Contextual Inverse Optimization: Offline and Online Learning

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Contextual Inverse Optimization

Standard data-driven decision processes framework:

- Given context, choose action, observe reward.
- In many settings, rewards cannot be observed.
 - Is there other type of feedback that we can use to learn?

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 - Is there other type of feedback that we can use to learn?
- In this work we consider problems where the reward is not observed but we observe, after-the-fact, what you should have done.
 - Contextual inverse optimization
- Applications:
 - Economics: learn from revealed preferences.
 - Robotics: teach a robot or AV by demonstration.
 - Medicine: learn from a doctor's decision-making.

Problem Formulation

In every *t*, you would like to solve:

 $\min_{x\in\mathcal{X}_t}f_t(x)'c^{\star}$

We **don't know** c^* , but we observe \mathcal{X}_t , $f_t(\cdot)$ and x_t^* (after period t):

 $x_t^{\star} \in \operatorname*{arg\,min}_{x \in \mathcal{X}_t} f_t(x)' c^{\star}$

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Example: Learning from Revealed Preferences

$$\mathbf{x}_t^{\star} = \arg\max_{\mathbf{x}\in\mathcal{X}_t} \mathbf{x}' Z_t \mathbf{c}^{\star} : \mathbf{x}' p_t \leq \mathbf{b}_t, \quad \mathcal{X}_t = \{0,1\}^{n_t}$$

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Related Literature: Inverse Optimization

Estimate cost vector based on optimal action

Ajuha and Orlin (OR 2001)

What if you have many data points?

- Esfahani, Shafieezadeh-Abadeh, Hanasuanto and Kuhn (MP 2018): closest to our offline model, stochastic framework
- Bärmann, Pokutta and Schneider (ICML 2017): closest to our online model, gradient descent approach

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Related Literature: Contextual Pricing and Search

Class of contextual bandit models where nature picks context adversarially and we choose action.

- Cohen, Lobel and Paes Leme (MS 2020): ellipsoid method
- ▶ Lobel, Paes Leme and Vladu (OR 2018): centroid and projection
- ▶ Paes Leme and Schneider (FOCS 2018): intrinstic volume
- Krishnamurthy, Lykouris, Podimata and Schapire (STOC 2021): irrational agents

We leverage ideas from this literature, but the problems are of a different nature (we have far less control on the feedback).

Related Literature: Structured Prediction and Inverse Reinforcement Learning

Optimization-based structured prediction is similar to inverse optimization but focuses on a different metric (prediction error).

- Taskar, Chatalbashev, Koller and Guestrin (ICML 2005): SVM-style approach called maximum margin planning
- Ratliff, Bagnell and Zinkevich (ICML 2006): online version

If you assign linear functionals to features, this approach can be used to learn a reward function in reinforcement learning.

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Abbeel and Ng (ICML 2004): apprenticeship learning

Main Results

Offline setting:

- ▶ We propose a geometric definition of data informativeness.
- Using this notion, we characterize the minimax regret.

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- Using this notion, we characterize the minimax regret.

Online setting:

- State-of-the-art: Bärmann et al. (ICML 2017) obtain $O(\sqrt{T})$ regret, assuming linear context functions.
- ▶ We obtain $O(d^4 \ln T)$ regret, assuming Lipschitz context functions.

In the offline setting, we have N observations, and for i = 1, ..., N, we have:

- A set of feasible actions $\mathcal{X}_i \subset \mathbb{R}^n$
- A context function $f_i : \mathcal{X}_i \to \mathbb{R}^d$
- An optimal action $x_i^{\star} \in \mathcal{X}_i$

 $x_i^* \in \underset{x \in \mathcal{X}_i}{\operatorname{arg min}} f_i(x)'c^*$ for some unknown c^*

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Given the data $\mathcal{D} = (\mathcal{X}_i, f_i, x_i^*)_{i=1,...,N}$ and initial knowledge set $c^* \in C_0$, the set of feasible cost vectors is:

$$C(\mathcal{D}) = \left\{ c \in C_0 : x_i^* \in \operatorname*{arg\,min}_{x \in \mathcal{X}_i} f_i(x)'c, \ i = 1, ..., N \right\}$$

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Policy and Objective

A policy $\pi \in \mathcal{P}$ is a mapping from $(\mathcal{D}, \mathcal{X}, f)$ to an action $x^{\pi} \in \mathcal{X}$

