Min Max Generalization for Deterministic Batch Mode Reinforcement Learning: Relaxation Schemes

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Goal

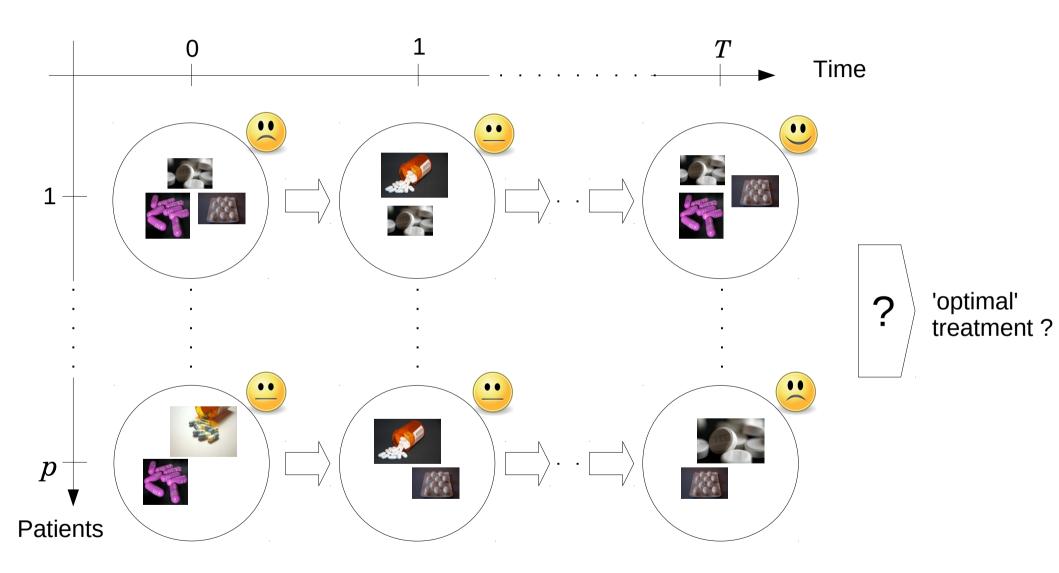


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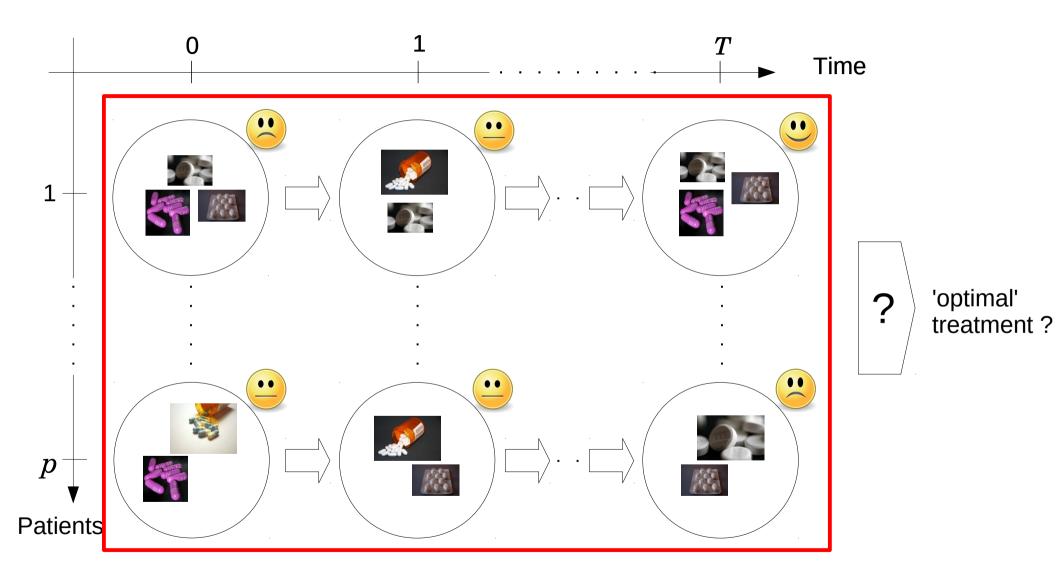
How to control a system so as to avoid the worst, given the knowledge of:

- A batch of (random) trajectories
- Maximal variations of the system, in the form of upper bounds on Lipschitz constants

A motivation: dynamic treatment regimes



A motivation: dynamic treatment regimes



Batch collection of trajectories of patients

Formalization

- Deterministic dynamics: $x_{t+1} = f\left(x_t, u_t\right)$ $t = 0, \ldots, T-1$
- Deterministic reward function: $r_t =
 ho\left(x_t, u_t
 ight) \in \mathbb{R}$
- Fixed initial state: $x_0 \in \mathcal{X}$
- Continuous sate space, finite action space: $\mathcal{U} = \left\{u^{(1)}, \dots, u^{(m)}\right\}$

$$\mathcal{X} \subset \mathbb{R}^d$$

Return of a sequence of actions:

$$J(u_0, \dots, u_{T-1}) \triangleq \sum_{t=0}^{T-1} \rho(x_t, u_t)$$

Optimal return:

$$J_T^* \triangleq \max_{(u_0, \dots, u_{T-1}) \in \mathcal{U}^T} J(u_0, \dots, u_{T-1})$$

The "batch" mode setting

Learning from trajectories

- System dynamics and reward function are unnkown
- For every action $u \in \mathcal{U}$, a **set of transitions** is known:

$$\mathcal{F}^{(u)} = \left\{ \left(x^{(u),k}, r^{(u),k}, y^{(u),k} \right) \right\}_{k=1}^{n^{(u)}}$$
$$y^{(u),k} = f\left(x^{(u),k}, u \right) \text{ and } r^{(u),k} = \rho\left(x^{(u),k}, u \right)$$

Each set of transition is non-empty:

$$\forall u \in \mathcal{U}, \qquad n^{(u)} > 0$$

Define:

$$\mathcal{F} = \mathcal{F}^{(1)} \cup \ldots \cup \mathcal{F}^{(m)}$$

Lipschitz continuity

Assumption about maximal variations

We assume that the system dynamics and reward function are Lipschitz continuous:

$$\forall (x, x') \in \mathcal{X}^2, \forall u \in \mathcal{U},$$

$$\|f(x, u) - f(x', u)\| \leq L_f \|x - x'\|$$

$$|\rho(x, u) - \rho(x', u)| \leq L_\rho \|x - x'\|$$

where $\| \cdot \|$ denotes the Euclidean norm over the state space

• We also assume that two constants L_f and $L_{
ho}$ satisfying the above equations are **known**

Min max generalization

One can define the sets of Lipschitz continuous functions compatible with the data:

$$\mathcal{L}_{\mathcal{F}}^{f} = \left\{ f': \mathcal{X} \times \mathcal{U} \to \mathcal{X} \middle| \begin{cases} \forall x', x'' \in \mathcal{X}, \forall u \in \mathcal{U}, \\ \|f'(x', u) - f'(x'', u)\| \leq L_f \|x' - x''\|, \\ \forall k, f'(x^{(u), k}, u) = f(x^{(u), k}, u) = y^{(u), k}, \end{cases} \right\}$$

$$\mathcal{L}_{\mathcal{F}}^{\rho} = \left\{ \rho' : \mathcal{X} \times \mathcal{U} \to \mathbb{R} \middle| \begin{cases} \forall x', x'' \in \mathcal{X}, \forall u \in \mathcal{U}, \\ |\rho'(x', u) - \rho'(x'', u)| \leq L_{\rho} ||x' - x''||, \\ \forall k, \rho'(x^{(u), k}, u) = \rho(x^{(u), k}, u) = r^{(u), k} \end{cases} \right\}$$

and the return associated with a couple of fonctions taken in those two ensembles :

$$J_{(f',\rho')}(u_0,\ldots,u_{T-1}) = \sum_{t=0}^{T-1} \rho'(x'_t, u_t)$$
$$x'_{t+1} = f'(x'_t, u_t)$$

