



Mathematics of statistical decision making

and applications to bariatric surgery

Patrick Saux

supervised by Odalric-Ambrym Maillard and Philippe Preux

30 January 2024

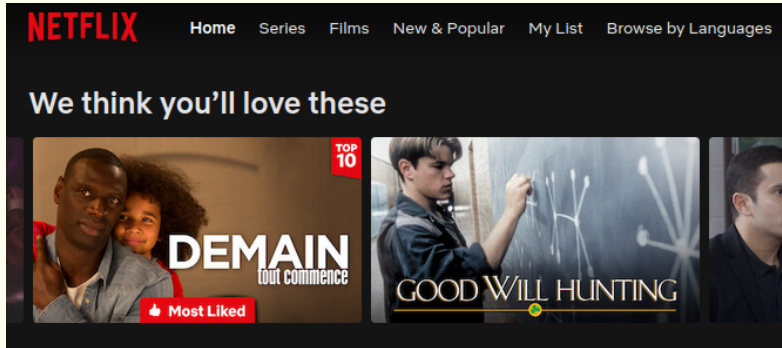


Towards recommender systems in healthcare

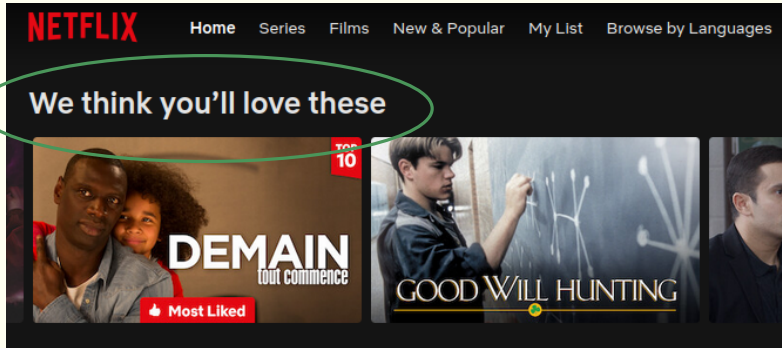
Inria



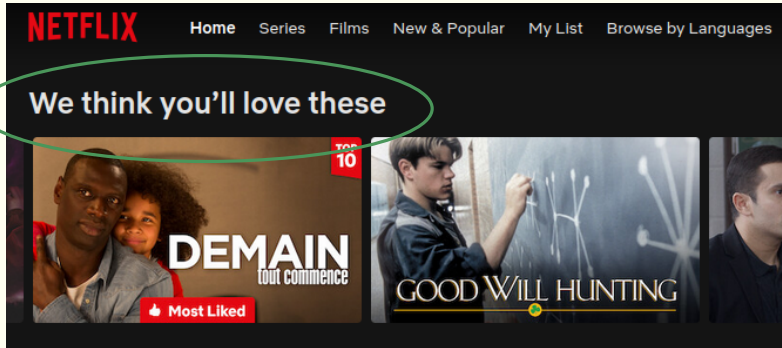
Online advertising



Online advertising

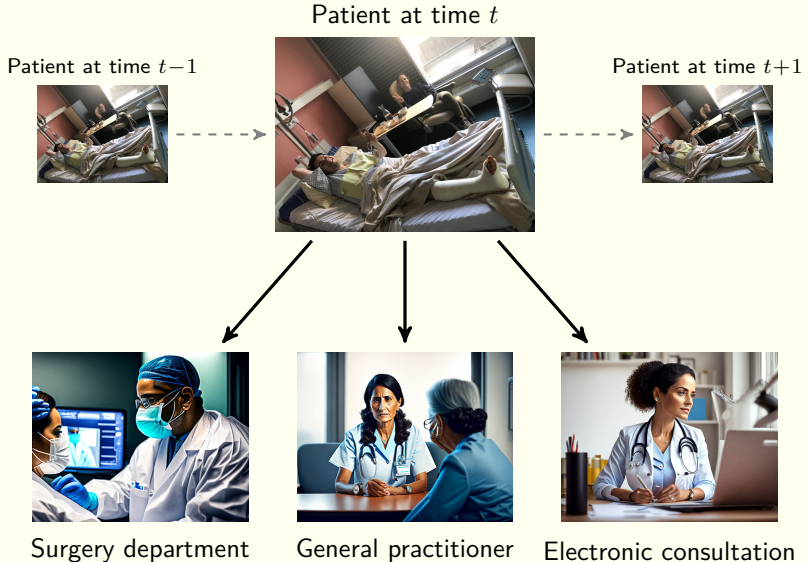


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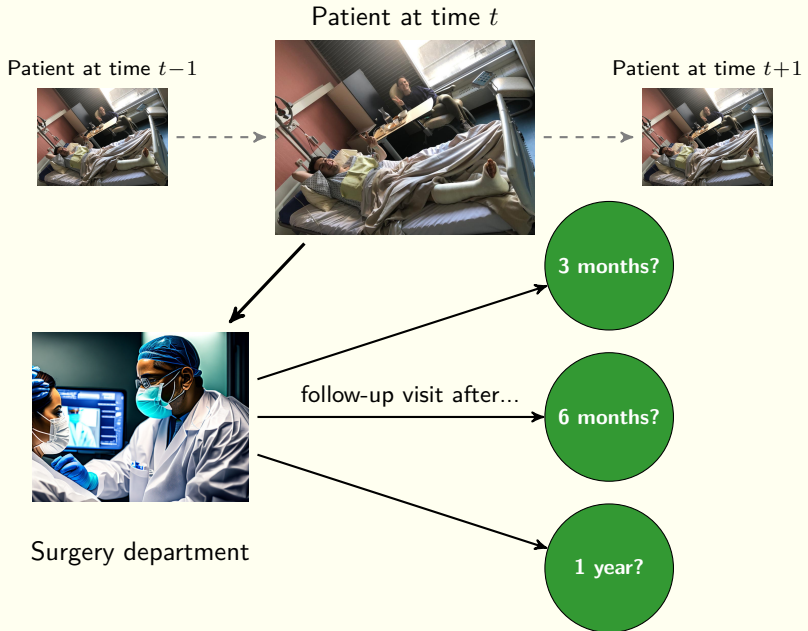


↪ from online marketing to healthcare recommendations.

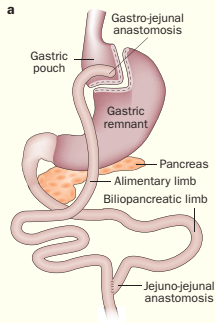
Postoperative follow-up: where to go?



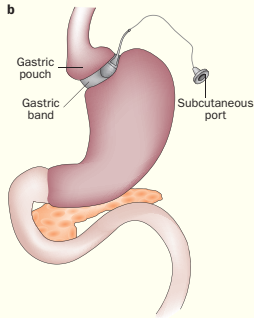
Postoperative follow-up: when to go?



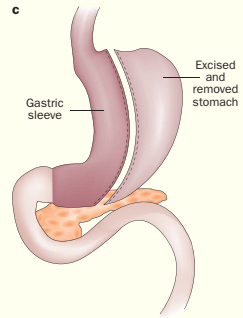
Bariatric surgery



Roux-en-Y
gastric bypass



Adjustable
gastric band



Sleeve
gastrectomy

↪ In France: 60 000 operations each year, 1% of adults.

Contributions in medical sciences




Publications in peer-reviewed journals

-  **PS**, Pierre Bauvin, Violeta Raverdy, Julien Teigny, Hélène Verkindt, Maxence Debert, Philippe Preux, François Pattou, et al. Development and validation of an interpretable machine learning based calculator for predicting 5 year-weight trajectories after bariatric surgery: a multinational retrospective cohort SOPHIA study.
The Lancet Digital Health, 2023