Our regret is given by:

$$\mathcal{R}^{\pi}(\boldsymbol{c}^{\star},\mathcal{X},f)=f(\boldsymbol{x}^{\pi})^{\prime}\boldsymbol{c}^{\star}-f(\boldsymbol{x}^{\star})^{\prime}\boldsymbol{c}^{\star}$$

Our **objective** is to find $\pi \in \mathcal{P}$ that minimizes the worst-case regret:

WCR^{$$\pi$$}(\mathcal{D}) = sup $_{c^{\star} \in C(\mathcal{D}), \ \mathcal{X} \in \mathcal{B}, \ f \in \mathcal{F}} \mathcal{R}^{\pi}(c^{\star}, \mathcal{X}, f)$

B: set of all measurable subsets of Rⁿ with diameter at most 1
 F: set of all 1-Lipschitz continuous functions from Rⁿ to R^d

Without distributional assumptions, we can't make claims about the convergence of the minimax regret as N grows.

▶ In a worst-case scenario (X_i and f_i are identical for all i = 1, ..., N), we wouldn't learn anything from observations 2, ..., N.

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What does it mean for the data to be informative?

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We need a bound that is strong if the data is informative.

What does it mean for the data to be informative?

We will build a **geometric** notion of what is an **informative** data set \mathcal{D} .

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Proxy Policies

We focus our attention on **proxy policies**, which are policies where we pick action x^{π} according to a **proxy cost vector** c^{π} :

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$$\mathcal{P}' = \left\{ \pi \in \mathcal{P} : \ \mathsf{x}^{\pi} \in \argmin_{x \in \mathcal{X}} f(x)' \mathbf{c}^{\pi}, \text{ for some } \mathbf{c}^{\pi} \in \mathbb{S}^{d} \right\}$$

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Given a proxy cost c^{π} and a true cost c^{\star} , our loss is bounded by:

$$\mathcal{L}(\boldsymbol{c}^{\pi},\boldsymbol{c}^{\star}) = \sup\left\{f(\boldsymbol{x}^{\pi})'\boldsymbol{c}^{\star} - f(\boldsymbol{x}^{\star})'\boldsymbol{c}^{\star} : \boldsymbol{x}^{\pi} \in \argmin_{\boldsymbol{x} \in \mathcal{X}} f(\boldsymbol{x})'\boldsymbol{c}^{\pi}, \mathcal{X} \in \mathcal{B}, f \in \mathcal{F}\right\}$$

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For any data set \mathcal{D} :

$$\inf_{\pi \in \mathcal{P}'} \operatorname{WCR}^{\pi}(\mathcal{D}) = \inf_{\mathbf{c}^{\pi} \in \mathbb{S}^d} \sup_{\mathbf{c}^{\star} \in \operatorname{C}(\mathcal{D})} \mathcal{L}(\mathbf{c}^{\pi}, \mathbf{c}^{\star})$$

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The Loss of a Proxy Policy

Lemma

Let θ be the angle between two vectors. For any c^{π} , $c^{\star} \in \mathbb{S}^d$:

$$\mathcal{L}(\boldsymbol{c}^{\pi}, \boldsymbol{c}^{\star}) = \begin{cases} \sin \theta(\boldsymbol{c}^{\pi}, \boldsymbol{c}^{\star}) & \text{if } \theta(\boldsymbol{c}^{\pi}, \boldsymbol{c}^{\star}) \leq \pi/2 \\ 1 & \text{otherwise} \end{cases}$$

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If the angle between the true cost c^* and the proxy cost c^{π} is small, the regret must also be small.

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We prove this lemma by showing that the problem of finding a worst-case loss is a semi-definite program.

Uncertainty Angle and Circumcenter

Definition

We define the **uncertainty angle** of a set C to be:

$$\alpha(C) = \inf_{\hat{c} \in \mathbb{S}^d} \sup_{c^{\star} \in C} \theta(\hat{c}, c^{\star}),$$

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The minimizer \hat{c} exists and we call it the **circumcenter** of C.

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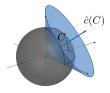
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The uncertainty angle and the circumcenter are the aperture and the axis of the smallest revolution cone containing C.