Min max generalization

One can then define:

$$B^*(\mathcal{F}, u_0, \dots, u_{T-1}) = \min_{(f', \rho') \in \mathcal{L}_{\mathcal{F}}^f \times \mathcal{L}_{\mathcal{F}}^\rho} \left\{ J_{(f', \rho')}(u_0, \dots, u_{T-1}) \right\}$$

And the solution of the min max generalization problem can be defined as follows:

$$(u_0, \dots, u_{T-1}) \in \underset{(u_0, \dots, u_{T-1}) \in \mathcal{U}^T}{\arg \max} B^*(\mathcal{F}, u_0, \dots, u_{T-1})$$

Reformulation

 According to previous research [1], we know that computing the optimal bound for a given sequence of actions can be reformalized as follows:

$$(\mathcal{P}(\mathcal{F}, L_{f}, L_{\rho}, x_{0}, u_{0}, \dots, u_{T-1})):$$

$$\min_{\hat{\mathbf{r}}_{0} \dots \hat{\mathbf{r}}_{T-1} \in \mathbb{R}} \sum_{t=0}^{T-1} \hat{\mathbf{r}}_{t},$$
subject to
$$(3.1)$$

$$\left| \hat{\mathbf{r}}_{t} - r^{(u_{t}), k_{t}} \right|^{2} \leq L_{\rho}^{2} \left\| \hat{\mathbf{x}}_{t} - x^{(u_{t}), k_{t}} \right\|^{2} \ \forall (t, k_{t}) \in \{0, \dots, T-1\} \times \{1, \dots, n^{(u_{t})}\},$$

$$(3.2)$$

$$\left\| \hat{\mathbf{x}}_{t+1} - y^{(u_{t}), k_{t}} \right\|^{2} \leq L_{f}^{2} \left\| \hat{\mathbf{x}}_{t} - x^{(u_{t}), k_{t}} \right\|^{2} \ \forall (t, k_{t}) \in \{0, \dots, T-1\} \times \{1, \dots, n^{(u_{t})}\},$$

$$(3.3) \quad \left| \hat{\mathbf{r}}_{t} - \hat{\mathbf{r}}_{t'} \right|^{2} \leq L_{\rho}^{2} \left\| \hat{\mathbf{x}}_{t} - \hat{\mathbf{x}}_{t'} \right\|^{2} \ \forall t, t' \in \{0, \dots, T-1 | u_{t} = u_{t'}\},$$

$$(3.4)$$

$$\left\| \hat{\mathbf{x}}_{t+1} - \hat{\mathbf{x}}_{t'+1} \right\|^{2} \leq L_{f}^{2} \left\| \hat{\mathbf{x}}_{t} - \hat{\mathbf{x}}_{t'} \right\|^{2} \ \forall t, t' \in \{0, \dots, T-2 | u_{t} = u_{t'}\},$$

$$(3.5) \qquad \hat{\mathbf{x}}_{0} = x_{0}.$$

^{[1] &}quot;Towards Min Max Generalization in Reinforcement Learning". R. Fonteneau, S.A. Murphy, L. Wehenkel and D. Ernst. Agents and Artificial Intelligence: International Conference, ICAART 2010, Valencia, Spain, January 2010, Revised Selected Papers. Series: Communications in Computed and Information Science (CCIS), Volume 129, pp. 61-77. Editors: J. Filipe, A. Fred, and B.Sharp. Springer, Heidelberg, 2011.