-  Robert Caiazzo, Pierre Bauvin, Camille Marciniak, **PS**, et al. Impact of robotic assistance on complications in bariatric surgery at expert laparoscopic surgery centers. a retrospective comparative study with propensity score.
Annals of Surgery, 2023




Contributions in statistics and machine learning



Publications in peer-reviewed international conferences with proceedings

-  Sayak Ray Chowdhury, **PS**, Odalric-Ambrym Maillard, and Aditya Gopalan. [Bregman deviations of generic exponential families.](#)
In [Conference On Learning Theory](#), 2023
-  **PS** and Odalric-Ambrym Maillard. [Risk-aware linear bandits with convex loss.](#)
In [International Conference on Artificial Intelligence and Statistics](#), 2023
-  Dorian Baudry, **PS**, and Odalric-Ambrym Maillard. [From optimality to robustness: Adaptive re-sampling strategies in stochastic bandits.](#)
[Advances in Neural Information Processing Systems](#), 2021b

Workshop presentations in peer-reviewed international conferences

-  **PS** and Odalric-Ambrym Maillard. [Risk-aware linear bandits with convex loss.](#)
In [European Workshop on Reinforcement Learning](#), 2022 (poster)

Ongoing

-  **PS**. [Empirical chernoff concentration: beyond bounded distributions](#)
-  **PS**, Romain Gautron, Odalric-Ambrym Maillard, Marc Corbeels, Chandra A. Madramootoo, and Nitin Joshi. [Quantifying the uncertainty of crop management decisions based on crop model simulations](#)

