

# A BNP Approach to the Multi-Armed Bandit **Problem for Traits Allocation Models**

Federico Camerlenghi Mario Beraha Claudio Del Sole

> University of Milano – Bicocca, Milan, Italy, claudio.delsole@unimib.it



#### Traits allocation models

Consider a **countable set** of **traits** or **features** (e.g. species, topics, genes):

- each observation displays a **finite subset** of traits, with a **level of belonging** (here, a count) for each trait;
- observations are collected from multiple populations, e.g. forests, books;
- the same trait may appear in different observations both within the same population and across populations  $\rightarrow$  the set of traits is shared among populations!

$$X_{11} =$$

$$X_{11} = X_{12} = X_{12}$$

$$X_{12} = X_{12} = X_{12}$$

$$X_{21} = X_{22} = X_{12}$$

$$X_{31} =$$

$$X_{41}=\ldots$$

$$X_{12} =$$

$$X_{32}=\ldots$$

$$X_{\it \Delta}$$

$$X_{43} = \dots$$

 $X_{13} = 1$ 

 $X_{23} = \text{empty}$ 

 $X_{33} =$ 

 $X_{13} = 1$ 

 $X_{23} = \text{empty}$ 

Consider d populations, with  $n_i$  observations collected from population  $j = 1, \ldots, d$ . The observation  $X_{ij}$  from population j is represented as

$$X_{ij} = \sum_{k>1} A_{ijk} \, \delta_{\psi_k}, \qquad i = 1, \dots, n_j,$$

where  $A_{ijk} \geq 0$  is the **count** for trait  $\psi_k$  in population j.

Nonparametric model: each observation  $X_{ij}$  is an i.i.d. realization of a Poisson process, driven by the finite discrete measure  $\mu_i$ :

$$A_{ijk} \overset{ind}{\sim} \mathsf{Poisson}(\lambda_{jk}), \qquad \mu_j = \sum_{k \geq 1} \lambda_{jk} \, \delta_{\psi_k}.$$

Some useful notation:

- the **total count** for trait  $X_k$  in population j is  $M_{jk} = \sum_{i=1}^{n_j} A_{ijk}$ ;
- the set of traits appearing at least once in population j is  $\mathcal{K}_i = \{k \geq 1 : M_{jk} > 0\}$ .

## Multi-armed bandit for traits discovery

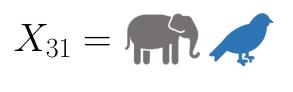
**Problem**: choose from which population to sample the next observation, with the goal of discovering new traits.

$$X_{11} =$$

$$X_{21} =$$













$$X_{32} =$$

$$X_{32} =$$

$$X_{33} =$$

$$X_{43} =$$

Multi-armed bandit formulation: sequentially select one among the possible actions (sampling from a certain population) to maximize the cumulative reward (the number of discovered traits).

The **random reward** of population j is the number of **new traits** discovered in a new observation:

$$R_j = \sum_{k \ge 1} \mathbb{1} \left( A_{(n_j+1)jk} > 0, \sum_{j=1}^d M_{jk} = 0 \right) = \sum_{k \notin \mathcal{K}} \mathbb{1} \left( A_{(n_j+1)jk} > 0 \right),$$

where  $\mathcal{K} = \bigcup_{j=1}^{d} \mathcal{K}_j$  is the set of traits appearing in **at least one** population.

Optimal strategy: choose the population maximizing the conditional expected reward, given the past observations,

$$\mathbb{E}\left[R_j \mid \mathbf{X}\right] = \sum_{k \notin \mathcal{K}} \left(1 - e^{-\lambda_{jk}}\right), \qquad j = 1, \dots, d.$$

**Statistical problem:** how to **estimate** the population **parameters**  $\mu_1, \ldots, \mu_d$ ?

#### Bayesian nonparametric approach

**Hierarchical prior**: the distribution of measures  $\mu_1, \ldots, \mu_d$  is a hierarchical **process**:

$$\mu_{j} = \sum_{k \geq 1} \lambda_{jk} \, \delta_{\psi_{k}}, \qquad \lambda_{jk} \mid \lambda_{0k} \stackrel{ind}{\sim} \operatorname{Gamma}(\theta_{j} \lambda_{0k}, 1), \qquad j = 1, \dots, d,$$

$$\mu_{0} = \sum_{k \geq 1} \lambda_{0k} \, \delta_{\psi_{k}} \, \sim \, \operatorname{CRM}(\theta_{0} \rho),$$

- where  $\theta_0, \theta_1, \dots, \theta_d > 0$  are concentration parameters,
- and  $\rho$  is the Lévy measure characterizing the **distribution of jumps**  $(\lambda_{0k})_{k\geq 1}$  in  $\mu_0$ .