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$$(\mathcal{P}(\mathcal{F}, L_f, L_\rho, x_0, u_0, \dots, u_{T-1})): \\ \min_{\substack{\hat{\mathbf{r}}_0 \ \dots \ \hat{\mathbf{r}}_{T-1} \in \mathbb{R} \\ \hat{\mathbf{x}}_0 \ \dots \ \hat{\mathbf{x}}_{T-1} \in \mathbb{R}}} \sum_{t=0}^{T-1} \hat{\mathbf{r}}_t, \\ \text{subject to} \\ \text{Subject to}$$

^{[1] &}quot;Towards Min Max Generalization in Reinforcement Learning". R. Fonteneau, S.A. Murphy, L. Wehenkel and D. Ernst. Agents and Artificial Intelligence: International Conference, ICAART 2010, Valencia, Spain, January 2010, Revised Selected Papers. Series: Communications in Computed and Information Science (CCIS), Volume 129, pp. 61-77. Editors: J. Filipe, A. Fred, and B.Sharp. Springer, Heidelberg, 2011.

Small simplification

One can show that type (3.3) constraints are redundant:

LEMMA 4.1. Consider $(\hat{\mathbf{r}}^*, \hat{\mathbf{x}}^*) \in \mathbb{R}^T \times \mathcal{X}^T$ an optimal solution to $\bar{\mathcal{P}}(\mathcal{F}, u_0, \dots, u_{T-1})$. Then, for all t, t' such that $u_t = u_{t'}$,

$$\|\hat{\mathbf{r}}_{t}^{*} - \hat{\mathbf{r}}_{t'}^{*}\|^{2} \le L_{\rho}^{2} \|\hat{\mathbf{x}}_{t}^{*} - \hat{\mathbf{x}}_{t'}^{*}\|^{2}$$
.

We can deduce the solution for time t=0 :

Lemma 4.2. The solution of the problem $(\mathcal{P}'(\mathcal{F}, u_0))$ is

$$\hat{\mathbf{r}}_0^* = \max_{k_0 \in \{1, \dots, n^{(u_0)}\}} r^{(u_0), k_0} - L_\rho \left\| x_0 - x^{(u_0), k_0} \right\|.$$

New problem

$$(\mathcal{P}''(\mathcal{F}, u_0, \dots, u_{T-1})): \min_{\substack{\hat{\mathbf{r}}_1 \dots \hat{\mathbf{r}}_{T-1} \in \mathbb{R} \\ \hat{\mathbf{x}}_0 \dots \hat{\mathbf{x}}_{T-1} \in \mathcal{X}}} \sum_{t=1}^{T-1} \hat{\mathbf{r}}_t,$$
subject to
$$(5.1) \left\| \hat{\mathbf{r}}_t - r^{(u_t), k_t} \right\|^2 \le L_\rho^2 \left\| \hat{\mathbf{x}}_t - x^{(u_t), k_t} \right\|^2 \ \forall (t, k_t) \in \{1, \dots, T-1\} \times \left\{1, \dots, n^{(u_t)}\right\},$$

$$(5.2) \left\| \hat{\mathbf{x}}_{t+1} - y^{(u_t), k_t} \right\|^2 \le L_f^2 \left\| \hat{\mathbf{x}}_t - x^{(u_t), k_t} \right\|^2 \ \forall (t, k_t) \in \{0, \dots, T-1\} \times \left\{1, \dots, n^{(u_t)}\right\},$$

$$(5.3) \left\| \hat{\mathbf{x}}_{t+1} - \hat{\mathbf{x}}_{t'+1} \right\|^2 \le L_f^2 \left\| \hat{\mathbf{x}}_t - \hat{\mathbf{x}}_{t'} \right\|^2 \ \forall t, t' \in \{0, \dots, T-2 | u_t = u_{t'}\},$$

$$(5.4) \qquad \hat{\mathbf{x}}_0 = x_0.$$

Complexity

- One can show that such a problem is NP-hard
- We propose relaxation schemes of polynomial complexity
- We want those relaxation schemes to preserve the philosophy of the original problem, i.e., to provide lower bounds
- We propose two types of relaxations:
 - The Intertwined Trust-Region (ITR) relaxation scheme
 - The Lagrangian relaxation scheme
- We show that those relaxations are more efficient than previous solution given in [1]