Software contributions

Bariatric Weight Trajectory Prediction

<https://bwtp.univ-lille.fr>



rlberry

<https://github.com/rlberry-py/rlberry>

concentration-lib

<https://pypi.org/project/concentration-lib>



Bariatric Weight Trajectory Prediction



Interpretable tree-based prediction model

Bariatric Weight Trajectory Prediction

SOPHIA Bariatric Weight Trajectory Prediction THE Digital Health

Patient

Weight

Height

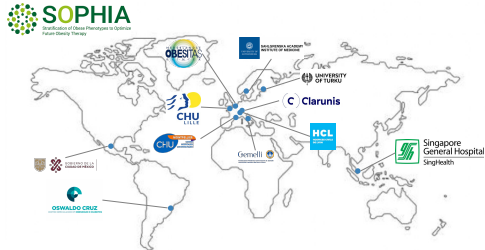
Age

Non-smoker ☐

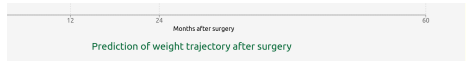
Type 2 diabetes
No diabetes ☒

Surgery

10k patients, 10 countries

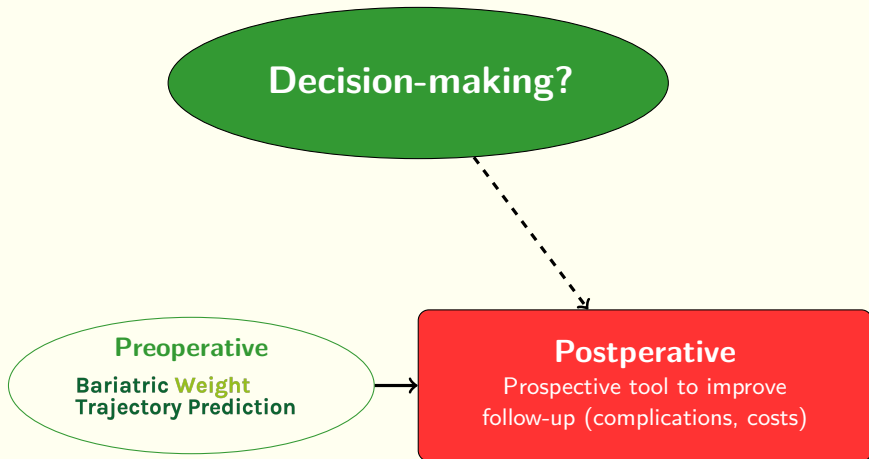


THE LANCET
Digital Health



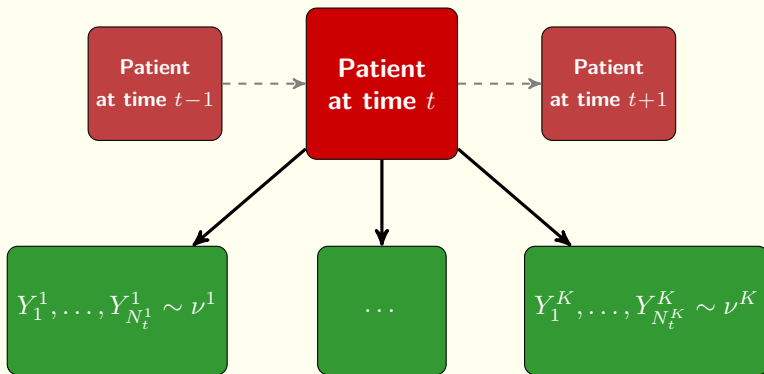
Interpretable tree-based prediction model

From preoperative to postoperative follow-up



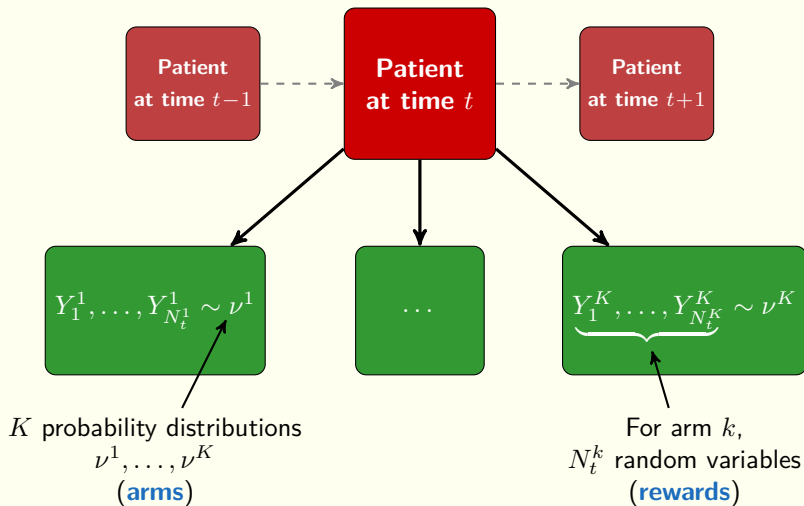
An abstract framework for decision-making

Stochastic bandit



An abstract framework for decision-making

Stochastic bandit



Stochastic bandits

$$Y_1^1, \dots, Y_{N_t^1}^1 \sim \nu^1$$

K probability distributions
 ν^1, \dots, ν^K
(**arms**)

$$\dots$$

$$\underbrace{Y_1^K, \dots, Y_{N_t^K}^K}_{N_t^k \text{ random variables}} \sim \nu^K$$

For arm k ,
 N_t^k random variables
(**rewards**)

👍 Active sampling of arm π_t .

Score (e.g. expectation)

👍 Minimise **regret** $\mathcal{R}_T = \sum_{t=1}^T \max_{k \in [K]} \rho(\nu^k) - \rho(\nu^{\pi_t})$.

👍 **Contextual bandits**: features X help predict rewards Y .

