new(lucb_policy, context_bandit)
lucb_agent
# Assign all agents to a list.
agents
                    <- list(ef_agent, eg_agent, lucb_agent)
# Initialize Simulator with agent list, horizon, and nr of simulations.
simulator
                    <- Simulator$new(agents, horizon, simulations)</pre>
# Now run the simulator.
history
                    <- simulator$run()
# And plot the cumulative reward rate again.
plot(history, type = "cumulative", regret = FALSE, rate = TRUE)
```

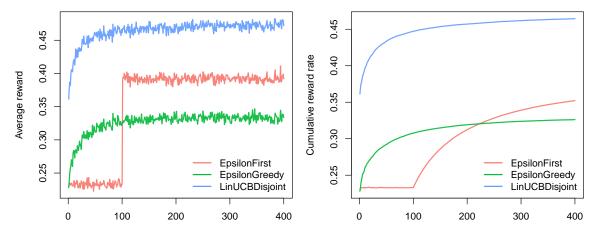


Figure 4: Average reward (left) and cumulative reward rate (equaling click-through rate, right) of LinUCB,  $\epsilon$ -first and  $\epsilon$ -greedy policies.

As can be observed in Figure 4, both context-free bandit's results do indeed not do better than before. On the other hand, LinUCBDisjointPolicy does very well, as it indeed proves able to map its rewards to the available contextual features.

Of course, the simulations in the current section are not very realistic. One way to ameliorate that would be to write a Bandit subclass with a more complex generative model. Section 6 shows how to get started with that. Another option would be to evaluate policies on an offline dataset—more on how to go about that in Section 7.

#### 4. Core classes

The current section offers additional background information on **contextual**'s class structure—both on the R6 class system Chang (2017) and on each of the six previously introduced core **contextual** classes. Together with the information in the next section, on bandit and policy implementation, this should be able to get you up and running with developing your own custom Bandit and Policy subclasses.

#### 4.1. Choice for the R6 class system

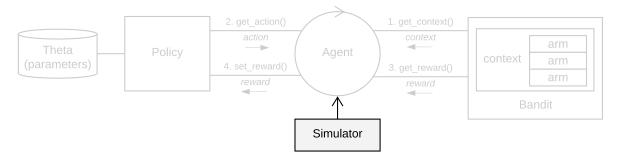
Though widely used as a procedural language, R offers several Object Oriented (OO) systems, which can significantly help in structuring the development of more complex packages. Out of the OO systems available (S3, S4, R5 and R6), we settled on R6, as it offered several advantages compared to the other options. Firstly, it implements a mature object-oriented design when compared to S3. Secondly, its classes can be accessed and modified by reference—which offers the added advantage that R6 classes are instantly recognizable for developers with a background in programming languages such as Java or C++. Finally, when compared to the older R5 reference class system, R6 classes are much lighter-weight and, as they do not make use of S4 classes, do not require the **methods** package.

#### 4.2. Main classes

In this section, we go over each of **contextual**'s six main classes in some more detail—with an emphasis on the Bandit and Policy classes. To clarify **contextual**'s class structure, we also include two UML diagrams (UML, or "unified modeling language" presents a standardized way to visualize the overall class structure and general design of a software application or framework (Rumbaugh, Jacobson, and Booch 2004)). The UML class diagram shown in Figure 13 on page 54 visualizes **contextual**'s static object model, showing how its classes inherit from, and interface with, each other. The UML sequence diagram in figure Figure 14 on page 55, on the other hand, illustrates how **contextual**'s classes interact dynamically over time.

<sup>&</sup>lt;sup>9</sup>In object-oriented programming, the developer compartmentalizes data into objects, whose behavior and contents are described through the declaration of classes. Its benefits include reusability, refactoring, extensibility, ease of maintenance and efficiency. See, for instance, Wirfs-Brock, Wilkerson, and Wiener (1990) for a general introduction to the princples of Object Oriented software design, and Wickham (2014) for more information of the use of OOP in R.

#### Simulator



A Simulator instance is the entry point of any **contextual** simulation. It encapsulates one or more **Agents**, clones them if necessary, runs the **Agents** (in parallel, by default), and saves the log of all of the **Agents** interactions to a **History** object:

history <- Simulator\$new(agents = agent, horizon = 10, simulations = 10)\$run()

By default, for performance reasons, a Simulator does not save context matrices and the (potentially deeply nested) theta list to its History log—though this can be changed by setting either save\_context and save\_theta arguments set to TRUE.

To specify how to run a simulation and which data is to be saved to a Simulator instance's History log, a Simulator object can be configured through, among others, the following arguments:

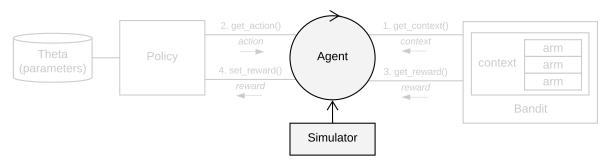
- agents [NULL] An Agent instance, or a list of Agent instances to be run by the instantiated Simulator.
- horizon [100] The T time steps to run the instantiated Simulator.
- simulations [100] How many times to repeat each agent's simulation with a new seed on each repeat (itself deterministically derived from set\_seed).
- save\_context [FALSE] Save context matrices X to the History log during a simulation?
- save\_theta [FALSE] Save the parameter list theta to the History log during a simulation?
- do\_parallel [TRUE] Run Simulator processes in parallel?
- worker\_max [NULL] Specifies how many parallel workers are to be used, when do\_parallel is TRUE. If unspecified, the amount of workers defaults to max(workers\_available)-1.
- set\_seed [0] Sets the seed of R's random number generator for the current Simulator.
- progress\_file [FALSE] If TRUE, Simulator writes progress.log and doparallel.log files to the current working directory, allowing you to keep track of workers, iterations, and potential errors when running a Simulator in parallel.
- include\_packages [NULL] List of packages that (one of) the policies depend on. If a Policy requires an R package to be loaded, this option can be used to load that package on each of the workers. Ignored if do\_parallel is FALSE.

• reindex [FALSE] If TRUE, removes empty rows from the History log, re-indexes the t column, and truncates the resulting data to the shortest simulation grouped by agent and simulation.

The Simulator class has been designed to make it as easy as possible to replace its default parallel backend for other **foreach** type backends. In the alt\_par\_backend\_examples subdirectory of **contextual**'s demo directory we offer examples of **doAzureParallel**, **doRedis** and **doMPI** Simulator subclasses. As a result of **contextual**'s object oriented setup, such Simulator subclasses can be implemented in just a few lines of code, for instance in the case of the **doMPI** subclass:

```
MPISimulator <- R6::R6Class(
  inherit = Simulator,
  public = list(
    register_parallel_backend = function() {
       super$cl <- doMPI::startMPIcluster()
       doMPI::registerDoMPI(super$cl)
       workers = foreach::getDoParWorkers()
       message(paste0("MPI workers: ", workers))
    },
    stop_parallel_backend = function() {
       doMPI::closeCluster(super$cl)
    }
  )
)</pre>
```

#### Agent



To ease the encapsulation of parallel Bandit and Policy simulations, Agent is responsible for the flow of information between and the running of one Bandit and Policy pair, for example:

It keeps track of t and makes sure that, at each time step t, all four main Bandit and Policy CMAB methods are called in correct order, one after the other:

```
Agent <- R6::R6Class(
  public = list(
    #...
    do_step = function() {
        t <- t + 1
        context = bandit$get_context(t)
        action = policy$get_action (t, context)
        reward = bandit$get_reward (t, context, action)
        theta = policy$set_reward (t, context, action, reward)
        list(context = context, action = action, reward = reward, theta = theta)
    }
    #...
)</pre>
```

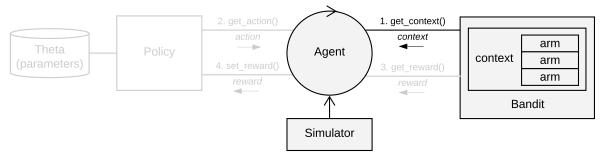
Its main function is do\_step(), generally called by a Simulator object (or, more specifically, by the Simulator-started parallel worker that is repsonsible for this particular Agent):

• do\_step() Completes one time step t by consecutively calling bandit\$get\_context(), policy\$get\_action(), bandit\$get\_reward() and policy\$set\_reward().

#### Bandit

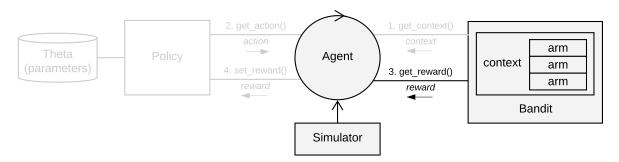
In **contextual**, any bandit implementation is expected to subclass and extend the Bandit superclass. It is then up to these subclasses themselves to provide an implementation for each of its abstract methods.

Bandits are responsible for the generation of (either synthetic or offline) contexts and rewards. On initialisation, a Bandit subclass has to define the number of arms self\$k and the number of contextual feature dimensions self\$d. For each  $t = \{1, ..., T\}$  a Bandit then generates a list containing current context in  $d \times k$  dimensional matrix ontext\$X, the number of arms in context\$k and the number of features in context\$d (Note: in context-free scenario's, context\$X can be omitted):



On receiving the index of a Policy-chosen arm through action\$choice, Bandit is expected to return a named list containing at least reward\$reward and, where computable, reward\$optimal:

<sup>&</sup>lt;sup>10</sup>For each *t*, a Bandit generated matrix describes both features shared by all arms and features that differ per arm. In other words, each column of this matrix represents a single arm's feature vector—combining, for instance, overall user and arm specific article weights. See also Section 2.1.



The following skeleton code gives an overview of how the above is implemented in **contextual**'s Bandit superclass:

```
Bandit <- R6::R6Class(</pre>
  portable = TRUE,
  class
           = FALSE,
  public
           = list(
                            # Number of arms (integer)
    k
                = NULL,
    d
                = NULL,
                            # Dimension of context feature vectors (integer)
                            # Pregenerate contexts & rewards? (boolean)
    precaching = FALSE,
    class_name = "Bandit", # Bandit name - required (character)
    initialize = function() {
      # Initialize Bandit. Set self$d and self$k here.
    },
    get_context = function(t) {
      stop("Bandit subclass needs to implement bandit$get_context()")
      # Return list with self$k, self$d & if applicable context matrix X.
      list(X = context, k = arms, d = features)
    },
    get_reward = function(t, context, action) {
      stop("Bandit subclass needs to implement bandit$get_reward()")
      # Return list with the reward.
      list(reward = reward_for_choice_made, optimal = optimal_reward_value)
    },
    . . .
  )
)
```

The main Bandit functions can be futher detailed as follows:

- new() generates and instantializes a new Bandit instance.
- get\_context(t)
  - t: [integer], time step t.

Returns a named list containing the current d x k dimensional matrix context\$X, the number of arms context\$k and the number of features context\$d.

- get\_reward(t, context, action)
  - t: [integer], time step t.
  - context: [list], containing the current context\$X (d x k context matrix), context\$k
     (number of arms) and context\$d (number of context features) (as set by bandit).
  - action: [list], containing action\$choice (as set by policy).

Returns a named list containing reward\$reward and, where computable, reward\$optimal (used by "oracle" policies and to calculate regret).

- post\_initialization() Called after class and seed initialisation, but before the start of the simulation. Set random values that remain available throughout the life of a Bandit here.
- generate\_bandit\_data() Called after class and seed initialisation, but before the start of a simulation. Only called when bandit\$precaching is set to TRUE (default FALSE). Pregenerate contexts and rewards here.

As already previously indicated in Table 2 in Section 3.1 Bandit, **contextual** already contains several predefined Bandits. For each of these Bandits, the package offers at least one example script, to be found in the package's demo directory:

- BasicBernoulliBandit: This basic (context-free) k-armed bandit synthetically generates rewards based on a weight vector.
- BasicGaussianBandit: Context-free Gaussian multi-armed bandit.
- ContextualBernoulliBandit: An example of a more complex and versatile synthetic bandit. It pregenerates both a randomized context matrix and reward vectors
- ContextualLinearBandit: Samples data from linearly parameterized arms.
- ContextualWheelBandit: The Wheel bandit game offers an artificial problem where the need for exploration is smoothly parameterized through an exploration parameter (Riquelme *et al.* 2018).
- ContextualLogitBandit: Samples data from a basic logistic regression model.
- ContinuumBandit: A basic example of a continuum bandit.
- OfflineReplayEvaluatorBandit: A basic example of a bandit that makes use of offline data as introduced by Li *et al.* (2010).

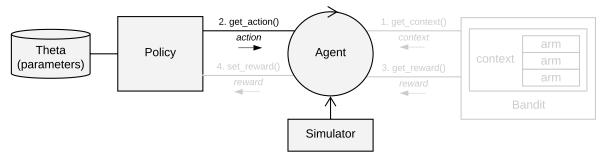
Any of these bandits can be deployed to run policies without further ado. They can, however, also be used as either examples or templates for your own custom Bandit implementation(s), or as superclasses for sub-subclass implementations.

#### **Policy**

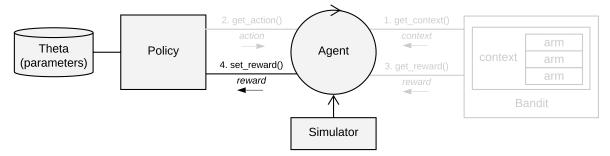
Policy is another often subclassed contexual superclass. Just like the Bandit superclass, Policy is an abstract class that declares methods without itself offering an implementation. Any Policy subclass is therefore expected to implement get\_action() and set\_reward(). Also, any parameters that keep track or summarize context, action and reward values are required to be saved to Policy's named list theta.

On every  $t = \{1, ..., T\}$ , a policy receives a  $d \times k$  dimensional matrix context\$X, the current number of Bandit arms in context\$k, and the current number of contextual features in context\$d. It has to compute which of the k Bandit arms to pull by taking into account this contextual information plus

the policy's current parameter values stored in the named list theta. On selecting an arm, the policy then returns its index as action\$choice:



On pulling a Bandit arm the policy receives a Bandit reward through reward\$reward. In combination with the current context\$X and action\$choice, this reward can then be used to update to the policy's parameters as stored in list theta:



Note: in context-free scenario's, context\$X can be omitted.

The following skeleton code gives an overview of how the above is implemented in **contextual**'s Policy superclass:

```
Policy <- R6::R6Class(</pre>
  portable = FALSE,
  class = FALSE,
  public = list(
    action
                  = NULL,
                                # action results (list)
                  = NULL.
                                # policy parameters theta (list)
    theta
                                # theta to arms "helper" (list)
    theta_to_arms = NULL,
                  = "Policy",
                                # policy name - required (character)
    class_name
    initialize = function() {
      self$theta <- list()</pre>
                                # initializes theta list
      self$action <- list()</pre>
                                # initializes action list
    },
    get_action = function(t, context) {
      # Selects arm based on theta & context, returns it in action$choice
      stop("Policy$get_action() has not been implemented.")
    },
    set_reward = function(t, context, action, reward) {
      # Updates parameters in theta based on reward awarded by bandit
      stop("Policy$set_reward() has not been implemented.")
```

```
},
...
)
```

Policy's main functions can be futher detailed as follows:

- new() Generates and initializes a new Policy object.
- get\_action(t, context)
  - t: [integer], time step t.
  - context: [list], containing the current context\$X (d x k context matrix), context\$k (number of arms) and context\$d (number of context features).

Computes which arm to play based on the current values in named list theta and the current context.

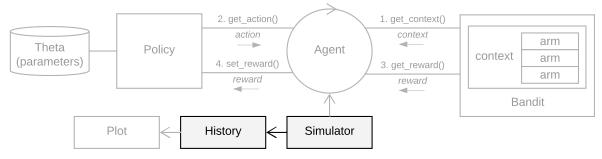
Returns a named list containing action\$choice, which holds the index of the arm to play.

- set\_reward(t, context, action, reward)
  - t: [integer], time step t.
  - context: [list], containing the current context\$X (d x k context matrix), context\$k (number of arms) and context\$d (number of context features).
  - action: [list], containing action\$choice (as set by policy).
  - reward: [list], containing reward\$reward and, if available, reward\$optimal (as set by bandit).

Returns the set of updated parameters in list theta.

• set\_parameters() Helper function, called during a Policy's initialisation, assigns the values it finds in list self\$theta\_to\_arms to each of the Policy's k arms. The parameters defined here can then be accessed by arm index in the following way: theta[[index\_of\_arm]]\$parameter\_name.

#### History



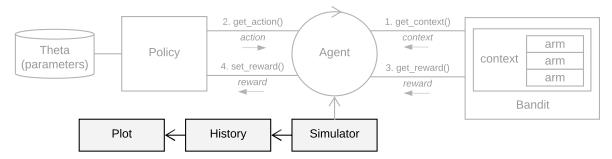
A Simulator aggregates the data acquired during a simulation in a History object's private data.table log. It also calculates per agent average cumulative reward, and, when the optimal outcome per t is known, per agent average cumulative regret. It is furthermore possible to plot() a History object, summarize() it, or obtain, for example, a data.frame() or a data.table() from any History instance:

```
history <- Simulator$new(agent)$run()
dt <- history$get_data_table()</pre>
```

Some other History functions:

- set(index, t, action, reward, policy\_name, simulation\_index, context\_value = NA, theta\_value = NA) Stores one row of simulation data. Generally not called directly, but rather through a Simulator instance.
- save(filename = NA) Writes History to a file with name filename.
- load(filename, interval = 0) Reads a History log file with name filename. If interval is larger than 0, every other interval row of data is read instead of the full data file.
- reindex(truncate = TRUE) Removes empty rows from the History log, reindexes the t column, and, when truncate is TRUE, truncates the resulting data to the number of rows of the shortest simulation.

#### Plot



The Plot class takes an History object and offers several ways to plot it, each optimized to be able to plot gigabytes worth of data, quickly:

- average: plots the average reward or regret over all simulations per Agent instance (that is, over each Bandit and Policy instance combo) over time.
- cumulative: plots the average reward or regret over all simulations per Agent instance over time.
- arms: plots ratio of arms chosen on average at each time step, in percentages, totaling 100

Plot objects can be instantiated directly, or, more commonly, by calling the plot() function. In either case, make sure to specify a History instance and one of the plot types specified above:

```
# plot a history object through default generic plot() function
plot(history, type = "arms")

# or call the Plot() directly
p1 <- Plot$new()$cumulative(history)
p2 <- Plot$new()$average(history)</pre>
```

Multiple Agent instances can be displayed within one Plot, and multiple plots can themselves again be combined into one graph<sup>11</sup>. Some example plots that illustrate many of Plot()'s features:

```
bandit
           <- ContextualBernoulliBandit$new(weights = c(0.9, 0.1, 0.1))</pre>
           <- list(Agent$new(RandomPolicy$new(), bandit),
agents
                   Agent$new(OraclePolicy$new(), bandit),
                   Agent$new(ThompsonSamplingPolicy$new(1.0, 1.0), bandit),
                   Agent$new(Exp3Policy$new(0.1), bandit),
                   Agent$new(GittinsBrezziLaiPolicy$new(), bandit),
                   Agent$new(UCB1Policy$new(), bandit))
history <- Simulator$new(agents,</pre>
                            horizon
                                        = 100,
                            simulations = 1000)$run()
par(mfrow = c(3, 2), mar = c(5, 5, 1, 1))
plot(history, type = "cumulative", use_colors = FALSE, no_par = TRUE)
plot(history, type = "cumulative", regret = FALSE, legend = FALSE,
     limit_agents = c("UCB1"), traces = TRUE, no_par = TRUE)
plot(history, type = "cumulative", regret = FALSE, rate = TRUE, disp = "sd",
     limit_agents = c("Exp3", "ThompsonSampling"),
     legend_position = "bottomright", no_par = TRUE)
plot(history, type = "cumulative", rate = TRUE, plot_only_ci = TRUE,
     disp = "var", limit_agents = c("UCB1", "GittinsBrezziLai"),
     smooth = TRUE, legend_position = "topright", no_par = TRUE)
plot(history, type = "average", disp = "ci", regret = FALSE, interval = 10,
     smooth = TRUE, legend_position = "bottomright", no_par = TRUE)
plot(history, limit_agents = c("ThompsonSampling"), type = "arms",
     interval = 20, no_par = TRUE)
```

<sup>&</sup>lt;sup>11</sup>To do so, call plot() with no\_par = TRUE. This enables the setting of custom plotting parameters through R's default par() functionality, allowing the formatting, layout and combination of single or multiple plots.

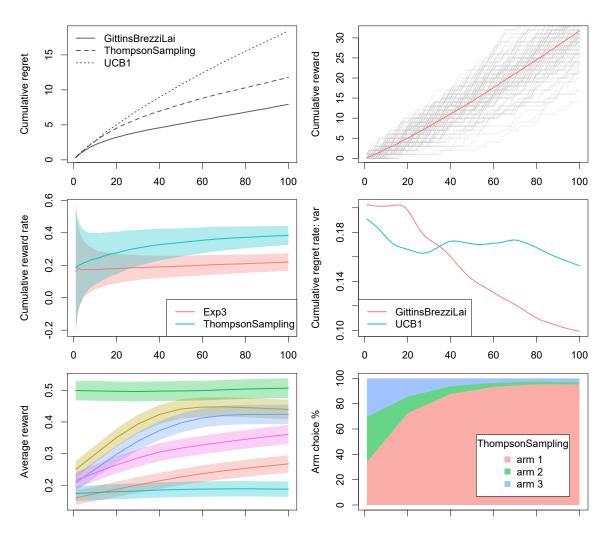


Figure 5: Overview hightlighting the versatility of contextual's Plot() class. From left to right, and top to bottom: 1. Grayscale plot 2. Plotting traces 3. Cumulative reward with SD 4. Dispersion plot (here, variance) 5. Color plot with 95% confidence interval 6. Arm choice percentage plot

## 5. Custom bandits and policies

The current section illustrates how to develop custom Bandit and Policy subclasses through an exploration of **contextual**'s BasicBernoulliBandit and its EpsilonFirst, EspilonGreedy, and LinUCB policy implementations.

#### 5.1. BasicBernoulliBandit: a minimal Bernoulli bandit

Where not otherwise noted, all Bandit implementations in the current paper refer to (or will be configured as) multi-armed Bandits with Bernoulli rewards. For Bernoulli Bandits, the reward received is either a zero or a one: on each t they offer either a reward of 1 with probability p or a reward of 0 with probability 1-p. In other words, a Bernoulli bandit has a finite set of arms k

 $\in \{1, ..., K\}$  where the rewards for each arm k is distributed Bernoulli with parameter  $p_k$ , the expected reward of the arm.

One example of a very simple context-free Bernoulli bandit is **contextual**'s minimal Bandit implementation, BasicBernoulliBandit:

```
BasicBernoulliBandit <- R6::R6Class(</pre>
  inherit = Bandit,
  portable = TRUE,
  class = FALSE,
  public = list(
    weights = NULL,
    class_name = "BasicBernoulliBandit",
    initialize = function(weights) {
      self$weights <- weights
      self$k
                        <- length(self$weights)
    },
    get_context = function(t) {
      context <- list(</pre>
        k = self k
      )
    },
    get_reward = function(t, context, action) {
                     <- as.double(runif(self$k) < self$weights)
      rewards
      optimal_arm
                     <- which.max(rewards)
      reward <- list(</pre>
                                  = rewards[action$choice],
        reward
        optimal_arm
                                  = optimal_arm,
        optimal_reward
                                  = rewards[optimal_arm]
      )
    }
  )
)
```

BasicBernoulliBandit expects a weight vector of probabilities, where every element in weight represents the probability of BasicBernoulliBandit returning a reward of 1 for one of its k arms.

#### **5.2.** EpsilonFirstPolicy

An important feature of **contextual** is that it eases the conversion from formal and pseudocode policy descriptions to clean R6 classes. We will give several examples of such conversions in the current paper, starting with the implementation of the  $\epsilon$ -first algorithm. In this context-free, "naive" policy, also known as AB(C) testing, a pure exploration phase is followed by a pure exploitation phase.

In that respect, the  $\epsilon$ -first algorithm is equivalent to a randomized controlled trial (RCT). An RCT, generally referred to as the gold standard clinical research paradigm, is a study design where subjects are allocated at random to receive one of several clinical interventions. On completion of an RCT, the interventions are compared. If one intervention proves significantly better than the others, that intervention is suggested to be the superior "evidence-based" option from then on.

In other words: an  $\epsilon$ -first policy starts out by exploring arms at random during the first  $\epsilon \cdot N$  time steps. The following  $(1 - \epsilon) \cdot N$  steps,  $\epsilon$ -first fully exploits the arm that proved the best during the previous  $\epsilon \cdot N$  exploration phase. In pseudocode:

#### **Algorithm 1** $\epsilon$ -first

```
Require: N \in \mathbb{Z}^+ - horizon of the experiment.

Require: \epsilon \in [0,1] - exploration tuning parameter n_k \leftarrow 0 for all actions a \in \{1, \dots, \mathcal{A}\} (count how many times an arm has been chosen) \hat{\mu}_k \leftarrow 0 for all actions a \in \{1, \dots, \mathcal{A}\} (estimate of expected reward per arm) for t = 1, \dots, T do

if t \leq \epsilon \cdot N then

play a random arm out of all actions a \in \{1, \dots, \mathcal{A}\} else

play action a_t = \arg\max_a \hat{\mu}_{t=\eta,a} with ties broken arbitrarily end if

observe real-valued payoff r_t

n_{a_t} \leftarrow n_{a_{t-1}} + 1 // Update count

\hat{\mu}_{t,a_t} \leftarrow \frac{r_t - \hat{\mu}_{t-1,a_t}}{n_{a_t}} // Update expected reward end for
```

And the above pseudocode converted to an EpsilonFirstPolicy class:

```
EpsilonFirstPolicy
                               <- R6::R6Class(
 inherit = Policy,
 public = list(
    first = NULL,
   class_name = "EpsilonFirstPolicy",
    initialize = function(epsilon = 0.1, N = 1000) {
      super$initialize()
      self$first
                                <- ceiling(epsilon*N)
   },
    set_parameters = function(context_params) {
                                <- list('n' = 0, 'mean' = 0)
      self$theta to arms
      # Here we define a list with 'n' and 'mean' theta parameters to each
      # arm through helper variable self$theta_to_arms. That is, when the
      # number of arms is 'k', the above would equal:
      # selftheta <- list(n = rep(list(0,k)), 'mean' = rep(list(0,k)))
      # ... which would also work just fine, but is much less concise.
      # When assigning both to self$theta directly & via self$theta_to_arms,
      # make sure to do it in that particular order.
```

```
},
    get_action = function(t, context) {
      if (sum_of(self$theta$n) < self$first) {</pre>
        action$choice
                                  <- sample.int(context$k, 1, replace = TRUE)
      } else {
        action$choice
                                 <- max_in(self$theta$mean)</pre>
      }
      action
    },
    set_reward = function(t, context, action, reward) {
                                  <- action$choice
      arm
                                  <- reward$reward
      reward
      inc(self$theta$n[[arm]]) <- 1</pre>
      if (sum_of(self$theta$n) < self$first - 1) {</pre>
        inc(self$theta$mean[[arm]]) <-</pre>
            (reward - self$theta$mean[[arm]]) / self$theta$n[[arm]]
      }
      self$theta
    }
 )
)
```

To evaluate this policy, instantiate both an EpsilonFirstPolicy and a ContextualBernoulliBandit <sup>12</sup>. Then add the Bandit/Policy pair to an Agent. Next, add the Agent to a Simulator. Finally, run the Simulator, and plot() the its History log:

```
horizon
                   <- 100
simulations
                   <- 1000
weights
                   <-c(0.6, 0.3, 0.3)
                   <- EpsilonFirstPolicy$new(epsilon = 0.5, N = horizon)
policy
bandit
                   <- ContextualBernoulliBandit$new(weights = weights)</pre>
agent
                   <- Agent$new(policy,bandit)
                   <- Simulator$new(agents = agent,
simulator
                                     horizon = horizon,
                                     simulations = simulations)
                   <- simulator$run()
history
plot(history, type = "cumulative", no_par = TRUE, legend_border = FALSE)
plot(history, type = "arms", no_par = TRUE)
```

 $<sup>^{12}</sup>$ A contextual version of the BasicBernoulliBandit subclass, introduced in Section 3.2.3. In contrast to the k dimensional weight vector BasicBernoulliBandit uses to generate its context-free rewards, ContextualBernoulliBandit generates both contexts and rewards based on some  $d \times k$  weight matrix. For implementation details, see **contextual**'s source code.

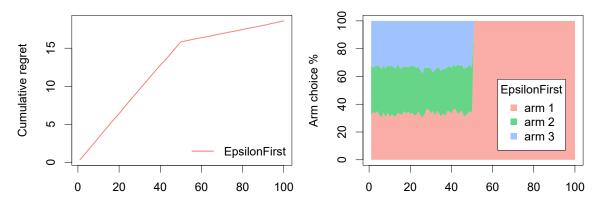


Figure 6: To the left, Epsilon First policy's cumulative regret over time. To the right, the percentage of simulations per time step for which each of the bandit's three arms where chosen. As can be observed in the arm choice plot, after fifty steps of exploration, the policy has settled overwhelmingly on arm one. On exploiting this arm, from thereon, it suffers significantly less regret than before.

#### 5.3. EpsilonGreedyPolicy

Contrary to the previously introduced  $\epsilon$ -first policy, an  $\epsilon$ -greedy algorithm (Sutton and Barto 1998) does not divide exploitation and exploration into two strictly separate phases—it explores with a probability of  $\epsilon$  and exploits with a probability of  $1 - \epsilon$ , right from the start. That is, an  $\epsilon$ -greedy policy with an  $\epsilon$  of 0.1 explores arms at random 10% of the time. The other  $1 - \epsilon$ , or 90% of the time, the policy "greedily" exploits the currently best-known arm.

This can be formalized in pseudocode as follows:

## **Algorithm 2** $\epsilon$ -greedy

```
Require: \epsilon \in [0,1] - exploration tuning parameter n_a \leftarrow 0 for all actions a \in \{1,\ldots,\mathcal{A}\} (count how many times an action has been chosen) \hat{\mu}_a \leftarrow 0 for all actions a \in \{1,\ldots,\mathcal{A}\} (estimate of expected reward per action) for t=1,\ldots,T do

if sample from unif(0,1) > \epsilon then

play action a_t = \arg\max_a \hat{\mu}_{t-1,a} with ties broken arbitrarily else

play a random action out of all actions a \in \{1,\ldots,\mathcal{A}\} end if

observe real-valued payoff r_t

n_{a_t} \leftarrow n_{a_{t-1}} + 1 // Update count

\hat{\mu}_{t,a_t} \leftarrow \frac{r_t - \hat{\mu}_{t-1,a_t}}{n_{a_t}} // Update expected reward end for
```

Converted to an EpsilonGreedyPolicy class:

```
EpsilonGreedyPolicy <- R6::R6Class(
  public = list(</pre>
```

```
epsilon = NULL,
    initialize = function(epsilon = 0.1) {
      super$initialize(name)
      self$epsilon <- epsilon</pre>
    },
    set_parameters = function() {
      self$theta_to_arms <- list('n' = 0, 'mean' = 0)</pre>
    },
    get_action = function(context, t) {
      if (runif(1) > epsilon) {
        action$choice <- max_in(theta$mean)</pre>
        action$choice <- sample.int(context$k, 1, replace = TRUE)</pre>
      }
      action
    },
    set_reward = function(context, action, reward, t) {
      arm <- action$choice</pre>
      reward <- reward$reward</pre>
      inc(theta$n[[arm]])
                               <- 1
      inc(theta$mean[[arm]]) <- (reward-theta$mean[[arm]]) / theta$n[[arm]]</pre>
      theta
    }
  )
)
```

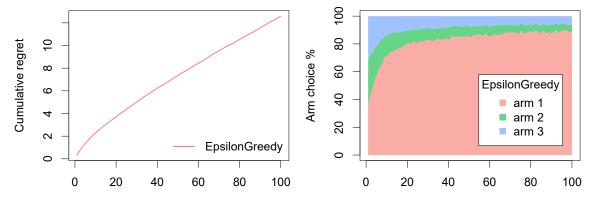


Figure 7: To the left, Epsilon Greedy policy's cumulative regret over time. To the right, the percentage of simulations per time step for which each of the bandit's three arms where chosen. The Epsilon Greedy policy starts to both explore and exploit right from the start, gradually choosing the best arm more and more.

Assign the new class, together with ContextualBernoulliBandit, to an Agent. Again, assign the Agent to a Simulator. Then run the Simulator and plot():

```
horizon <- 100 simulations <- 1000
```

```
weights
                   <-c(0.6, 0.3, 0.3)
policy
                   <- EpsilonGreedyPolicy$new(epsilon = 0.1)
bandit
                   <- ContextualBernoulliBandit$new(weights = weights)</pre>
agent
                   <- Agent$new(policy,bandit)
simulator
                   <- Simulator$new(agents = agent,
                                     horizon = horizon,
                                     simulations = simulations)
history
                   <- simulator$run()
plot(history, type = "cumulative", no_par = TRUE)
plot(history, type = "arms", no_par = TRUE)
```

## 5.4. Contextual Bandit: LinUCB with linear disjoint models

As a final example of how to subclass **contextual**'s Bandit superclass, we move from context-free algorithms to a contextual one. As described in Section 1, contextual bandits make use of side information to help them choose the current best arm to play. For example, contextual information such as a website visitors' location may be related to which article's headline (or arm) on the frontpage of the website will be clicked on most.

Here, we show how to implement and evaluate probably one of the most cited out of all contextual policies, the LinUCB algorithm with Linear Disjoint Models Li *et al.* (2010). The policy is more complicated than the previous two bandits, but when following its pseudocode description to the letter, it translates nicely to yet another Bandit subclass.

The LinUCBDisjoint algorithm runs one online ridge regression model per arm, using context features to predict rewards. Importantly, the algorithm also generates a confidence interval for this predicted payoff. The policy then chooses the arm with the highest upper confidence bound. In pseudocode, following Algorithm 1 from Li *et al.* (2010):

#### Algorithm 3 LinUCB with linear disjoint models

```
Require: \alpha \in \mathbb{R}^+, exploration tuning parameter for t = 1, \ldots, T do

Observe features of all actions a \in \mathcal{A}_t : x_{t,a} \in \mathbb{R}^d for a \in \mathcal{A} do

if a is new then

A_a \leftarrow I_d \text{ (d-dimensional identity matrix)}
b_a \leftarrow 0_{d \times 1} \text{ (d-dimensional zero vector)}
end if

\hat{\theta}_a \leftarrow A_a^{-1}b_a
p_{t,a} \leftarrow \hat{\theta}_a^T + \alpha \sqrt{x_{t,a}^T A_a^{-1} x_{t,a}}
end for

Play action a_t = \arg\max_a p_{t,a} with ties broken arbitrarily and observe real-valued payoff r_t
A_{a_t} \leftarrow A_{a_t} + x_{t,a_t} x_{t,a_t}^T
b_{a_t} \leftarrow b_{a_t} + r_t x_{t,a_t}
end for
```

Next, translating the above pseudocode into a well organized Bandit subclass:

```
LinUCBDisjointPolicy <- R6::R6Class(</pre>
  public = list(
    alpha = NULL,
    initialize = function(alpha = 1.0) {
      super$initialize(name)
      self$alpha <- alpha
    },
    set_parameters = function() {
      self$theta_to_arms <- list( 'A' = diag(1,self$d,self$d),</pre>
                                     b' = rep(0, self$d)
    },
    get_action = function(context, t) {
      expected_rewards <- rep(0.0, context$k)</pre>
      for (arm in 1:self$k) {
                    <- context$X[,arm]</pre>
        Α
                    <- theta$A[[arm]]</pre>
                    <- theta$b[[arm]]</pre>
        A_inv
                    <- solve(A)
         theta_hat <- A_inv %*% b
                    <- X %*% theta_hat
        mean
                    <- sqrt(tcrossprod(X %*% A_inv, X))
         expected_rewards[arm] <- mean + alpha * sd</pre>
      }
      action$choice <- max_in(expected_rewards)</pre>
      action
    },
```

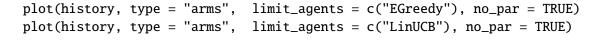
```
set_reward = function(context, action, reward, t) {
    arm <- action$choice
    reward <- reward$reward
    Xa <- context$X[,arm]

    inc(theta$A[[arm]]) <- outer(Xa, Xa)
    inc(theta$b[[arm]]) <- reward * Xa

    theta
}
)
)</pre>
```

Let us now evaluate the above LinUCBDisjointPolicy using a Bernoulli ContextualBernoulliBandit with three arms and three context features. In the code below we define each of ContextualBernoulliBandit's arms to be, on average, equally probable to return a reward. As can be confirmed in the two plots to the right below, where EpsilonGreedyPolicy and LinUCBDisjointPolicy actually show no difference in their overall arm preference. Yet LinUCBDisjointPolicy's awareness of the changing context allows it to learn the relationships between arms, rewards, and features, and select the right arm in the right context nevertheless.