Relaxation schemes

First approach: remove constraints until the problem becomes polynomial

$$(\mathcal{P}''(\mathcal{F}, u_0, \dots, u_{T-1})): \\ \min_{\hat{\mathbf{r}}_1 \dots \dots \hat{\mathbf{r}}_{T-1} \in \mathbb{R}} \sum_{t=1}^{T-1} \hat{\mathbf{r}}_t, \\ \hat{\mathbf{x}}_0 \dots \hat{\mathbf{x}}_{T-1} \in \mathcal{X} \\ \text{subject to} \\ (5.1) \\ \left\| \hat{\mathbf{r}}_t - r^{(u_t), k_t} \right\|^2 \le L_\rho^2 \left\| \hat{\mathbf{x}}_t - x^{(u_t), k_t} \right\|^2 \ \forall (t, k_t) \in \{1, \dots, T-1\} \times \left\{1, \dots, n^{(u_t)}\right\}, \\ (5.2) \\ \left\| \hat{\mathbf{x}}_{t+1} - y^{(u_t), k_t} \right\|^2 \le L_f^2 \left\| \hat{\mathbf{x}}_t - x^{(u_t), k_t} \right\|^2 \ \forall (t, k_t) \in \{0, \dots, T-1\} \times \left\{1, \dots, n^{(u_t)}\right\}, \\ (5.3) \\ \left\| \hat{\mathbf{x}}_{t+1} - \hat{\mathbf{x}}_{t'+1} \right\|^2 \le L_f^2 \left\| \hat{\mathbf{x}}_t - \hat{\mathbf{x}}_{t'} \right\|^2 \ \forall t, t' \in \{0, \dots, T-2 | u_t = u_{t'}\}, \\ (5.4) \qquad \hat{\mathbf{x}}_0 = x_0.$$

We get the ITR problem:

$$(\mathcal{P}''_{ITR}(\mathcal{F}, u_0, \dots, u_{T-1}, \bar{k}_0, \dots, \bar{k}_{T-1})):$$

$$\min_{\hat{\mathbf{r}}_1, \dots, \hat{\mathbf{r}}_{T-1} \in \mathbb{R}} \sum_{t=1}^{T-1} \hat{\mathbf{r}}_t$$

$$\hat{\mathbf{x}}_0, \dots, \hat{\mathbf{x}}_{T-1} \in \mathcal{X}$$
subject to
$$(5.5) \qquad \left| \hat{\mathbf{r}}_t - r^{(u_t), \bar{k}_t} \right|^2 \le L_\rho^2 \left\| \hat{\mathbf{x}}_t - x^{(u_t), \bar{k}_t} \right\|^2, \qquad t \in \{1, \dots, T-1\},$$

$$(5.6) \qquad \left\| \hat{\mathbf{x}}_t - y^{(u_{t-1}), \bar{k}_{t-1}} \right\|^2 \le L_f^2 \left\| \hat{\mathbf{x}}_{t-1} - x^{(u_{t-1}), \bar{k}_{t-1}} \right\|^2, \qquad t \in \{1, \dots, T-1\},$$

$$(5.7) \qquad \hat{\mathbf{x}}_0 = x_0.$$

A closed-form solution of this problem can be obtained

THEOREM 5.4. The solution to $(\mathcal{P}''_{ITR}(\mathcal{F}, u_0, \dots, u_{T-1}, \bar{k}_0, \dots, \bar{k}_{T-1}))$ is given by

$$B_{ITR}''(\mathcal{F}, u_0, \dots, u_{T-1}, \bar{k}_0, \dots, \bar{k}_{T-1}) = \sum_{t=1}^{T-1} \mathbf{\hat{r}}_t^*,$$