Stochastic bandits

$$Y_1^1, \dots, Y_{N_t^1}^1 \sim \nu^1$$

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$$\dots$$

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For arm k ,
 N_t^k random variables
(**rewards**)

👍 Regret lower bound ($T \rightarrow +\infty$):

$$\mathcal{R}_T = \Omega(\sqrt{T}) \quad \text{or} \quad \mathcal{R}_T \geq \log(T) \sum_{k \in [K]} \frac{\rho^* - \rho(\nu^k)}{\mathcal{K}_{\text{inf}}(\nu; \rho^*)}.$$

Worst case

Instance-dependent

$$\mathcal{K}_{\text{inf}}(\nu; \rho^*) = \inf_{\nu'} \{ \text{KL}(\nu \parallel \nu'), \rho(\nu') > \rho^* \}$$

Exploration versus exploitation

$$Y_1^1, \dots, Y_{N_t^1}^1 \sim \nu^1$$

K probability distributions
 ν^1, \dots, ν^K
(**arms**)

...

$$\underbrace{Y_1^K, \dots, Y_{N_t^K}^K}_{\text{For arm } k, N_t^k \text{ random variables}} \sim \nu^K$$

For arm k ,
 N_t^k random variables
(**rewards**)

Greed is **not** good!

$$\text{✗ } \pi_{t+1} \neq \underset{k \in [K]}{\operatorname{argmax}} \hat{\rho}_t^k.$$

Need to **explore**:

- ✓ Deterministic:
 $\hat{\rho}_t^k + \text{confidence set.}$
- ✓ Randomised:
 $\hat{\rho}_t^k + \text{noise.}$



Challenges of healthcare recommendations



Online advertising

- ✓ Huge volume of data.
- ✓ Easy to model (Bernoulli, logistic...).
- ✓ Limited risks ($\rho = \mathbb{E}$).

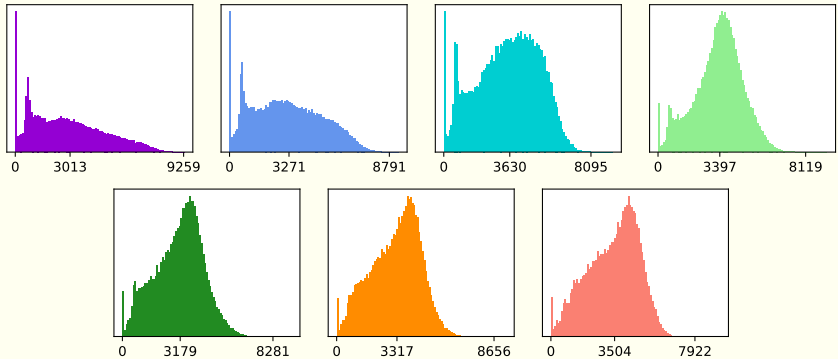


Healthcare

- ✗ Slow and scarce data.
- ✗ Nonparametric models.
- ✗ Risky.

Example distributions

Grain yield distributions (=rewards)



I. Efficient deterministic exploration

👍 Quantify uncertainty for the score ρ from i.i.d. Y_1, \dots, Y_N .

? Confidence sets: $\forall n \in \mathbb{N}, \mathbb{P}(\rho \in \hat{\Theta}_n) \geq 1 - \delta$ (e.g. $\delta = 5\%$).

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✗ **p-hacking**: incompatible with random (active, data-dependent) N .

✓ **Anytime valid** confidence sequence:

$$\forall \text{ stopping time } N, \mathbb{P}(\rho \in \hat{\Theta}_N) \geq 1 - \delta.$$

I. Concentration bounds

Method	Assumption	Variance adaptive	Random N
t -test	Gaussian (or $N \rightarrow +\infty$)	✓	✗
Method of mixtures (MM) supermartingale inequality	Sub-Gaussian	✗	✓

Robbins and Pitman. [Application of the method of mixtures to quadratic forms in normal variates](#). 1949.

Peña, Lai, and Shao. [Self-normalized processes: Limit theory and statistical applications](#). 2009.

I. Concentration bounds

Method	Assumption	Variance adaptive	Random N
t -test	Gaussian (or $N \rightarrow +\infty$)	✓	✗
Method of mixtures (MM) supermartingale inequality	Sub-Gaussian	✗	✓
Bregman MM	Exp. families	✓	✓
Empirical Chernoff MM	Second order sub-Gaussian	✓	✓

Robbins and Pitman. Application of the method of mixtures to quadratic forms in normal variates. 1949.

Peña, Lai, and Shao. Self-normalized processes: Limit theory and statistical applications. 2009.

I. Bregman concentration

Parameter θ points to θ in the equation.

Feature function $F(y)$ points to $F(y)$ in the equation.

Log-partition function $\mathcal{L}(\theta)$ points to $\mathcal{L}(\theta)$ in the equation.

👍 Exponential family: $p_{\theta}(y) = h(y) \exp(\langle \theta, F(y) \rangle - \mathcal{L}(\theta))$.

👍 Bregman divergence:

$$\mathcal{B}(\theta', \theta) = \mathcal{L}(\theta') - \mathcal{L}(\theta) - \langle \theta' - \theta, \nabla \mathcal{L}(\theta) \rangle = \text{KL}(p_{\theta} \parallel p_{\theta'}).$$

Family	Known anytime valid concentration
Bernoulli, Gaussian (known variance)	✓
Gaussian, Chi-square, Poisson, Pareto, etc.	✗

I. Bregman concentration

$$\hat{\Theta}_n^\delta = \left\{ \theta_0 \in \Theta : (n+c) \mathcal{B}_{\mathcal{L}} \left(\theta_0, \hat{\theta}_{n,c}(\theta_0) \right) \leq \log \frac{1}{\delta} + \gamma_{n,c}(\theta_0) \right\}$$

is an anytime valid confidence sequence for this exponential family.