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Definition

We call the proxy policy that uses the circumcenter as the proxy cost the **circumcenter policy**.

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Theorem

The optimal proxy policy is the circumcenter policy. It achieves:

$$\inf_{\pi \in \mathcal{P}'} \operatorname{WCR}^{\pi}(\mathcal{D}) = \begin{cases} \sin \alpha(\mathcal{C}(\mathcal{D})) & \text{if } \alpha(\mathcal{C}(\mathcal{D})) \leq \pi/2 \\ 1 & \text{otherwise} \end{cases}$$

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The uncertainty angle determines the worst-case regret.

▶ Nontrivial bounds iff *D* implies feasible costs live in a **pointed cone**.

In the online setting, at each period t = 1, ..., T, we are given:

- A set of feasible actions $\mathcal{X}_t \subset \mathbb{R}^n$
- A context function $f_t : \mathcal{X}_t \to \mathbb{R}^d$

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At the end of period t, we observe an optimal action $x_t^{\star} \in \mathcal{X}_t$

Our data at the start of period t is given by

$$\mathcal{I}_t = (\mathcal{X}_i, f_i, x_i^{\star}, x_i^{\pi})_{i=1,...,t-1} \cup (\mathcal{X}_t, f_t)$$

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The set of cost vectors compatible with our data at period t is:

$$C(\mathcal{I}_t) = \left\{ c \in C_0 : x_i^* \in \operatorname*{arg\,min}_{x \in \mathcal{X}_i} f_i(x)'c, \ i = 1, ..., t-1 \right\}$$

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Policy and Objective

A policy $\pi \in \mathcal{P}$ is a mapping from \mathcal{I}_t to an action $x_t^{\pi} \in \mathcal{X}_t$

Our cumulative regret is given by:

$$\mathcal{R}_{T}^{\pi}\left(\boldsymbol{c}^{\star}, \boldsymbol{\vec{\mathcal{X}}}, \boldsymbol{\vec{f}}\right) = \sum_{t=1}^{T} \left(f_{t}(\boldsymbol{x}_{t}^{\pi})'\boldsymbol{c}^{\star} - f_{t}(\boldsymbol{x}_{t}^{\star})'\boldsymbol{c}^{\star}\right)$$

Our **objective** is to find $\pi \in \mathcal{P}$ that minimizes the worst-case regret:

WCR^{$$\pi$$}(C_0) = sup
 $c^* \in C_0, \ \vec{\mathcal{X}} \in \mathcal{B}^T, \ \vec{f} \in \mathcal{F}^T \ \mathcal{R}^\pi\left(c^*, \vec{\mathcal{X}}, \vec{f}\right)$

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• The actions $\{x_t^{\pi}\}$ do not appear in the information set:

$$\boldsymbol{c}^{\star} \in \mathcal{C}(\mathcal{I}_{t}) = \left\{ \boldsymbol{c} \in \mathcal{C}_{0} : \boldsymbol{x}_{i}^{\star} \in \operatorname*{arg\,min}_{\boldsymbol{x} \in \mathcal{X}_{i}} f_{i}(\boldsymbol{x})^{\prime}\boldsymbol{c}, \ i = 1, ..., t-1 \right\}$$

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Perhaps we should ignore the dynamics and use a greedy policy.
Greedy = circumcenter policy.

The Circumcenter Policy Fails in the Online Setting

Theorem

There exists a C_0 such that, if the decision-maker uses the circumcenter policy, nature can cause regret that is linear in T.

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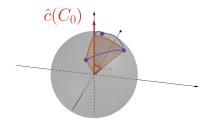
Nature can construct instances where there the decision-maker simultaneously incurs large regret and learns essentially nothing.