where

$$\hat{\mathbf{r}}_{t}^{*} = r^{(u_{t}), \bar{k}_{t}} - L_{\rho} \left\| \hat{\mathbf{x}}_{t}^{*}(\bar{k}_{0}, \dots, \bar{k}_{t}) - x^{(u_{t}), \bar{k}_{t}} \right\|,
\hat{\mathbf{x}}_{t}^{*}(\bar{k}_{0}, \dots, \bar{k}_{t}) \doteq y^{(u_{t-1}), \bar{k}_{t-1}}
+ L_{f} \frac{\left\| \hat{\mathbf{x}}_{t-1}^{*}(\bar{k}_{0}, \dots, \bar{k}_{t-1}) - x^{(u_{t-1}), \bar{k}_{t-1}} \right\|}{\left\| y^{(u_{t-1}), \bar{k}_{t-1}} - x^{(u_{t}), \bar{k}_{t}} \right\|} \left(y^{(u_{t-1}), \bar{k}_{t-1}} - x^{(u_{t}), \bar{k}_{t}} \right)
if $y^{(u_{t-1}), \bar{k}_{t-1}} \neq x^{(u_{t}), \bar{k}_{t}}$$$

and, if $y^{(u_{t-1}),\bar{k}_{t-1}} = x^{(u_t),\bar{k}_t}$, $\hat{\mathbf{x}}_t^*(\bar{k}_0,\ldots,\bar{k}_t)$ can be any point of the sphere centered in $y^{(u_{t-1}),\bar{k}_{t-1}} = x^{(u_t),\bar{k}_t}$ with radius $L_f \|\hat{\mathbf{x}}_{t-1}^*(\bar{k}_0,\ldots,\bar{k}_{t-1}) - x^{(u_{t-1}),\bar{k}_{t-1}}\|$.

- The ITR problem can be solved for any selection of constraints
- One can thus define a maximal ITR bound :

DEFINITION 5.5 (ITR bound $B_{ITR}(\mathcal{F}, u_0, \dots, u_{T-1})$).

$$B_{ITR}(\mathcal{F}, u_0, \dots, u_{T-1}) \triangleq \hat{\mathbf{r}}_0^*$$
+
$$\max_{\bar{k}_{T-1} \in \{1, \dots, n^{(u_{T-1})}\}} B_{ITR}''(\mathcal{F}, u_0, \dots, u_{T-1}, \bar{k}_0, \dots, \bar{k}_{T-1})$$

$$\dots$$

$$\bar{k}_0 \in \{1, \dots, n^{(u_0)}\}$$

(II) Lagrangian relaxation

$$(\mathcal{P}''_{LD}(\mathcal{F}, u_0, \dots, u_{T-1})): \max_{\substack{\nu_{t,t'} \in \mathbb{R} \\ \lambda_{t,k_t} \in \mathbb{R} \\ \mu_{t,k_t} \in \mathbb{R}}} \hat{\mathbf{r}}_{1}, \dots, \hat{\mathbf{r}}_{T-1} \in \mathbb{R} \\ \sum_{\substack{\lambda_{t,k_t} \in \mathbb{R} \\ \mu_{t,k_t} \in \mathbb{R}}} \hat{\mathbf{x}}_{1}, \dots, \hat{\mathbf{x}}_{T-1} \in \mathcal{X}$$

$$\hat{\mathbf{r}}_{1} + \dots + \hat{\mathbf{r}}_{T-1} + \sum_{\substack{(t,k_t) \in \{1,\dots,T-1\} \times \{1,\dots,n^{(u_t)}\} \\ (t,k_t) \in \{1,\dots,T-1\} \times \{1,\dots,n^{(u_t)}\}}} \mu_{t,k_t} \left(\left\| \hat{\mathbf{r}}_{t} - r^{(u_t),k_t} \right\|^2 - L_{\rho}^2 \left\| \hat{\mathbf{x}}_{t} - x^{(u_t),k_t} \right\|^2 \right) + \sum_{\substack{(t,k_t) \in \{1,\dots,T-1\} \times \{1,\dots,n^{(u_t)}\} \\ t,t' \in \{0,\dots,T-2|u_t=u_{t'}\}}} \nu_{t,t'} \left(\left\| \hat{\mathbf{x}}_{t+1} - \hat{\mathbf{x}}_{t'+1} \right\|^2 - L_{f}^2 \left\| \hat{\mathbf{x}}_{t} - \hat{\mathbf{x}}_{t'} \right\|^2 \right).$$

Polynomial complexity

Comparison with the relaxation proposed in [1]:

Definition 5.8 (CGRL bound $B_{CGRL}(\mathcal{F}, u_0, \dots, u_{T-1})$).

