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

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November, 29th, 2013
Maastricht, The Nederlands
Goal

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

Time

Patients

'optimal' treatment?
A motivation: dynamic treatment regimes

Batch collection of trajectories of patients
Formalization

- Deterministic dynamics:  
  \[ x_{t+1} = f(x_t, u_t) \quad t = 0, \ldots, T - 1 \]

- Deterministic reward function:  
  \[ r_t = \rho(x_t, u_t) \in \mathbb{R} \]

- Fixed initial state:  
  \[ x_0 \in \mathcal{X} \]

- Continuous state space, finite action space:  
  \[ \mathcal{U} = \{ u^{(1)}, \ldots, u^{(m)} \} \]
  \[ \mathcal{X} \subset \mathbb{R}^d \]

- Return of a sequence of actions:
  \[
  J(u_0, \ldots, u_{T-1}) \triangleq \sum_{t=0}^{T-1} \rho(x_t, u_t)
  \]

- Optimal return:
  \[
  J_T^* \triangleq \max_{(u_0, \ldots, u_{T-1}) \in \mathcal{U}^T} J(u_0, \ldots, u_{T-1})
  \]
The "batch" mode setting

Learning from trajectories

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

\[
\mathcal{F}(u) = \left\{ (x^{(u),k}, r^{(u),k}, y^{(u),k}) \right\}_{k=1}^{n^{(u)}}
\]

\[
y^{(u),k} = f \left( x^{(u),k}, u \right) \quad \text{and} \quad r^{(u),k} = \rho \left( x^{(u),k}, u \right)
\]

- Each set of transition is non-empty:

\[
\forall u \in \mathcal{U}, \quad n^{(u)} > 0
\]

- 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 \( L_\rho \) satisfying the above equations are known.
Min max generalization

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

\[
\mathcal{L}^f_{\mathcal{F}}(f') = \left\{ f' : \mathcal{X} \times \mathcal{U} \to \mathcal{X} \mid \begin{array}{l}
\forall x', x'' \in \mathcal{X}, \forall u \in \mathcal{U}, \\
\quad \|f'(x', u) - f'(x'', u)\| \leq L_f \|x' - x''\|,
\end{array} \\
\forall k, f'(x(u), k, u) = f(x(u), k, u) = y(u), k
\right\}
\]

\[
\mathcal{L}^\rho_{\mathcal{F}}(\rho') = \left\{ \rho' : \mathcal{X} \times \mathcal{U} \to \mathbb{R} \mid \begin{array}{l}
\forall x', x'' \in \mathcal{X}, \forall u \in \mathcal{U}, \\
\quad |\rho'(x', u) - \rho'(x'', u)| \leq L_{\rho} \|x' - x''\|,
\end{array} \\
\forall k, \rho'(x(u), k, u) = \rho(x(u), k, u) = r(u), k
\right\}
\]

and the return associated with a couple of functions 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:

\[
B^*(\mathcal{F}, u_0, \ldots, u_{T-1}) = \min_{(f', \rho') \in \mathcal{L}_f \times \mathcal{L}_\rho} \left\{ J(f', \rho') (u_0, \ldots, u_{T-1}) \right\}
\]

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

\[
(u_0, \ldots, u_{T-1}) \in \arg \max_{(u_0, \ldots, u_{T-1}) \in \mathcal{U}^T} B^*(\mathcal{F}, u_0, \ldots, u_{T-1})
\]
Reformulation

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

\[
(P(F, L_f, L_\rho, x_0, u_0, \ldots, u_{T-1})):
\]

\[
\min_{\hat{r}_0, \ldots, \hat{r}_{T-1} \in \mathbb{R}} \sum_{t=0}^{T-1} \hat{r}_t,
\]

subject to

\[
(3.1) \quad \left| \hat{r}_t - r(u_t, k_t) \right|^2 \leq L^2_\rho \left| \hat{x}_t - x(u_t, k_t) \right|^2 \quad \forall (t, k_t) \in \{0, \ldots, T - 1\} \times \{1, \ldots, n^{(u_t)}\};
\]

\[
(3.2) \quad \left\| \hat{x}_{t+1} - y(u_t, k_t) \right\|^2 \leq L^2_f \left\| \hat{x}_t - x(u_t, k_t) \right\|^2 \quad \forall (t, k_t) \in \{0, \ldots, T - 1\} \times \{1, \ldots, n^{(u_t)}\};
\]