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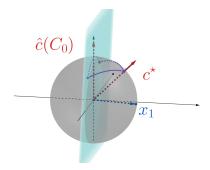
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Learning Nothing While Incurring Regret

- Feasible actions $\mathcal{X} = \{0, x_1\}$ and context function f(x) = x
- Proxy cost of $\hat{c}(C_0)$ implies x_1 is better
- With true cost c^* , the actual optimal action is $x^* = 0$
- Regret is substantial: x₁'c*
- Feedback is marginal: $x_1'c^* \ge x^{*'}c^* = 0$



Let us assume $f_t(x_t^*) \neq f_t(x_t^{\pi})$ (otherwise we don't incur regret)

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By the optimality of x_t^{\star} : $f_t(x_t^{\star})'c^{\star} \leq f_t(x_t^{\pi})'c^{\star}$

▶ That is, we can add constraint $(f_t(x_t^*) - f_t(x_t^{\pi}))'c^* \leq 0$ to $C(\mathcal{I}_{t+1})$

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 - $(f_t(x_t^{\star}) f_t(x_t^{\pi}))$ must satisfy $(f_t(x_t^{\star}) f_t(x_t^{\pi}))'c_t^{\pi} \ge 0$

Let us assume $f_t(x_t^*) \neq f_t(x_t^{\pi})$ (otherwise we don't incur regret)

By the optimality of x_t^* : $f_t(x_t^*)'c^* \leq f_t(x_t^{\pi})'c^*$

▶ That is, we can add constraint $(f_t(x_t^*) - f_t(x_t^{\pi}))'c^* \leq 0$ to $C(\mathcal{I}_{t+1})$

We do have some control over the vector $(f_t(x_t^{\star}) - f_t(x_t^{\pi}))$

- By the optimality of x_t^{π} : $f_t(x_t^{\star})'c_t^{\pi} \ge f_t(x_t^{\pi})'c_t^{\pi}$
 - $\blacktriangleright (f_t(x_t^*) f_t(x_t^{\pi})) \text{ must satisfy } (f_t(x_t^*) f_t(x_t^{\pi}))' c_t^{\pi} \ge 0$

The constraints $(f_t(x_t^{\star}) - f_t(x_t^{\pi}))'c^{\star} \leq 0$ and $(f_t(x_t^{\star}) - f_t(x_t^{\pi}))'c_t^{\pi} \geq 0$ jointly imply that either $c_t^{\pi} \notin C(\mathcal{I}_{t+1})$ or $c_t^{\pi} \in \partial C(\mathcal{I}_{t+1})$

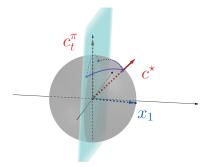
When We Don't Learn Much

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For nature to cause regret in period t, it needs to either remove c_t^{π} from $C(\mathcal{I}_t)$ or at least cut the knowledge set through it

Nature is able to cause significant and little learning when the proxy cost is at or near the boundary of C₀.



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Inverse Exploration

We don't have any direct control over the information gain in our problem

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We don't have any direct control over the information gain in our problem To cause regret, nature needs to cut c_t^{π} or move it to a boundary of $C(\mathcal{I}_{t+1})$

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If we choose c_t^{π} that is away from all the boundaries of $C(\mathcal{I}_t)$, nature needs to at least cut through c_t^{π} , giving us a lot of information

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We call this process of forcing nature to choose between causing regret and impeding learning **inverse exploration**

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The knowledge set evolves by incorporating new halfspace cuts

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- The knowledge set evolves by incorporating new halfspace cuts
- But the circumcenter of a polyhedral cone can easily lie on its boundary

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- Ellipsoidal cone: circumcenter = axis (farthest point from all borders)

EllipsoidalCones is a first step towards our final algorithm

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Types of periods:

No update: we incur low regret

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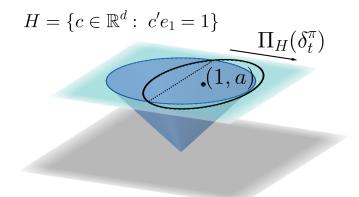
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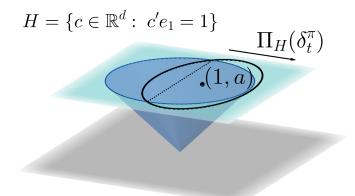
- No update: we incur low regret
- Cone update: we gain valuable information about c*

Why Periods Without Updates?



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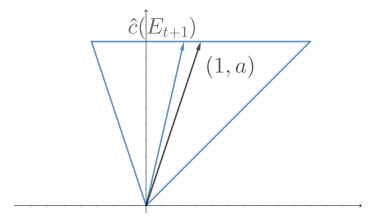
Why Periods Without Updates?



The ellipsoid method runs the risk of making the ellipsoid ill-conditioned (long and skinny). No-update periods prevent that from happening.