• ITR versus [1] :

THEOREM 5.9.

$$B_{CGRL}(\mathcal{F}, u_0, \dots, u_{T-1}) \leq B_{ITR}(\mathcal{F}, u_0, \dots, u_{T-1})$$

Sketch of proof:

Compute the ITR relaxation with the constraints used by the CGRL bound

Lagrangian relaxation versus ITR :

THEOREM 5.17.

$$B_{ITR}(\mathcal{F}, u_0, \dots, u_{T-1}) \le B_{LD}(\mathcal{F}, u_0, \dots, u_{T-1})$$

Sketch of proof:

- Strong duality holds for the Lagrangian relaxation of the ITR problem

• Synthesis:

$$B_{CGRL}(\mathcal{F}, u_0, \dots, u_{T-1}) \leq B_{ITR}(\mathcal{F}, u_0, \dots, u_{T-1})$$

$$\leq B_{LD}(\mathcal{F}, u_0, \dots, u_{T-1})$$

$$\leq B^*(\mathcal{F}, u_0, \dots, u_{T-1})$$

$$\leq J(u_0, \dots, u_{T-1}).$$

 All these bounds converge to the actual return of sequences of actions when the dispersion decreases towards zero

Illustration

• Dynamics:
$$\forall (x, u) \in \mathcal{X} \times \mathcal{U}, \qquad f(x, u) = x + 3.1416 \times u \times 1_d$$

• Reward function:
$$\forall (x,u) \in \mathcal{X} \times \mathcal{U}, \qquad \rho(x,u) = \sum_{i=1}^{a} x(i)$$

• Initial state:
$$x_0 = 0.5772 \times 1_d$$

• Decision space:
$$\mathcal{U} = \{0, 0.1\}$$

Grid :

$$\forall u \in \mathcal{U}, \mathcal{F}_{c_i}^{(u)} = \left\{ \left(\left[\frac{i_1}{i}; \frac{i_2}{i} \right], u, \rho \left(\left[\frac{i_1}{i}; \frac{i_2}{i} \right], u \right), f \left(\left[\frac{i_1}{i}; \frac{i_2}{i} \right], u \right) \right) \middle| (i_1, i_2) \in \{1, \dots, i\}^2 \right\}$$

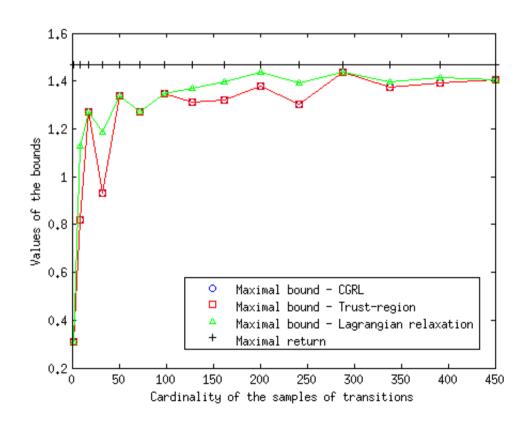
• 100 samples of transitions drawn uniformly at random