```
horizon
            <- 100L
simulations <- 300L
                       # k=1 k=2 k=3
                                                    -> columns represent arms
weights
            <- matrix(c(0.8, 0.1, 0.1,
                                            # d=1 -> rows represent
                         0.1, 0.8, 0.1,
                                            # d=2
                                                       context features.
                         0.1, 0.1, 0.8),
                                            \# d=3
                        nrow = 3, ncol = 3, byrow = TRUE)
bandit
            <- ContextualBernoulliBandit$new(weights</pre>
                                                          = weights,
                                              precaching = TRUE)
            <- EpsilonGreedyPolicy$new(0.1)
eg_policy
lucb_policy <- LinUCBDisjointPolicy$new(0.6)</pre>
            <- list(Agent$new(eg_policy, bandit, "EGreedy"),
agents
                    Agent$new(lucb_policy, bandit, "LinUCB"))
simulation <- Simulator$new(agents, horizon, simulations)</pre>
history
            <- simulation$run()
plot(history, type = "cumulative", no_par = TRUE, legend_border = FALSE)
```



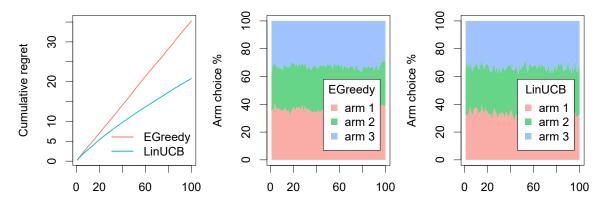


Figure 8: To the left, both policies' cumulative regret over time. Middle and right, Epsilon Greedy and LinUCB policies' cumulative regret over time. As can be observed in both arm choice percentage plots, on average, both policies choose each of the three arms about equally often. However, the cumulative regret plot clearly shows that, in contrast to the Epsilon Greedy policy, the LinUCB policy is able to map the contextual information available to it to its rewards, suffering less and less regret over time.

## 6. Subclassing bandits and policies

**contextual**'s extensibility does not limit itself to the subclassing of Policy classes. Through its R6 based object system it is easy to extend and override any **contextual** super- or subclass. Below, we demonstrate how to apply that extensibility to sub-subclass one Bandit and one Policy subclass. First, we extend BasicBernoulliBandit, replacing its Bernoulli based reward function with a Poisson based one (Presman 1991). Next, we implement an EpsilonGreedyAnnealingPolicy version of the  $\epsilon$ -greedy policy introduced in Section 5.3—where its EpsilonGreedyAnnealingPolicy subclass introduces a gradual reduction ("annealing") of the policy's *epsilon* parameter over T (Cesa-Bianchi and Fischer 1998; Kirkpatrick, Gelatt, and Vecchi 1983), in effect making the policy more exploitative over time.

```
BasicPoissonBandit <- R6::R6Class(
  inherit = BasicBernoulliBandit,
  portable = TRUE,
  class = FALSE,
  public = list(
    weights = NULL,
    class_name = "BasicPoissonBandit",
    # OVerride get_reward & generate Poisson based rewards
    get_reward = function(t, context, action) {
      reward_means = rep(2,self$k)
      rpm <- rpois(self$k, reward_means)
      rewards <- matrix(rpm < self$weights, self$k, 1)*1</pre>
```

```
<- which.max(rewards)</pre>
      optimal_arm
      reward <- list(</pre>
                                  = rewards[action$choice],
        reward
        optimal_arm
                                  = optimal_arm,
        optimal_reward
                                  = rewards[optimal_arm]
      )
    }
  )
)
EpsilonGreedyAnnealingPolicy <- R6::R6Class(</pre>
  # Class extends EpsilonGreedyPolicy
  inherit = EpsilonGreedyPolicy,
  portable = FALSE,
  public = list(
    class_name = "EpsilonGreedyAnnealingPolicy",
    # Override EpsilonGreedyPolicy's get_action, use annealing epsilon
    get_action = function(t, context) {
      self$epsilon <- 1 / log(t + 0.0000001)
      super$get_action(t, context)
    }
  )
)
weights <- c(7,1,2)
horizon <- 200
simulations <- 1000
bandit <- BasicPoissonBandit$new(weights)</pre>
eg_policy <- EpsilonGreedyPolicy$new(0.1)</pre>
ega_policy <- EpsilonGreedyAnnealingPolicy$new(0.1)</pre>
agents <- list(Agent$new(ega_policy, bandit, "EG Annealing"),</pre>
               Agent$new(eg_policy, bandit, "EG"))
simulation <- Simulator$new(agents, horizon, simulations, do_parallel = FALSE)</pre>
history <- simulation$run()</pre>
plot(history, type = "cumulative", no_par = TRUE, legend_border = FALSE,
              legend_position = "bottomright")
plot(history, type = "arms",
                               limit_agents = c("EG Annealing"), no_par = TRUE,
              interval = 25)
plot(history, type = "arms", limit_agents = c("EG"), no_par = TRUE,
              interval = 25)
```

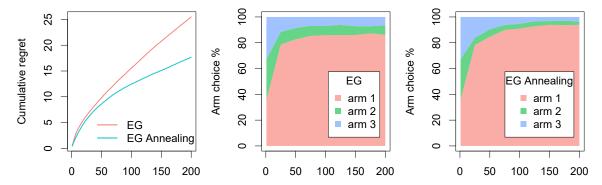


Figure 9: To the left, both policies' cumulative regret over time. Middle and right, the percentage of simulations per time step for which each of the bandit's three arms where chosen. In the rightmost plot, it can be observed that, in contrast to its non-annealing cousin, the annealing policy is able to explore the sub-optimal arms less and less over time.

## 7. Offline evaluation

Though it is, as demonstrated in the previous section, relatively easy to create basic synthetic Bandits to evaluate simple MAB and CMAB policies, the creation of more elaborate simulations that generate more complex contexts for more demanding policies can become very complicated very fast. To such an extent, that the implementation of such simulators regularly becomes more intricate than the analysis and implementation of the policies themselves (Strehl, Li, Wiewiora, Langford, and Littman 2006a). Moreover, even when succeeding in surpassing these technical challenges, it remains an open question if an evaluation based on simulated data reflects real-world applications—as modeling by definition introduces bias (Li *et al.* 2012, 2011).

It is, of course, possible to evaluate policies by running them in a live setting. Such live evaluations would deliver unbiased, realistic estimates of a policy's effectiveness. Running an evaluation on live data is, however, generally much slower than an offline evaluation, as online evaluations are dependent on active user interventions. (Mandel, Liu, Brunskill, and Popovic 2016; Tewari and Murphy 2017). Furthermore, the testing of policies on a live target audience, such as patients or customers, with potentially suboptimal policies, could become either dangerous or very expensive (Bastani and Bayati 2015).

Fortunately, there is also the option to evaluate bandit policies on offline interaction logs. To be of use in CMAB evaluation, such logs would, of course, need to contain observed contexts, rewards, and actions  $D = (x_{t,a_t}, a_t, r_{t,a_t})$ . As, among others, ad placement systems, web search engines, and recommendation engines habitually keep interactions logs, such data is widely available. There is a catch though; offline data only contains "bandit feedback", and as such, is "partially labeled" with respect to the bandit policies under evaluation(Strehl, Langford, Li, and Kakade 2010). That is, with logged data, we only know the reward values of the specific action that was chosen for each time step t.

As a result, we need some type of counterfactual estimator to evaluate "off-policy" logged actions. Off-policy, as we evaluate policies against logged bandit feedback gathered by some other policy (Li *et al.* 2012, 2011). And counterfactual, as we seek to estimate how these other policies perform against the logged data as if they were themselves in control of the action selection process (Bottou, Peters,

Quiñonero-Candela, Charles, Chickering, Portugaly, Ray, Simard, and Snelson 2013; Swaminathan and Joachims 2015).

In the next section, we introduce one example of such a counterfactual estimator by demonstrating contextual's implementation of Li *et al.* (2011)'s "replay" method (Nicol 2014). In a subsequent section, we demonstrate how this "replay" method is sensitive to bias—and how inverse propensity weighting can help remove this bias.

#### 7.1. The replay method

One approach to the use of offline data in off-policy evaluation is to recognize that we need to limit our evaluation to those rows of data where the action taken by the original logging policy equals the action suggested by the policy under evaluation (Li *et al.* 2012, 2011). In pseudocode, following Algorithm 2 from Li *et al.* (2011):

#### Algorithm 4 Replay Policy Evaluator

