

Collecting the **right** data:

A machine learning theory perspective on A/B testing

Wouter M. Koolen

AI020, April 24 2024

Welcome! A bit about me



Senior Researcher, Machine Learning group, Centrum Wiskunde & Informatica

Professor of Mathematical Machine Learning, University of Twente

Welcome! A bit about me



Senior Researcher, Machine Learning group, Centrum Wiskunde & Informatica

Professor of Mathematical Machine Learning, University of Twente

Lecturer *Machine Learning Theory* for MasterMath

Lecturer *Graphical Models and Causality* at UT

Welcome! A bit about me



Senior Researcher, Machine Learning group, Centrum Wiskunde & Informatica

Professor of Mathematical Machine Learning, University of Twente

Lecturer *Machine Learning Theory* for MasterMath

Lecturer *Graphical Models and Causality* at UT

Keywords: Machine Learning, Online Learning, Statistics, Game theory, Optimisation

The idea of this workshop



I'll sketch a PhD project trajectory.

Please interrupt!

What is a PhD project



- Typically 4 years
- One or more supervisors
- Training to be an independent researcher ...
- ... by doing actual research
- Large academic freedom
- Join community: conferences, workshops, summer schools, internship

How to start a PhD project

Need a **supervisor** with an open position

Don't **wait** for the perfect vacancy. Engage!

Check out the **PhD program** of the **European Laboratory for Learning and Intelligent Systems** (ELLIS). They do central recruiting for top AI/ML in Europe.



It all starts with a question

Suppose we are excited about autonomous driving.

It all starts with a question

Suppose we are excited about autonomous driving.

As you may know, training AI systems (e.g. deep neural networks) takes a lot of data.

It all starts with a question

Suppose we are excited about autonomous driving.

As you may know, training AI systems (e.g. deep neural networks) takes a lot of data.

Yet not all data are equally valuable/useful.

It all starts with a question

Suppose we are excited about autonomous driving.

As you may know, training AI systems (e.g. deep neural networks) takes a lot of data.

Yet not all data are equally valuable/useful.

Let's optimise and automate the data collection.

It all starts with a question

Suppose we are excited about autonomous driving.

As you may know, training AI systems (e.g. deep neural networks) takes **a lot** of data.

Yet not all data are equally valuable/useful.

Let's **optimise and automate** the data collection.

Where should I send my prototype for training?

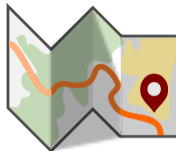


Dragons everywhere

Where should I send my prototype for training?

- AI system is huge parameterised model
- Lots of possible environments to drive in
- Multiple objectives (safety, efficiency, ...)
- Feedback (crash/intervention) is very one-sided

Dragons everywhere



Where should I send my prototype for training?

- AI system is huge parameterised model
- Lots of possible environments to drive in
- Multiple objectives (safety, efficiency, ...)
- Feedback (crash/intervention) is very one-sided

Distilled goal:

- Identify parameters that cause fewest crashes in natural environment mix.

Simplify

Close-by parameters in close-by environments result in close-by outcomes

Simplify

Close-by parameters in close-by environments result in close-by outcomes

Often true, but too complicated. Let's **discretise!**

Simplify

Close-by parameters in close-by environments result in close-by outcomes

Often true, but too complicated. Let's **discretise!**

Environments



Simplify

Close-by parameters in close-by environments result in close-by outcomes

Often true, but too complicated. Let's **discretise!**

Environments



Parameters



Simplify

Close-by parameters in close-by environments result in close-by outcomes

Often true, but too complicated. Let's **discretise!**

Environments



Parameters



Outcomes



World model (Stochastic Bandit)

The world *simplifies* to vector + table:

World model (Stochastic Bandit)

The world **simplifies** to vector + table:

Known natural environment mix

$$\mathbb{P} \left(\text{Traffic} \right) = 40\%$$

$$\mathbb{P} \left(\text{Road} \right) = 30\%$$

$$\mathbb{P} \left(\text{City} \right) = 15\%$$

$$\mathbb{P} \left(\text{Park} \right) = 10\%$$

$$\mathbb{P} \left(\text{Desert} \right) = 5\%$$

World model (Stochastic Bandit)