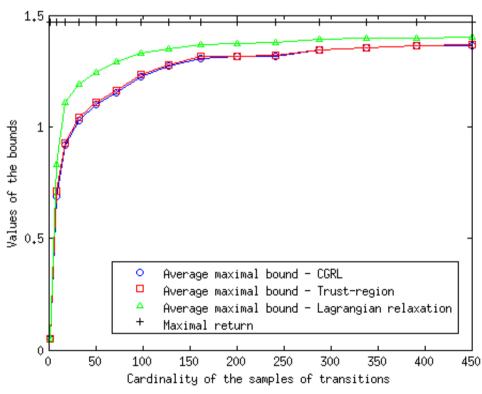
Illustration

Maximal bounds

Grid

Empirical average over random samples



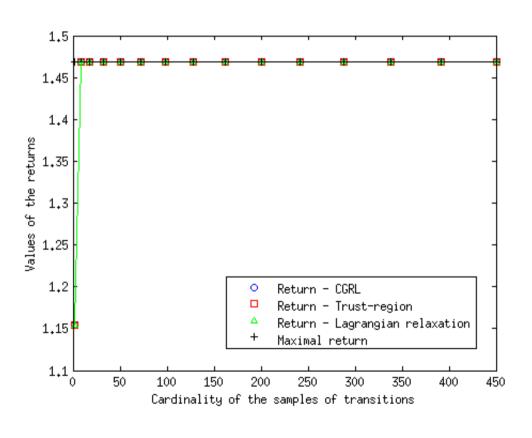


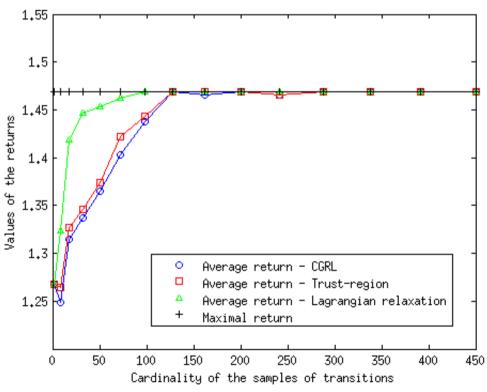
Illustration

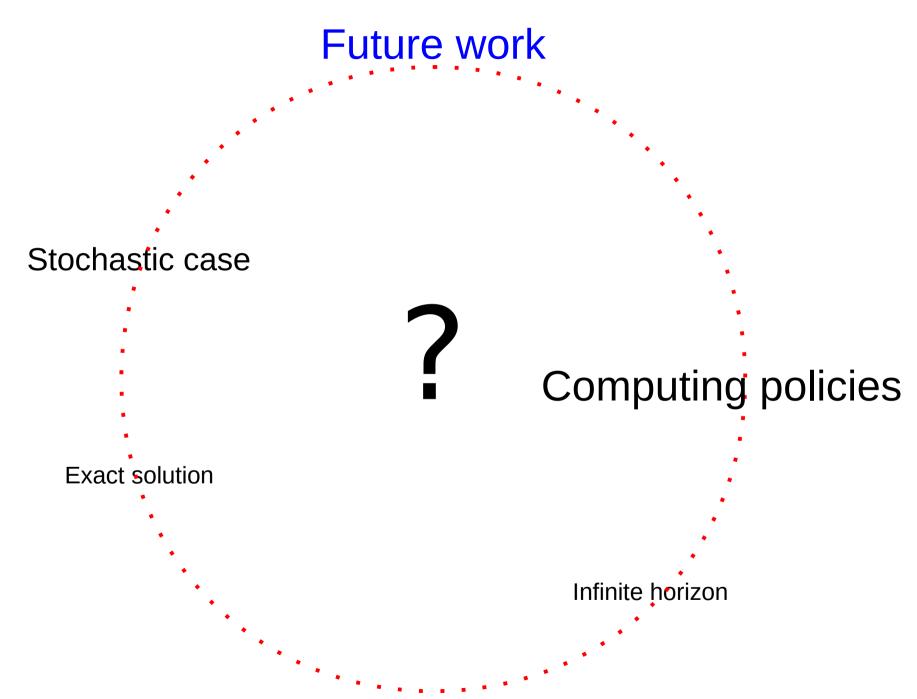
Returns of sequences

Grid

Empirical average over random samples







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