Ellipsoid Method for Ellipsoidal Cones

- The variation of the ellipsoid method we developed for cones is novel
- It required finding the best-fit new ellipsoidal cone after an update



Theorem

Consider any C_0 with $\alpha(C_0) < \pi/2$. Then, EllipsoidalCones incurs regret:

WCR(C_0) = $\mathcal{O}(d^2 \ln(T \tan \alpha(C_0)))$.

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First ln(T) regret bound for this problem.

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Can we relax this assumption?

What If we Started From a Nonpointed Set?

If d = 1 or 2, we reach a pointed set after 2 periods where $f_t(x_t^{\pi}) \neq f_t(x_t^{\star})$

What If we Started From a Nonpointed Set?

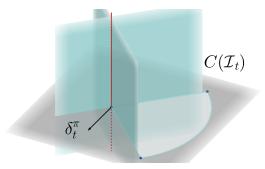
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If $d \ge 3$, nature can stop the knowledge set from becoming pointed

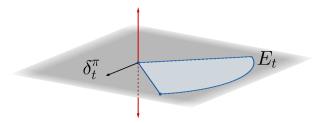
What If we Started From a Nonpointed Set?

If d = 1 or 2, we reach a pointed set after 2 periods where $f_t(x_t^{\pi}) \neq f_t(x_t^{\star})$ If $d \ge 3$, nature can stop the knowledge set from becoming pointed This occurs if natures avoids 1 or more dimensions



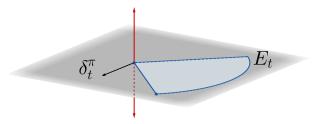
If nature decides not to use a dimension, we don't incur regret from it

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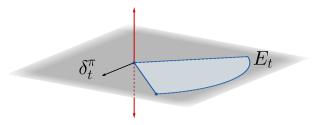
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We do this by keeping track of subspace Δ_t where the projection of $C(\mathcal{I}_t)$ onto Δ_t lives inside a pointed cone

If nature decides not to use a dimension, we don't incur regret from it We can safely ignore such dimensions until nature decides to use them



We do this by keeping track of subspace Δ_t where the projection of $C(\mathcal{I}_t)$ onto Δ_t lives inside a pointed cone

We ignore all information we have about costs orthogonal to Δ_t

► As long as we collect δ_t^{π} close enough to the subspace Δ_t , we proceed with a robustified version of the EllipsoidalCones

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- Otherwise we update Δ_{t+1} (increase the dimension) and fit a new cone

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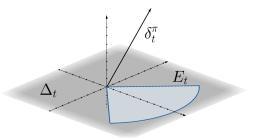
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Types of periods:

- No update: Low regret
- **Cone update**: Sufficient learning within the subspace
- **Dimension update**: Construct a pointed cone in a higher dimension

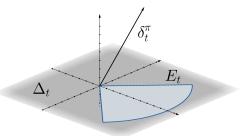
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By performing a dimension update only if δ_t^{π} is sufficiently far from Δ_t , we obtain a higher-dimensional knowledge set that fits inside a pointed cone.



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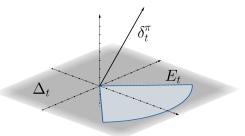
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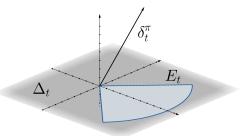
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A bigger gap improves subspace updates (more pointed cone)

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There is a tradeoff in how to set the minimum gap from Δ_t for an update.

- A bigger gap improves subspace updates (more pointed cone)
- A smaller gap improves cone updates (less robustness needed)

Performance of ProjectedCones

Theorem

For any C₀, ProjectedCones incurs regret:

 $\operatorname{WCR}(C_0) = \mathcal{O}(d^4 \ln T)$

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First logarithmic regret bound for this class of models.



Feedback from optimal actions:

Rich class of problems at the frontier of OR and ML



Takeaways

Feedback from optimal actions:

- Rich class of problems at the frontier of OR and ML
- This kind of feedback arises in a wide class of domains

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Gives rise to a novel family of algorithms

Takeaways

Feedback from optimal actions:

- Rich class of problems at the frontier of OR and ML
- This kind of feedback arises in a wide class of domains
- Gives rise to a novel family of algorithms
- Imitation learning is quite different from statistical learning:

inverse exploration vs. classical exploration-exploitation

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