\[
(3.3) \quad \left| \hat{r}_t - \hat{r}_{t'} \right|^2 \leq L^2_\rho \left\| \hat{x}_t - \hat{x}_{t'} \right\|^2 \quad \forall t, t' \in \{0, \ldots, T - 1\} | u_t = u_{t'}\};
\]

\[
(3.4) \quad \left\| \hat{x}_{t+1} - \hat{x}_{t'+1} \right\|^2 \leq L^2_f \left\| \hat{x}_t - \hat{x}_{t'} \right\|^2 \quad \forall t, t' \in \{0, \ldots, T - 2\} | u_t = u_{t'}\};
\]

\[
(3.5) \quad \hat{x}_0 = x_0.
\]

Reformulation

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

\[
\begin{align*}
(\mathcal{P}(F, L_f, L_p, x_0, u_0, \ldots, u_{T-1})) : \\
\min_{\hat{r}_0 \ldots \hat{r}_{T-1} \in \mathbb{R}} \sum_{t=0}^{T-1} \hat{r}_t, \\
\text{s.t. } \hat{x}_0 \ldots \hat{x}_{T-1} \in \mathcal{X}
\end{align*}
\]

[1] proposes a lower bound on the optimal bound (computed independently from this reformulation)

Here, we directly target this problem in order to find a bound tighter than [1]
Small simplification

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

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

\[ |\hat{r}^*_t - \hat{r}^*_{t'}|^2 \leq L^2_{\rho} \|\hat{x}^*_t - \hat{x}^*_{t'}\|^2. \]

- We can deduce the solution for time t=0:

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

\[ \hat{r}^*_0 = \max_{k_0 \in \{1, \ldots, n(u_0)\}} r^{(u_0),k_0} - L_{\rho} \|x_0 - x^{(u_0),k_0}\|. \]
New problem

\[(\mathcal{P}''(\mathcal{F}, u_0, \ldots, u_{T-1})):\]

\[\begin{align*}
\min & \quad \sum_{t=1}^{T-1} \hat{r}_t, \\
\hat{r}_1 & \ldots \hat{r}_{T-1} \in \mathbb{R} \\
\hat{x}_0 & \ldots \hat{x}_{T-1} \in \mathcal{X}
\end{align*}\]

subject to

\[(5.1) \quad \left| \hat{r}_t - r(u_t, k_t) \right|^2 \leq L^2_\rho \left\| \hat{x}_t - x(u_t, k_t) \right\|^2 \quad \forall (t, k_t) \in \{1, \ldots, T-1\} \times \{1, \ldots, n(u_t)\},
\]

\[(5.2) \quad \left\| \hat{x}_{t+1} - y(u_t, k_t) \right\|^2 \leq L^2_f \left\| \hat{x}_t - x(u_t, k_t) \right\|^2 \quad \forall (t, k_t) \in \{0, \ldots, T-1\} \times \{1, \ldots, n(u_t)\},
\]

\[(5.3) \quad \left\| \hat{x}_{t+1} - \hat{x}_{t'} \right\|^2 \leq L^2_f \left\| \hat{x}_t - \hat{x}_{t'} \right\|^2 \quad \forall t, t' \in \{0, \ldots, T-2\} | u_t = u_{t'},
\]

\[(5.4) \quad \hat{x}_0 = x_0.\]
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
(I) Intertwined trust-region

- First approach: remove constraints until the problem becomes polynomial

\[
(P''(F, u_0, \ldots, u_{T-1})):
\]

\[
\min \sum_{t=1}^{T-1} \hat{r}_t, \quad \hat{r}_1, \ldots, \hat{r}_{T-1} \in \mathbb{R}, \quad \hat{x}_0, \ldots, \hat{x}_{T-1} \in X
\]

subject to

\[
|\hat{r}_t - r(u_t, k_t)|^2 \leq L^2_{\rho} \|\hat{x}_t - x(u_t, k_t)\|^2 \quad \forall (t, k_t) \in \{1, \ldots, T-1\} \times \{1, \ldots, n(u_t)\},
\]

Only one constraint

\[
|\hat{x}_{t+1} - y(u_t, k_t)|^2 \leq L^2_f \|\hat{x}_t - x(u_t, k_t)\|^2 \quad \forall (t, k_t) \in \{0, \ldots, T-1\} \times \{1, \ldots, n(u_t)\},
\]

\[
\|\hat{x}_{t+1} - \hat{x}_{t'+1}\|^2 \leq L^2_f \|\hat{x}_t - \hat{x}_{t'}\|^2 \quad \forall t, t' \in \{0, \ldots, T-2\}, u_t = u_{t'}
\]