```
Require: Policy \pi
   Data stream of events S of length T
   h_0 \leftarrow \emptyset An initially empty history log
   R_{\pi} \leftarrow 0 An initially zero total cumulative reward
   L \leftarrow 0 An initially zero length counter of valid events
   for t = 1, \ldots, T do
      Get the t-th event (x_{t,a_t}, a_t, r_{t,a_t}) from S
      if \pi(h_{t-1}, x_{t,a_t}) = a_t then
         h_t \leftarrow \text{CONCATENATE}(h_{t-1}, (x_{t,a_t}, a_t, r_{t,a_t}))
         R_{\pi} = R_{\pi} + r_{t,a_t}
         L = L + 1
      else
         h_t \leftarrow h_{t-1}
      end if
   end for
   Output: rate of cumulative regret R_{\pi}/L
```

Below, an implementation of this algorithm (a version of **contextual**'s OfflineReplayEvaluatorBandit), followed by an offline evaluation of **contextual**'s LinUCBHybridPolicy. We feed the replay bandit a dataset that consists of 570061 rows, where every row represents a page view of a user browsing a web store's products (Kaptein, McFarland, and Parvinen 2018). For each page view, a product was presented with one of four persuasion strategies: no strategy (control group), authority (e.g., "recommended product"), social proof (e.g., "bestseller"), and scarcity (e.g., "almost out of stock"). Adding a product on a page to a shopping basket was counted as a success (rewarded by 1), not adding a product as a failure (rewarded by 0).

```
library(contextual)
library(data.table)
setwd(here("demo","paper_jss_replication_package"))
OfflineReplayEvaluatorBandit <- R6::R6Class(</pre>
```

```
inherit = Bandit,
  portable = TRUE,
  class = FALSE,
  private = list(
    S = NULL
  ),
  public = list(
    class_name = "OfflineReplayEvaluatorBandit",
    randomize = NULL,
    initialize = function(data_stream, k, d) {
                 <- k
      self$k
                                 # Number of arms (integer)
      self$d
                <- d
                                # Dimension context features (integer)
      private$S <- data_stream # Data stream, as data.table</pre>
    },
    post_initialization = function() {
      private$S <- private$S[sample(nrow(private$S))]</pre>
    get_context = function(index) {
      context <- list(</pre>
        k = self k,
        d = self d,
        X = matrix(private$S$daypart[[index]], self$d, self$k)
      )
      context
    },
    get_reward = function(index, context, action) {
                        <- as.double(private$S$reward[[index]])</pre>
      if (private$S$choice[[index]] == action$choice) {
        list(
          reward = reward
        )
      } else {
        NULL
      }
    }
  )
data_url <- "https://raw.githubusercontent.com"</pre>
data_url <- paste0(data_url,"/Nth-iteration-labs/contextual_data/master")</pre>
data_url <- paste0(data_url,"/data_persuasion_api/persuasion_api_daypart.csv")</pre>
data
         <- data.table::fread(data_url)</pre>
horizon <- nrow(data)</pre>
sims
       <- 10L
bandit <- OfflineReplayEvaluatorBandit$new(data, k = 4, d = 1)</pre>
```

See Figure 10 for a plot of the resulting click-through rate over time.

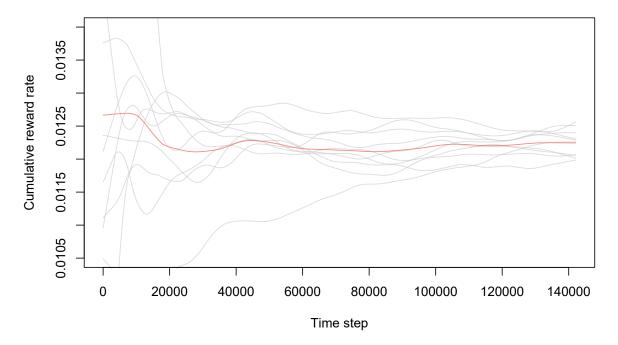


Figure 10: LinUCBHybridPolicy evaluated with OfflineReplayEvaluatorBandit. The offline bandit samples from 570061 rows with clicks for rewards and the display of one of four "persuasive strategies" to users of an online store representing the offline bandit's four arms. The context is a one dimensional context feature representing whether the page is shown during night or day.

### 7.2. Inverse propensity scoring

The replay method works well for unbiased logs—that is, logs where each arm is chosen at random, independent from its context, and where the original logging policy is known. In the current section, we will use Simpson's Paradox to demonstrate how replaying a biased dataset propagates this bias—and then illustrate how correct this bias through the use of inverse propensity scoring.

Imagine a popular website with sports and movie related articles. The unbiased click-through rate (CTR) per article category for both for male and female visitor is presented to the left in Table 3.

	Sport	Movie
Male	0.4 x 0.5	0.3 x 0.5
Female	0.8 x 0.5	0.7 x 0.5
Per category CTR	0.6	0.5

	Sport	Movie
Male	0.4 x 0.75	0.3 x 0.25
Female	0.8 x 0.25	0.7 x 0.75
Per category CTR	0.5	0.6

Table 3: To the left, a table with unbiased per category click-through rates for male and female visitors to a website. Here, visitors are randomly assigned to article categories. For example, male visitors click-through to sports articles four out of ten times, and three out of ten times to movie articles—displaying each type of article 50% of the time. To the right, a table representing the same site with the same visitors where the assignement of visitor types to categories is skewed. For instance, here, male visitors are shown sports type articles 75% and movie articles 25% of the time, and female visitors vice versa.

Clearly, both male and female visitors prefer sports over movie related articles, which is reflected by the overall CTR per article category. A scenario that can be converted to a **contextual** bandit scenario with much difficulty, with article categories for arms, and male and female visitors for context:

```
horizon
            <- 5000L
simulations <- 1L
                      S----M-----> Arm 1:
                                                    Sport
#
                            1
                                           Arm 2:
                                                    Movie
                           1
weights \leftarrow matrix( c(0.4, 0.3, #----> Context: Male
                     0.8, 0.7), #----> Context: Female
                     nrow = 2, ncol = 2, byrow = TRUE)
policy
            <- RandomPolicy$new()
bandit
            <- ContextualBasicBandit$new(weights = weights)</pre>
            <- Agent$new(policy, bandit)
agent
simulation <- Simulator$new(agent, horizon, simulations, save_context = TRUE)</pre>
history
            <- simulation$run()
u_dt
            <- history$get_data_table()</pre>
print(paste("Sport:",sum(u_dt[choice==1]$reward)/nrow(u_dt[choice==1])))
print(paste("Movie:",sum(u_dt[choice==2]$reward)/nrow(u_dt[choice==2])))
[1] "Sport: 0.592259577795152"
[1] "Movie: 0.502457002457002"
```

Great—our simulation did indeed generate the expected unbiased CTR per article category! Let us now run a replay type bandit and evaluate the CTR of both arms on this offline dataset:

Again, the correct, unbiased CTR per category.

Let us now suggest that the editor of this website just "knows' that men like sport type articles, and women like movie type articles, without taking a look at the actual data. So the editor has some lines of code added to the site that assigns movie related articles, on average, to 75% of female visitors and sport articles, on average, to 75% of the male visitors. See Table 3, to the right, for an overview of this setup. Surprisingly, even though overall both male and female visitors still prefer sports over movie related articles, the resulting (now biased) click-through rate (CTR) per article category is suddenly reversed: overall, visitor's now seem to prefer sports articles! This unexpected result, known as "Simpson's Paradox", serves as a perfect backdrop for a demonstation of the use of propensity scores in offline bandit evaluation. To do so, we first need to implement a policy that assigns male and female visitors to articles according to the editor's wishes:

```
BiasedPolicy <- R6::R6Class(</pre>
  portable = FALSE,
  class = FALSE,
  inherit = RandomPolicy,
  public = list(
    class_name = "BiasedPolicy",
    get_action = function(t, context) {
      if(context$X[1,1]==1) { # 1: Male, 0: Female.
        prob < c(0.75,0.25) # Editor thinks men like sports
      } else {
        prob < c(0.25,0.75) # Editor thinks women like movies
                         <- sample.int(context$k, 1, replace = TRUE, prob = prob)</pre>
      action$choice
      # Store the propensity score for the current action too:
      action$propensity <- prob[action$choice]</pre>
      action
    }
  )
)
```

There is one element in this code that has not been introduced yet: next to action\$choice, this policy also calculates the probability  $p_t$  of selecting this action, returning it in action\$propensity. This propensity can then:

- Be used for inverse propensity matching or weighting Austin (2011) to estimate the action's causal effect by accounting for contextual covariates Imbens and Rubin (2015); Pearl (2009).
- Stored in the log, resulting in  $D = (x_{t,a_t}, a_t, r_{t,a_t}, p_a)$ , and then be used to estimate average rewards using inverse propensity scoring (ips) by computing

$$ips(\pi) = \frac{1}{N} \sum_{t=1}^{N} \mathbb{1} \{ \pi(x_t) = a_t \} r_t / p_t$$
 (3)

where the indicator is 1 when  $\pi$ 's action matches the action in the logs (Kruijswijk *et al.* 2018). See for example Agarwal, Hsu, Kale, Langford, Li, and Schapire (2014); Dudík *et al.* (2011) and Swaminathan and Joachims (2015) for a comprehensive discussion of *ips* and other offline evaluation methods.

In other words, inverse propensity scoring can reduce bias in arm choice by controlling for the existence of confounding factors that skew random arm assignment. So let us again generate data for the same bandit—but this time round, generated by our editor's biased policy:

```
policy <- BiasedPolicy$new()</pre>
```

bandit <- ContextualBasicBandit\$new(weights = weights)</pre>

agent <- Agent\$new(policy, bandit, "Random")</pre>

simulation <- Simulator\$new(agent, horizon, simulations, save\_context = TRUE)</pre>

history <- simulation\$run()</pre>

b\_dt <- history\$get\_data\_table()

print(paste("Sport:",sum(b\_dt[choice==1]\$reward)/nrow(b\_dt[choice==1])))
print(paste("Movie:",sum(b\_dt[choice==2]\$reward)/nrow(b\_dt[choice==2])))

[1] "Sport: 0.497419610956729" [1] "Movie: 0.60217654171705"

Clearly, Simpson's Paradox is at work here: overall, visitor's do indeed seem to prefer sports articles now. Even worse, when we use this data to evaluate another policy, the bias propagates itself:

```
bandit <- OfflineReplayEvaluatorBandit$new(b_dt,2,2)</pre>
```

policy <- EpsilonGreedyPolicy\$new(0.1)
agent <- Agent\$new(policy, bandit, "rb")</pre>

simulation <- Simulator\$new(agent, horizon, simulations, reindex = TRUE)</pre>

history <- simulation\$run()</pre>

rb\_dt <- history\$get\_data\_table()</pre>

print(paste("Sport:",sum(rb\_dt[choice==1]\$reward)/nrow(rb\_dt[choice==1])))
print(paste("Movie:",sum(rb\_dt[choice==2]\$reward)/nrow(rb\_dt[choice==2])))

[1] "Sport: 0.511053315994798"
[1] "Movie: 0.618181818181818"

Simpson's Paradox all over again. Yet when we make one minor change to our original replay evaluator, implementing *ips* though the multiplaction of rewards by 1 / action\$propensity (see **contextual**'s OfflineReplayEvaluatorBandit for the full implementation), we are able to correct for the editor's bias:

```
bandit
                        <- OfflinePropensityWeightingBandit$new(b_dt,2,2)
policy
                        <- EpsilonGreedyPolicy$new(0.1)
                        <- Agent$new(policy, bandit, "prop")
agent
                        <- Simulator$new(agent, horizon, simulations, reindex = TRUE)</pre>
simulation
history
                        <- simulation$run()
                        <- history$get_data_table()</pre>
prop_dt
print(paste("Sport:",sum(prop_dt[choice==1]$reward)/nrow(prop_dt[choice==1])))
print(paste("Movie:",sum(prop_dt[choice==2])reward)/nrow(prop_dt[choice==2])))
[1] "Sport: 0.601543859649123"
[1] "Movie: 0.519125683060109"
```

# 8. Replication of Li et al 2010

In the current section, we demonstrate how **contextual** facilitates the comparison of bandit policies on big offline datasets by running a partial replication of Li *et al.* (2010). The paper describes how the authors made use of offline Yahoo! click-through rate data to evaluate and compare the effectiveness of several context-free and contextual policies—therein introducing both the offline policy evaluator outlined in the previous section and the LinUCB algorithm introduced in Section 5.4.

# 8.1. Description of the data

The dataset used in the Li *et al.* (2010) paper has been made available at the Yahoo! lab's website<sup>13</sup>. It contains the click-through rate from the Today news module on Yahoo!'s homepage over the course of several days in May 2009, totaling 45,811,883 separate events.

Each row in the dataset describes an interaction event (click or no click) of users shown a randomly chosen article. Each of these events contains the following information:

- 1. The ID's of each of a varying subset of 19 to 25 articles selected by human editors from a pool of 217 articles.
- 2. The ID of an article randomly chosen from the subset defined in 1. and positioned at the story position (that is, at the top of the Yahoo!'s website's "Today" segment).
- 3. Six features per article for each of the articles shown.
- 4. Six user features (with a distinct user for each event).
- 5. Whether or not a user clicked on the article at the story position.

<sup>&</sup>lt;sup>13</sup>At https://webscope.sandbox.yahoo.com/catalog.php?datatype=r&did=49

That is, for each event t an article represents one of A actions (that is, one of the 271 articles observed within the course of the 10 days covered by the dataset) with  $\mathbb{R}^6$  features  $X_{t,a}$  per arm, and another  $\mathbb{R}^6$  features  $X_{t,u}$  per unique visitor. Together, the flattened outer product of the user and article feature vector creates a  $\mathbb{R}^{36}$  feature vector  $X_t$  for each user and article pair with outcome value or reward  $r_t$  click (1) or no click (0). For the further details on the data structure and the general setup of the experiment, we refer the reader to Chu *et al.* (2009) and to the original Li *et al.* (2010) paper.

# 8.2. Data import

As the Yahoo data is too large to fit into memory, we imported most<sup>14</sup> of the dataset's CSV files into a **MonetDB** (Idreos, Groffen, Nes, Manegold, Mullender, and Kersten 2012) instance—a fast, open source column-oriented database management system with excellent R support<sup>15</sup>. The import script, example import scripts for several other databases (**MySQL**, **SQLite**, **Postgresql**) and all other source code related to this replication can be found in the package's demo/replication\_li\_2010 directory.

# 8.3. Custom bandit and policies

With the Yahoo! data imported into the MonetDB server, the next step was to create a custom offline YahooBandit plus seven Policy subclasses implementing the policies described in the Li *et al.* (2010) paper. Though most of these policies were already implemented in **contextual**, the fact that only a subset of all 271 articles or arms are shown to a visitor at a time meant we needed to make some minor changes to **contextual**'s exisiting classes to make the policies run smoothly on a continually shifting pool of active arms.

To facilitate these shifting arms, YahooBandit makes use of an self\$arm\_lookup table listing all 271 arms. This table enables the bandit to look up the currently active arms' indexes from the shifting set of article ID's as specified in the dataset for each time step t, and return these indexes to the policies under evaluation:

```
get_context = function(index) {
  # Retrieve the index of all arms this row/event.
  arm_indices_this_event <- seq(10, 184, by = 7)</pre>
  article_ids
                           <- row[arm_indices_this_event]</pre>
                           <- article_ids[!is.na(article_ids)]
  article ids
  article ids
                           <- match(article_ids,self$arm_lookup)</pre>
  context <- list(</pre>
    k = self k.
    d = self d.
    unique = self$unique, # Indexes of disjoint arms (user features)
    shared = self$shared, # Indexes of shared arms (article features)
                           # Indexes of arms this event.
    arms = article ids.
```

<sup>&</sup>lt;sup>14</sup>The first two CSV files of the Yahoo! dataset are somewhat irregular, as they contain articles with more than six features. We, therefore, decided to leave these two CSV files out of our import, resulting in 37,450,196 imported events, instead of the 45,811,883 events used in the original paper.

<sup>&</sup>lt;sup>15</sup>MonetDB can be downloaded at https://www.monetdb.org/

```
X = X
)
```

The policy classes then use this information to select and update only the currently active subset of arms. For instance, in YahooEpsilonGreedyPolicy's get\_action():

On completing the implementation of the aforementioned seven custom policy subclasses (Random, EGreedy, EGreedySeg, LinUCBDis, LinUCBHyb, UCB1 and UCB1Seg<sup>16</sup>) we then assigned them to six simulations—one for each of the six (0, 30, 20, 10, 5 and 1 percent) levels of sparsity defined in the original paper. This resulted in  $7 \times 6 = 42$  Agents, which were then run on the offline dataset as follows:

<sup>&</sup>lt;sup>16</sup>EGreedyDis and EGreedyHyb policies were too summarily described for us to be able to replicate them with confidence.