The world **simplifies** to vector + table:

Known natural environment mix

$$\mathbb{P} \left(\text{Traffic Jam} \right) = 40\%$$

$$\mathbb{P} \left(\text{Open Road} \right) = 30\%$$

$$\mathbb{P} \left(\text{City Street} \right) = 15\%$$

$$\mathbb{P} \left(\text{Park Road} \right) = 10\%$$

$$\mathbb{P} \left(\text{Desert Road} \right) = 5\%$$

Unknown crash probabilities

$$\mathbb{P} \left(\text{Sad Face} \mid \text{Traffic Jam}, \text{Yellow Car} \right) = 0.1\%$$

$$\mathbb{P} \left(\text{Sad Face} \mid \text{Open Road}, \text{Silver Car} \right) = 0.3\%$$

$$\mathbb{P} \left(\text{Sad Face} \mid \text{City Street}, \text{Red Car} \right) = 0.03\%$$

⋮

$$\mathbb{P} \left(\text{Sad Face} \mid \text{Desert Road}, \text{Blue Car} \right) = 2.7\%$$

World model (Stochastic Bandit)

The world **simplifies** to vector + table:

Known natural environment mix

$$\mathbb{P} \left(\text{Traffic Jam} \right) = 40\%$$

$$\mathbb{P} \left(\text{Open Road} \right) = 30\%$$

$$\mathbb{P} \left(\text{City Street} \right) = 15\%$$

$$\mathbb{P} \left(\text{Park Road} \right) = 10\%$$

$$\mathbb{P} \left(\text{Desert Road} \right) = 5\%$$

Unknown crash probabilities

$$\mathbb{P} \left(\text{Sad Face} \mid \text{Traffic Jam}, \text{Yellow Car} \right) = 0.1\%$$

$$\mathbb{P} \left(\text{Sad Face} \mid \text{Open Road}, \text{Silver Car} \right) = 0.3\%$$

$$\mathbb{P} \left(\text{Sad Face} \mid \text{City Street}, \text{Red Car} \right) = 0.03\%$$

⋮

$$\mathbb{P} \left(\text{Sad Face} \mid \text{Desert Road}, \text{Blue Car} \right) = 2.7\%$$

Together these determine the **best parameter** on average. Say .

Learning the best Parameter by Driving: Example Interaction

Learning the best Parameter by Driving: Example Interaction

1



Learning the best Parameter by Driving: Example Interaction

1



2



Learning the best Parameter by Driving: Example Interaction





Learning the best Parameter by Driving: Example Interaction
























Learning the best Parameter by Driving: Example Interaction



Learning the best Parameter by Driving: Example Interaction

1			
2			
3			
4			
5			
⋮	⋮	⋮	⋮
65535			
65536			

Learning the best Parameter by Driving: Example Interaction

1			
2			
3			
4			
5			
⋮	⋮	⋮	⋮
65535			
65536			
65537			



So how do we build that learning algorithm?

- Reliable
- Data efficient

Theory: Characteristic Time and Oracle Weights

Answering correctly in world μ requires data rejecting all worlds with a different answer.

Theory: Characteristic Time and Oracle Weights

Answering correctly in world μ requires data rejecting all worlds with a different answer.

Theorem (Garivier and Kaufmann, 2016; Russac et al., 2021)

Any δ -correct testing algorithm must, for any world μ , take samples at least

$$\text{samples}(\mu) \geq \ln \frac{1}{\delta} \cdot \frac{1}{\max_{\text{par+env proportions } w} \min_{\substack{\text{world } \lambda \text{ with answer} \\ \text{different from that of } \mu}} \sum_{\text{par } p, \text{ env } e} w_{p,e} \text{KL}(\mu_{p,e}, \lambda_{p,e})}$$

Theory: Characteristic Time and Oracle Weights

Answering correctly in world μ **requires data** rejecting all worlds with a different answer.

Theorem (Garivier and Kaufmann, 2016; Russac et al., 2021)










Any δ -correct testing algorithm must, for any world μ , take samples at least

$$\text{samples}(\mu) \geq \ln \frac{1}{\delta} \cdot \frac{1}{\max_{\text{par+env proportions } w} \min_{\substack{\text{world } \lambda \text{ with answer} \\ \text{different from that of } \mu}} \sum_{\text{par } p, \text{ env } e} w_{p,e} \text{KL}(\mu_{p,e}, \lambda_{p,e})}$$

Why should we care?