I. Bregman concentration

Regularised estimator

$$\hat{\theta}_{n,c}(\theta_0) = (\nabla \mathcal{L})^{-1} \left(\frac{1}{n+c} \left(\sum_{j=1}^n F(Y_j) + c \nabla \mathcal{L}(\theta_0) \right) \right)$$

$$\hat{\Theta}_n^\delta = \left\{ \theta_0 \in \Theta : (n+c) \mathcal{B}_{\mathcal{L}} \left(\theta_0, \hat{\theta}_{n,c}(\theta_0) \right) \leq \log \frac{1}{\delta} + \gamma_{n,c}(\theta_0) \right\}$$

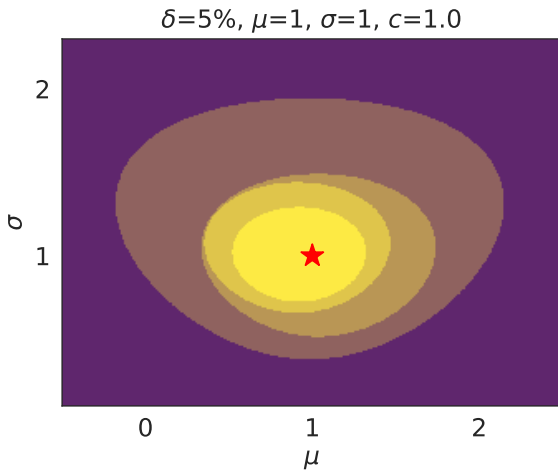
Bregman divergence

Bregman information gain

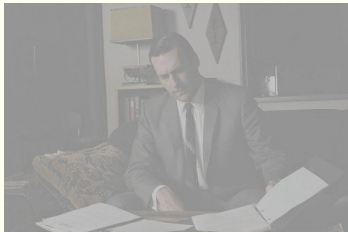
$$\gamma_{n,c}(\theta_0) = \log \left(\frac{\int_{\Theta} \exp(-c \mathcal{B}_{\mathcal{L}}(\theta', \theta_0)) d\theta'}{\int_{\Theta} \exp(-(n+c) \mathcal{B}_{\mathcal{L}}(\theta', \hat{\theta}_{n,c}(\theta_0))) d\theta'} \right)$$

is an anytime valid confidence sequence for this exponential family.

I. Bregman concentration



Challenges of healthcare recommendations



Online advertising

- ✓ Huge volume of data.
- ✓ Easy to model (Bernoulli, logistic...).
- ✓ Limited risks ($\rho = \mathbb{E}$).



Healthcare

- ✓ Slow and scarce data.
- ✗ Nonparametric models.
- ✗ Risky.

II. Nonparametric: bootstrapping from data only

👍 Greedy policy:

$$\pi_{t+1} = \operatorname{argmax}_{k \in [K]} \frac{1}{N_t^k} \sum_{j=1}^{N_t^k} Y_j^k.$$

Empirical average



II. Nonparametric: bootstrapping from data only

👍 Greedy policy:

$$\pi_{t+1} = \operatorname{argmax}_{k \in [K]} \sum_{j=1}^{N_t^k} w_{j,t}^k Y_j^k.$$

Empirical average

$$w_{j,t}^k = \frac{1}{N_t^k}$$

II. Nonparametric: bootstrapping from data only

👉 Greedy policy with fictitious rewards:

$$\pi_{t+1} = \operatorname{argmax}_{k \in [K]} \sum_{j=1}^{N_t^k} w_{j,t}^k Y_j^k + \tilde{w}_t^k \tilde{Y}_t^k.$$

Empirical average

Fictitious reward

$$w_{j,t}^k, \tilde{w}_t^k = \frac{1}{N_t^k + 1}$$

II. Nonparametric: bootstrapping from data only



Randomised greedy policy with fictitious rewards:

Randomised average

$$\pi_{t+1} = \operatorname{argmax}_{k \in [K]} \sum_{j=1}^{N_t^k} w_{j,t}^k Y_j^k + \tilde{w}_t^k \tilde{Y}_t^k.$$

$w_{j,t}^k, \tilde{w}_t^k \in [0, 1]$ random

$$\sum_{j=1}^{N_t^k} w_{j,t}^k + \tilde{w}_t^k = 1$$

Fictitious reward

II. Nonparametric: bootstrapping from data only

👉 Nonparametric Thompson sampling:

$$\pi_{t+1} = \operatorname{argmax}_{k \in [K]} \sum_{j=1}^{N_t^k} w_{j,t}^k Y_j^k + \tilde{w}_t^k \tilde{Y}_t^k.$$

Dirichlet average

$w_{j,t}^k, \tilde{w}_t^k \sim \operatorname{Dir}(1, \dots, 1)$
(uniform distribution on the simplex)

Fictitious reward
(\approx reward upper bound)

II. Nonparametric: bootstrapping from data only

👉 Nonparametric Thompson sampling:

$$\pi_{t+1} = \operatorname{argmax}_{k \in [K]} \sum_{j=1}^{N_t^k} w_{j,t}^k Y_j^k + \tilde{w}_t^k \tilde{Y}_t^k.$$

Dirichlet average

$w_{j,t}^k, \tilde{w}_t^k \sim \operatorname{Dir}(1, \dots, 1)$
(uniform distribution on the simplex)

Fictitious reward
(\approx reward upper bound)

Beyond bounded rewards (with known bounds)?