```
list (Agent$new(YahooLinUCBDisjointPolicy$new(0.2),
                  bandit, name = "LinUCB Dis", sparse = 0.99),
        Agent$new(YahooLinUCBHybridPolicy$new(0.2),
                  bandit, name = "LinUCB Hyb", sparse = 0.99),
        Agent$new(YahooEpsilonGreedyPolicy$new(0.3),
                  bandit, name = "EGreedy",
                                                  sparse = 0.99),
        Agent$new(YahooEpsilonGreedySegPolicy$new(0.3),
                  bandit, name = "EGreedySeg", sparse = 0.99),
        Agent$new(YahooUCB1AlphaPolicy$new(0.4),
                  bandit, name = "UCB1",
                                                  sparse = 0.99),
        Agent$new(YahooUCB1AlphaSegPolicy$new(0.4),
                  bandit, name = "UCB1Seg",
                                                 sparse = 0.99),
        Agent$new(YahooRandomPolicy$new(),
                  bandit, name = "Random"))
simulation <- Simulator$new(</pre>
    agents,
    simulations = simulations,
    horizon = horizon,
    do_parallel = TRUE,
    worker_max = worker_max.
    reindex = TRUE,
    progress_file = TRUE,
    include_packages = c("MonetDB.R"))
history <- simulation$run()</pre>
. . .
```

#### 8.4. Results

We were able to complete the full  $7 \times 6 = 42$  agent simulation over all of the 37,450,196 events in our database within 22 hours on a 64 core Intel Xeon Unbuntu server with 256GB of memory. We then proceeded to analyse the results of the first 4.7 million events (following the original paper, representing about a day worth of events) to reproduce Li *et al.* (2010)'s Figure 4b: "CTRs in evaluation data with varying data sizes in the learning bucket.". Just like the original paper, the replicated Figure 11 reports each algorithm's relative CTR for all of the defined data sparsity levels, that is, each algorithm's CTR divided by the random policy's CTR.

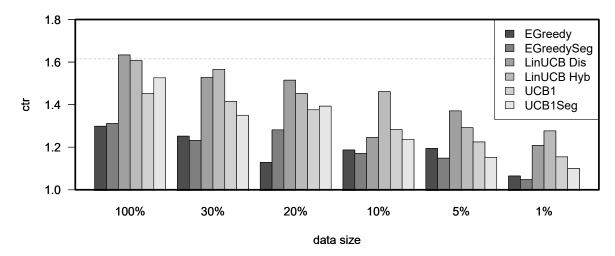


Figure 11: Replication of Figure 4b on Yahoo! dataset's day three: "CTRs in evaluation data with varying data sizes in the learning bucket." from Li *et al.* (2010).

As can be observed in Figure 11, after one day of learning, the conclusions of the original paper still stand. First, features again prove to be of use at all levels of sparsity, as LinUCB policies outperform the others consistently. Second, UCB policies generally outperform  $\epsilon$ -greedy ones. And third, Hybrid LinUCB again shows benefits when the data is small, as can be deduced from it doing better in the 1% bucket. Still, as we started our simulation on the third day instead of the first, our results are close to, but not quite the same as those reported in the original paper. Particularly the third conclusion, that of the relative advantage of Hybrid LinUCB with sparse data, seems to be slightly less convincing in our Figure 11.

So we decided to run a simulation that continued to learn beyond the first day for the sparse (1%) data condition to test whether Hybrid LinUCB's reported relative advantage would prove stable over time.

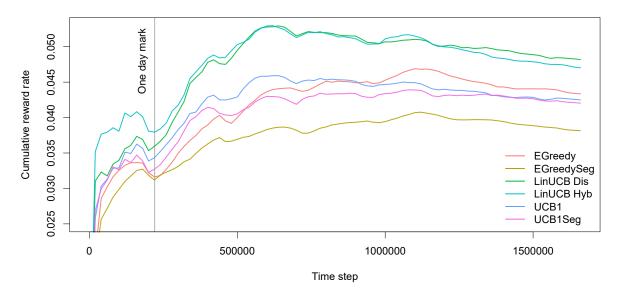


Figure 12: A plot of the cummulative reward rate (equals click-through rate) for EGreedy, EGreedySeg, LinUCB Dis, LinUCB Hyb, UCB1 and UCB1Seg policies over eight days of events from the Yahoo dataset at 1% sparsity. The plot's sinoidal wave pattern reflects visitors' average cyclical daily waxing and waning click-through tendendy.

On closer examiniation of the resulting plot in Figure 12, it becomes clear that the policies did not settle after one day of training. For one, on inspection of the full span of about eight days of learning, Hybrid LinUCB's advantage over Disjoint LinUCB gradually diminishes and turns into an advantage for the Disjoint version. Also, surprisingly, over the full eight days, the  $\epsilon$ -greedy policy goes from the worst to third best policy overall, becoming the best context-free policy—clearly outperforming both context-free UCB policies. Though we intend to further analyze these discrepancies, for now, these results seem to pose questions for two out of three conclusions drawn in the original paper—leaving only the first outcome, the superiority of the contextual LinUCB in comparison to several context-free ones. Underlining the benefits of **contextual**, as it enabled us to replicate and confirm the original Li *et al.* (2010) paper, and then explore it further: extending Bandit and Policy classes, running simulations in parallel on an offline dataset and plotting and analyzing the results—within 48 hours.

## 9. Discussion and future work

Statistical computational methods, in R or otherwise, are regularly made available through single-use scripts or basic, isolated code packages (Gandrud 2016). Usually, such code examples are meant to give a basic idea of a statistical method, technique or algorithm in the context of a scientific paper (Stodden, Guo, and Ma 2013). Such code examples offer their scientific audience a first inroad towards the comparison and further implementation of their underlying methods (Buckheit and Donoho 1995). However, when a set of well-researched interrelated algorithms, such as MAB and CMAB policies, find growing academic, practical and commercial adoption, it becomes crucial to offer a more standardized and more accessible way to compare such methods and algorithms (Mesirov 2010).

It is on that premise that we decided to develop the **contextual** R package—a package that would offer an open bandit framework with easily extensible bandit and policy libraries. To us, it made the most sense to create such a package in R (R Core Team 2018), as R is currently the de facto language for

the dissemination of new statistical methods, techniques, and algorithms (Tippmann 2015)—while it is at the same time finding ever-growing adoption in industry (Muenchen 2012). The resulting lively exchange of R related code, data, and knowledge between scientists and practitioners offers precisely the kind of cross-pollination that **contextual** intends to facilitate.

As the package is intended to be usable by practitioners, scientists and students alike, we started our paper with a general introduction to the (contextual) multi-armed bandit problem, followed by a compact formalization. We then demonstrated how our implementation flows naturally from this formalization, with Agents that cycle Bandits and Policies through four function calls: get\_context(), get\_action(), get\_reward() and set\_reward(). Next, we evaluated some of contextual's built-in policies, delved deeper into contextual's class structure, extended contextual's Bandit and Policy superclasses, demonstrated how to evaluate Policies on offline datasets, and, finally replicated a frequently cited CMAB paper.

Though the package is fully functional and we expect no more changes to its core architecture and API, there is ample room to further improve and extend **contextual**. We intend to expand **contextual**'s documentation and tests. We expect to include more bandit paradigms, such as dueling and combinatorial bandits. We expect to add other offline bandit types, such as a doubly robust bandit (Dudík *et al.* 2011). We are interested in growing our policy library—possibly by creating a separate repository where both existing and new CMAB policies are shared, evaluated and compared. Finally, we hope that the package will find an active community of users and developers, thereby introducing more and more people to the refined sequential decision strategies offered by contextual bandit policies and algorithms.

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# 10. Appendix A: UML diagrams

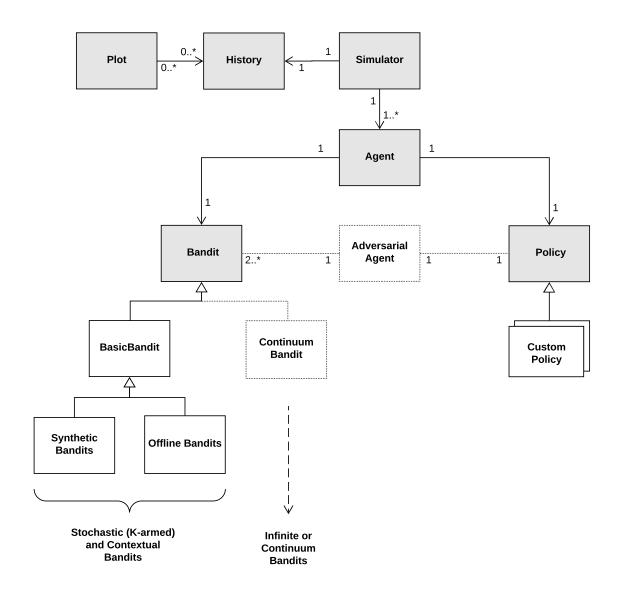


Figure 13: contextual UML Class Diagram

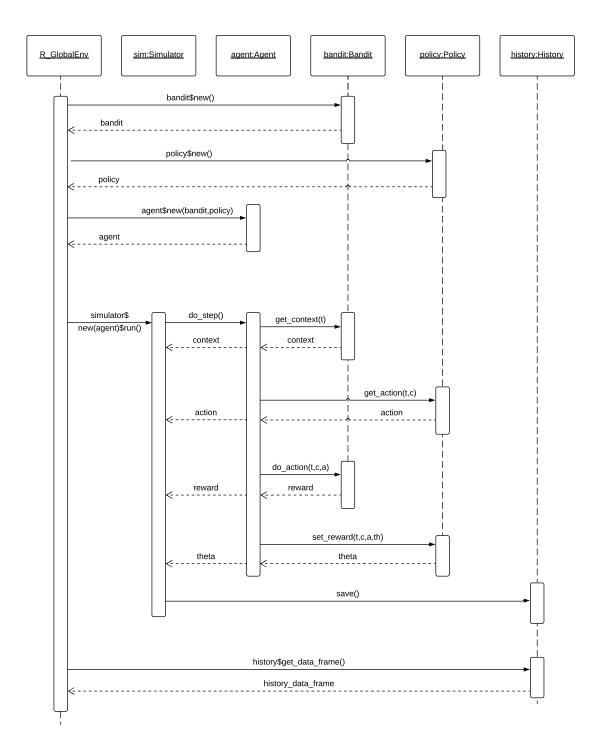


Figure 14: contextual UML Sequence Diagram

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