**Posterior distribution**: the posterior of the parameters for the unseen traits is tractable:

$$\mu_j^* = \sum_{k \notin \mathcal{K}} \lambda_{jk} \, \delta_{\psi_k}, \qquad \lambda_{jk} \mid \lambda_{0k}, \boldsymbol{X}_j \stackrel{ind}{\sim} \operatorname{Gamma}(\theta_j \lambda_{0k}, 1 + n_j), \qquad j = 1, \dots, d,$$

$$\mu_0^* = \sum_{k \notin \mathcal{K}} \lambda_{0k} \, \delta_{\psi_k} \mid \boldsymbol{X} \sim \operatorname{CRM}(\theta_0 \rho^*), \qquad \rho^*(\mathrm{d}s) = \prod_{j=1}^d (1 + n_j)^{-\theta_j s} \, \rho(\mathrm{d}s).$$

Important remarks:

- the posterior parameters of unseen traits depend exclusively on the number of observations in each population!
- to model **biodiversity** across populations, consider exponential **hyperpriors** on concentration parameters  $\theta_0, \theta_1, \dots, \theta_d$ .

#### Thompson sampling for traits discovery

Since population parameters are **unknown**, common **heuristic** strategies balance:

- exploration, selecting less sampled populations to learn their parameters;
- exploitation, selecting populations with highest chances of seeing new traits.

**Thompson sampling**: choose the population randomly, according to the posterior probability of maximizing the conditional expected reward:

$$p_j = \int \mathbb{1} \left( j = \arg \max_{\ell} \mathbb{E} \left[ R_{\ell} \mid \boldsymbol{X}, \boldsymbol{\mu} \right] \right) p(\boldsymbol{\mu} \mid \boldsymbol{X}).$$

In practice, consider two possible **implementations**:

- standard Thompson sampling:
- 1. sample posterior measures  $\mu_1, \ldots, \mu_d$ ;
- 2. select the population  $j^* = \arg\max_j \mathbb{E}\left[R_j \mid \boldsymbol{X}, \boldsymbol{\mu}, \boldsymbol{\theta}\right] = \arg\max_j \sum_{k \notin \mathcal{K}} \left(1 e^{-\lambda_{jk}}\right)$
- partially marginalized Thompson sampling:
- 1. sample posterior parameters  $\theta_1, \ldots, \theta_d$ ;
- 2. select the population  $j^* = \arg \max_j \mathbb{E}[R_j \mid \boldsymbol{X}, \boldsymbol{\theta}] \approx \arg \max_j \theta_j \log \left(1 + \frac{1}{1+n_i}\right)$ .

**Idea**: the more you marginalize, the more you exploit!

### Trees species in Japanese forests

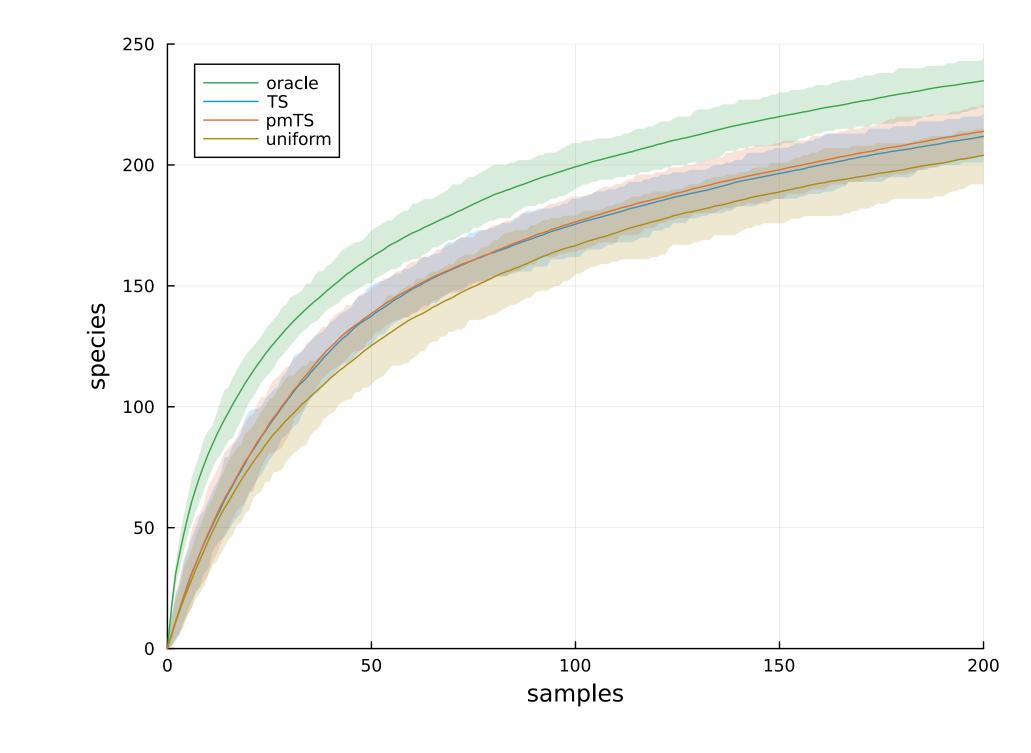
Dataset containing trees species counts from ecological survey plots collected in various forest sites in Japan:

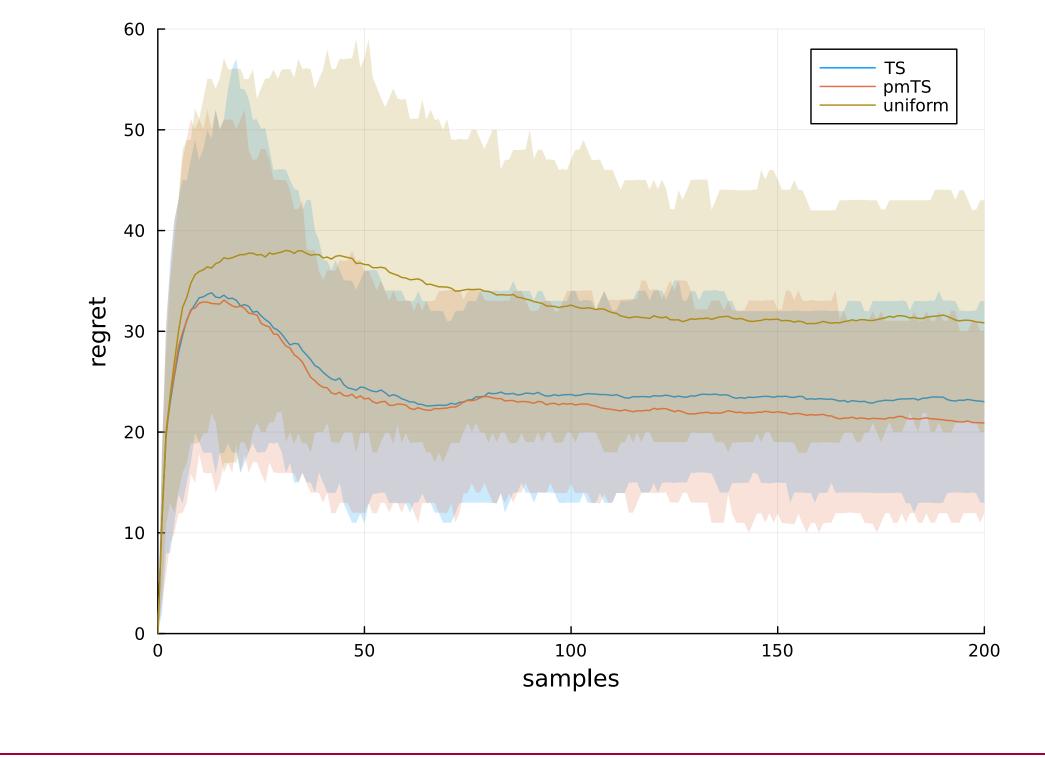
- consider d=41 populations (forest plots) classified in 4 macro-types;
- around 100 **observations** per forest  $\rightarrow$  trees counts in  $10 \times 10$  m areas;
- records for 365 **species** across forest sites.

Preliminary analysis:

- → number of **discovered** species;
- → regret from optimal strategy.

Results are averaged over 100 experiments.





- [1] Battiston, Favaro & Teh (2018). Multi-Armed Bandit for Species Discovery: A Bayesian Nonparametric Approach. Journal of the American Statistical Association.
- [2] Camerlenghi, Dumitrascu, Ferrari, Engelhardt & Favaro (2020). Nonparametric Bayesian Multiarmed Bandits for Single-Cell Experiment Design. The Annals of Applied Statistics.
- [3] Auer, Cesa-Bianchi, Fisher (2002). Finite-time Analysis of the Multiarmed Bandit Problem. Machine Learning.
- [4] Masoero, Camerlenghi, Favaro, Broderick (2023). Posterior representations of hierarchical completely random measures in trait allocation models. NeurIPS Workshop.