Kveton, Szepesvari, et al. [ICML](#), 2019.

Riou and Honda. [ALT](#), 2020.

II. Regret guarantees for Dirichlet sampling

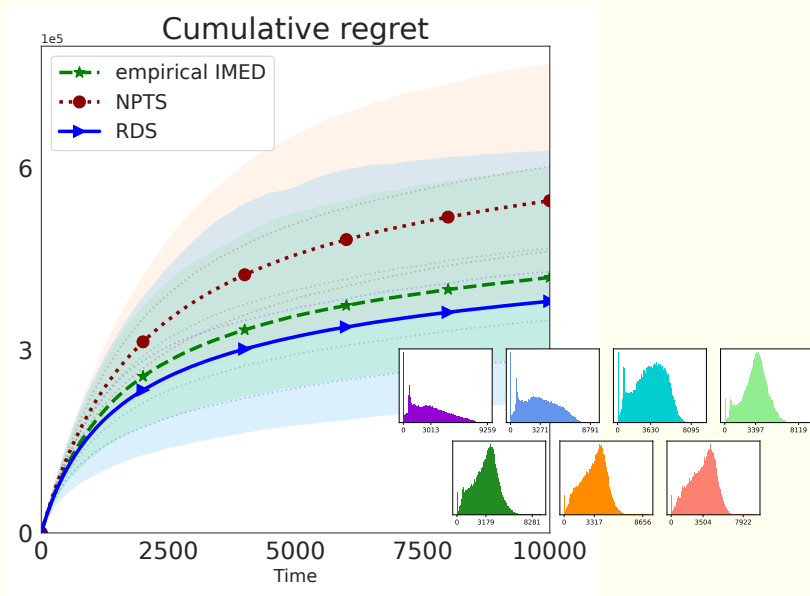
$$\pi_{t+1} = \operatorname{argmax}_{k \in [K]} \sum_{j=1}^{N_t^k} w_{j,t}^k Y_j^k + \tilde{w}_t^k \tilde{Y}_t^k.$$

👍 Regret guarantees (instance-dependent)

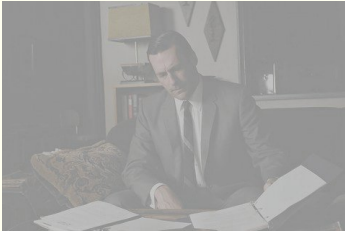
✓ Optimal in several settings
(bounded, bounded detectable, semibounded + quantile condition)

💡 **Light tailed:** $\mathcal{R}_T = \mathcal{O}(\log(T) \log \log(T)).$

II. Dirichlet sampling



Challenges of healthcare recommendations



Online advertising

- ✓ Huge volume of data.
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Healthcare

- ✓ Slow and scarce data.
- ✓ Nonparametric models.
- ✗ Risky.

III. From risk-neutral to risk-aware

👉 Non-contextual bandits:

- ▶ Maillard. Robust risk-averse stochastic multi-armed bandits. ALT, 2013.
- ▶ Baudry, Gautron, et al. Optimal Thompson sampling strategies for support-aware CVAR bandits. ICML, 2021a.

👉 Contextual bandits?

III. From risk-neutral to risk-aware

👉 Classical linear bandit $Y = \langle \theta^*, X \rangle + \text{zero-mean noise}$:

$$\hat{\theta}_{t+1} = \min_{\theta \in \Theta} \sum_{s=1}^t (Y_s - \langle \theta, X_s \rangle)^2 + \text{exploration}.$$

Estimator of
 $\rho(\nu) = \mathbb{E}_{\nu} [Y \mid X]$

III. From risk-neutral to risk-aware

👉 Classical linear bandit $Y = \langle \theta^*, X \rangle +$ zero-mean noise:

$$\hat{\theta}_{t+1} = \min_{\theta \in \Theta} \sum_{s=1}^t \mathcal{L}(Y_s, \langle \theta, X_s \rangle) + \text{exploration}.$$

Estimator of
 $\rho(\nu) = \min_{\theta} \mathbb{E}_{\nu} [\mathcal{L}(Y, \langle \theta, X \rangle) \mid X]$
(M-estimator)

$$\mathcal{L}(y, \xi) = (y - \xi)^2$$

III. From risk-neutral to risk-aware

👉 Elicitable risk measure linear bandit $Y \approx \langle \theta^*, X \rangle + \text{zero } \rho\text{-noise}$:

$$\hat{\theta}_{t+1} = \min_{\theta \in \Theta} \sum_{s=1}^t \mathcal{L}(Y_s, \langle \theta, X_s \rangle) + \text{exploration}.$$

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\mathcal{L} (strongly) convex mapping

III. From risk-neutral to risk-aware

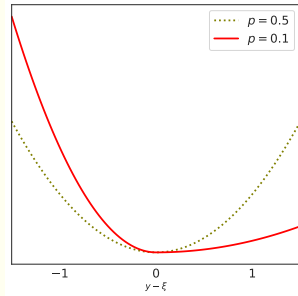
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Estimator of
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\mathcal{L} (strongly) convex mapping

Expectile: $\mathcal{L}(y, \xi) = |p - \mathbb{1}_{y < \xi}| (y - \xi)^2$
(\neq loss for negative and positive rewards).