- Characterises* complexity of **each world** μ
- Optimal testing algorithm **must** sample with proportions $\arg \max_w$

What are those oracle weights $w^*(\mu)$

$w_{e,p}^*(\mu)$				
	0.05	0.01	0.13	...
				
				
				
			...	0.08

Instance-Optimal Algorithms

Sample complexity lower bound at world μ governed by max-min problem:

$$\max_{\text{par+env proportions } w} \min_{\substack{\text{world } \lambda \text{ with answer} \\ \text{different from that of } \mu}} \sum_{\text{par } p, \text{ env } e} w_{p,e} \text{KL}(\mu_{p,e}, \lambda_{p,e})$$

Main challenge: driving with proportions $w^*(\mu) = \arg \max_w$ **without knowing** world μ .

Instance-Optimality: Iterative Saddle Point Approach

Approx. solve saddle point problem iteratively: $w_1, w_2, \dots \rightarrow w^*(\mu)$



Instance-Optimality: Iterative Saddle Point Approach

Approx. solve saddle point problem iteratively: $w_1, w_2, \dots \rightarrow w^*(\mu)$

Main pipeline:

- Get current w_t from saddle point solver.
- Pick parameter and environment $(P_t, E_t) \sim w_t$, see outcome X_t
- Update estimate $\hat{\mu}_t$ of world.
- Advance the saddle point solver **one** iteration.
- Add optimism to gradients to induce exploration ($\hat{\mu}_t \rightarrow \mu$).
- Regret bounds + concentration + optimism \Rightarrow finite-time guarantee:



Instance-Optimality: Iterative Saddle Point Approach

Approx. solve saddle point problem iteratively: $w_1, w_2, \dots \rightarrow w^*(\mu)$

Main pipeline:

- Get current w_t from saddle point solver.
- Pick parameter and environment $(P_t, E_t) \sim w_t$, see outcome X_t
- Update estimate $\hat{\mu}_t$ of world.
- Advance the saddle point solver **one** iteration.
- Add optimism to gradients to induce exploration ($\hat{\mu}_t \rightarrow \mu$).
- Regret bounds + concentration + optimism \Rightarrow finite-time guarantee:

Theorem (Degenne, Koolen, and Ménard, 2019)

For every $\delta \in (0, 1)$ and world μ , the above scheme takes samples bounded by

$$\text{samples}(\mu) \leq \boxed{\text{char. time}} \cdot \ln \frac{1}{\delta} + o(\ln \frac{1}{\delta})$$



Lessons

Content:

- Optimal data collection can be achieved by learning algorithms
- It is inefficient follow the natural environment mix
- It will take many samples to see small differences between good parameters
- Discretising parameters finer makes learning harder ...
- ...while finer discretisation of environments can help

Lessons




Content:

- Optimal data collection can be achieved by learning algorithms
- It is inefficient follow the natural environment mix
- It will take many samples to see small differences between good parameters
- Discretising parameters finer makes learning harder ...
- ...while finer discretisation of environments can help

Meta:

- It will go deep
- Learning/AI/ML will require mix of algorithms, statistics, game theory, optimisation
- Need to zoom out, scale up and iterate. This is hard!

References

-  Degenne, R., W. M. Koolen, and P. Ménard (Dec. 2019). **“Non-Asymptotic Pure Exploration by Solving Games”**. In: *Advances in Neural Information Processing Systems (NeurIPS) 32*, pp. 14492–14501.
-  Garivier, A. and E. Kaufmann (2016). **“Optimal Best arm Identification with Fixed Confidence”**. In: *Proceedings of the 29th Conference On Learning Theory (COLT)*.
-  Russac, Y., C. Katsimerou, D. Bohle, O. Cappé, A. Garivier, and W. M. Koolen (Dec. 2021). **“A/B/n Testing with Control in the Presence of Subpopulations”**. In: *Advances in Neural Information Processing Systems (NeurIPS) 34*.