III. Risk-aware policies

👍 Deterministic exploration:

$$\pi_{t+1} = \operatorname{argmax}_x \langle \hat{\theta}_{t+1}, x \rangle + \text{UCB}(x),$$

Worst case: $\mathcal{R}_T = \tilde{\mathcal{O}}(\sqrt{T})$.

👍 Randomised Dirichlet exploration:

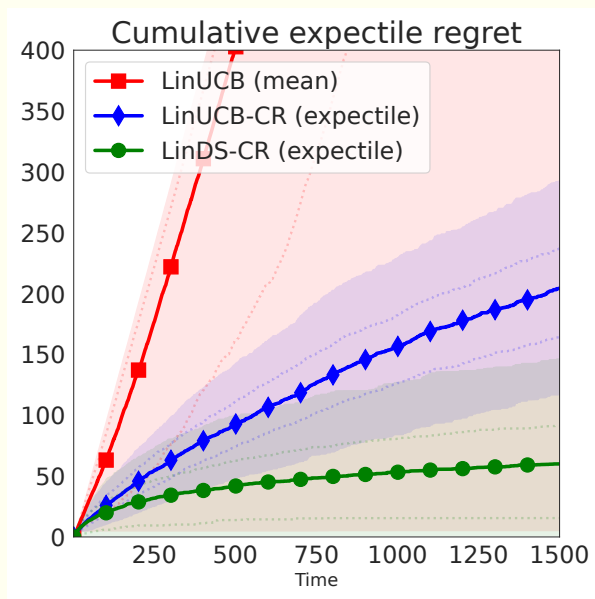
$$\tilde{\theta}_{t+1} = \min_{\theta \in \Theta} \sum_{s=1}^t w_s^t \mathcal{L}(Y_s, \langle \theta, X_s \rangle) + \tilde{w}_{t+1}^t \mathcal{L}(\tilde{Y}, \langle \theta, \tilde{X} \rangle),$$

$$\pi_{t+1} = \operatorname{argmax}_x \langle \tilde{\theta}_{t+1}, x \rangle,$$

Worst case: $\mathcal{R}_T \stackrel{?}{=} \tilde{\mathcal{O}}(\sqrt{T})$.

Linear Gaussian Thompson sampling?
(strong approximation of weighted bootstrap)

III. Risk-aware policies



Challenges of healthcare recommendations



Online advertising

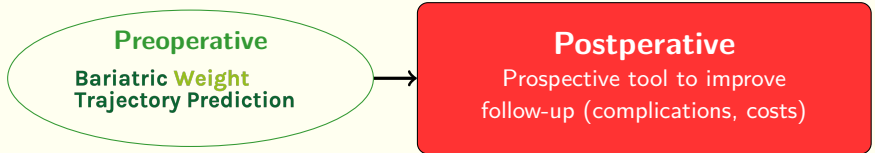
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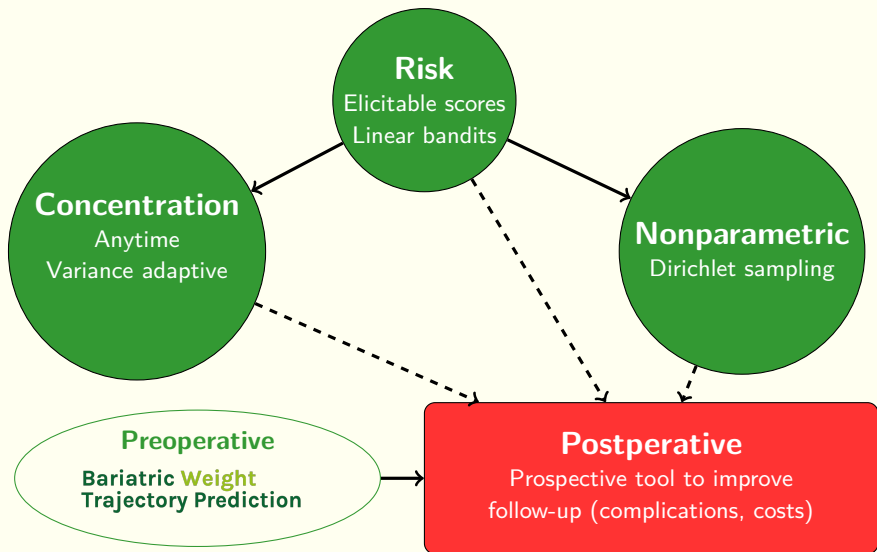
Healthcare

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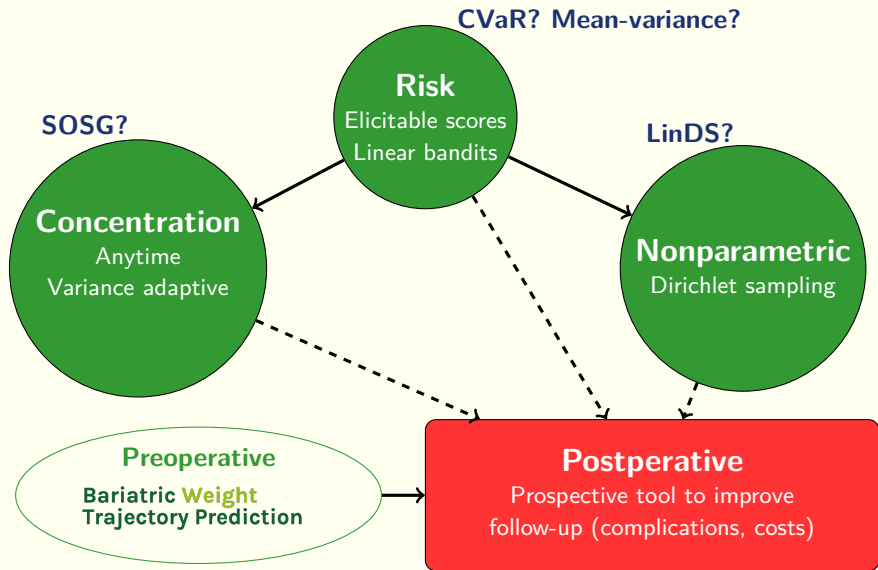
Conclusion and future works



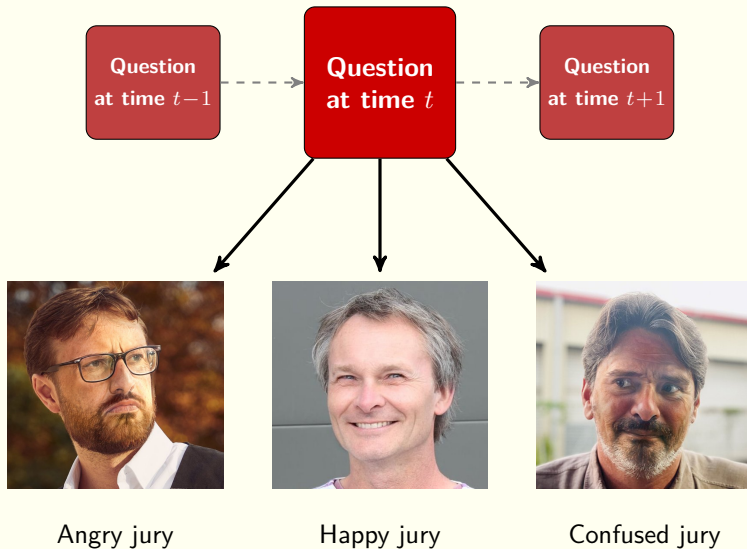
Conclusion and future works



Conclusion and future works



Questions





Empirical Chernoff concentration

👍 Sub-Gaussian (SG): $\forall \lambda \in \mathbb{R}, \log \mathbb{E} [e^{\lambda(Y-\mu)}] \leq \frac{\lambda^2 R^2}{2}$.

👍 Second order sub-Gaussian (SOSG):

$$\forall \lambda \in \mathbb{R}_+, \log \mathbb{E} [e^{-\lambda(Y-\mu)^2}] \leq -\frac{1}{2} \log (1 + 2\lambda(\rho R)^2).$$

Second to first order variance ratio ($\rho \in (0, 1]$)

Family	Known anytime valid concentration
Gaussian (unknown variance)	×
Uniform, symmetric triangular (unknown support)	×
Other nonparametric distributions	×

Empirical Chernoff concentration

$$\hat{\Theta}_n^\delta = \left[\hat{\mu}_n \pm \sqrt{\frac{2}{n} \left(1 + \frac{\alpha}{n}\right) \overset{\text{Proxy variance}}{R^2} \log \left(\frac{2\sqrt{1+\frac{n}{\alpha}}}{\delta} \right)} \right]$$

is an anytime valid confidence sequence for SG.

Empirical Chernoff concentration

$$\hat{\Theta}_{n,\rho}^{\delta} = \left[\hat{\mu}_n \pm \sqrt{\frac{2}{n} \left(1 + \frac{\alpha}{n}\right) \frac{\lfloor n/2 \rfloor V_{\lfloor n/2 \rfloor}^I}{\rho^2 \left(G_{\beta,\gamma,\zeta,\lfloor n/2 \rfloor}^T\right)^{-1} \left(\frac{3}{\delta}\right)} \log \left(\frac{3\sqrt{1+\frac{n}{\alpha}}}{\delta} \right)} \right]$$

is an anytime valid confidence sequence for SOSG.

Empirical Chernoff concentration

Empirical variance estimator

$$\hat{\Theta}_{n,\rho}^{\delta} = \left[\hat{\mu}_n \pm \sqrt{\frac{2}{n} \left(1 + \frac{\alpha}{n}\right) \frac{\lfloor n/2 \rfloor V_{\lfloor n/2 \rfloor}^I}{\rho^2 \left(G_{\beta,\gamma,\zeta,\lfloor n/2 \rfloor}^T\right)^{-1} \left(\frac{3}{\delta}\right)} \log \left(\frac{3\sqrt{1+\frac{n}{\alpha}}}{\delta} \right)} \right]$$

Second to first order
variance ratio

$$G_{\beta,\gamma,\zeta,\lfloor n/2 \rfloor}^T(z) = \frac{U\left(\beta, \gamma + \frac{t}{2}; \zeta + \frac{z}{2}\right)}{U(\beta, \gamma; \zeta)}$$

$$U(b, c; z) = \frac{1}{\Gamma(b)} \int_0^{+\infty} u^{b-1} (1+u)^{c-b-1} e^{-zu} du$$

(Tricomi's confluent hypergeometric function)

is an anytime valid confidence sequence for SOSG.

Empirical Chernoff concentration