(5.4) \( \hat{x}_0 = x_0 \).
(I) Intertwined trust-region

- We get the ITR problem:

\[
(\mathcal{P}_{ITR}''(F, u_0, \ldots, u_{T-1}, k_0, \ldots, k_{T-1})) : \quad \min_{\hat{r}_1, \ldots, \hat{r}_{T-1} \in \mathbb{R}} \quad \sum_{t=1}^{T-1} \hat{r}_t \\
\text{subject to} \\
(5.5) \quad \left\| \hat{r}_t - r(u_t, k_t) \right\|^2 \leq L^2_\rho \left\| \hat{x}_t - x(u_t, k_t) \right\|^2, \quad t \in \{1, \ldots, T-1\}, \\
(5.6) \quad \left\| \hat{x}_t - y(u_{t-1}, k_{t-1}) \right\|^2 \leq L^2_f \left\| \hat{x}_{t-1} - x(u_{t-1}, k_{t-1}) \right\|^2, \quad t \in \{1, \ldots, T-1\}, \\
(5.7) \quad \hat{x}_0 = x_0.
\]

- A closed-form solution of this problem can be obtained
(I) Intertwined trust-region

**Theorem 5.4.** The solution to \( (P''_{ITR}(F, u_0, \ldots, u_{T-1}, k_0, \ldots, k_{T-1})) \) is given by

\[
B''_{ITR}(F, u_0, \ldots, u_{T-1}, k_0, \ldots, k_{T-1}) = \sum_{t=1}^{T-1} \hat{r}_t^*,
\]

where

\[
\hat{r}_t^* = r^{(u_t), k_t} - L_P \left\| \hat{x}_t^*(k_0, \ldots, k_t) - x^{(u_t), k_t} \right\|
\]

\[
\hat{x}_t^*(k_0, \ldots, k_t) \doteq y^{(u_{t-1}), k_{t-1}}
\]

\[
+ L_f \frac{\left\| \hat{x}_{t-1}^*(k_0, \ldots, k_{t-1}) - x^{(u_{t-1}), k_{t-1}} \right\|}{\left\| y^{(u_{t-1}), k_{t-1}} - x^{(u_t), k_t} \right\|} \left( y^{(u_{t-1}), k_{t-1}} - x^{(u_t), k_t} \right)
\]

if \( y^{(u_{t-1}), k_{t-1}} \neq x^{(u_t), k_t} \)

and, if \( y^{(u_{t-1}), k_{t-1}} = x^{(u_t), k_t} \), \( \hat{x}_t^*(k_0, \ldots, k_t) \) can be any point of the sphere centered in \( y^{(u_{t-1}), k_{t-1}} = x^{(u_t), k_t} \) with radius \( L_f \left\| \hat{x}_{t-1}^*(k_0, \ldots, k_{t-1}) - x^{(u_{t-1}), k_{t-1}} \right\|. \)
(I) Intertwined trust-region

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

**Definition 5.5** (ITR bound $B_{ITR}(\mathcal{F}, u_0, \ldots, u_{T-1})$).

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

\[
\bar{k}_0 \in \{1, \ldots, n^{(u_0)}\}
\]

\[
\bar{k}_0 \in \{1, \ldots, n^{(u_0)}\}
\]
(II) Lagrangian relaxation

\[ (\mathcal{P}_{LD}''(\mathcal{F}, u_0, \ldots, u_{T-1})) : \]

\[
\begin{align*}
\max_{\nu_{t,t'} \in \mathbb{R}} & \quad \min_{\hat{r}_1, \ldots, \hat{r}_{T-1} \in \mathbb{R}} \\
\sum_{(t,k_t) \in \{1, \ldots, T-1\} \times \{1, \ldots, n(u_t)\}} & \quad \mu_{t,k_t} \left( \left\| \hat{r}_t - r(u_t,k_t) \right\|^2 - L^2_{\rho} \left\| \hat{x}_t - x(u_t,k_t) \right\|^2 \right) \\
+ \sum_{(t,k_t) \in \{1, \ldots, T-1\} \times \{1, \ldots, n(u_t)\}} & \quad \lambda_{t,k_t} \left( \left\| \hat{x}_{t+1} - y(u_t,k_t) \right\|^2 - L^2_{f} \left\| \hat{x}_t - x(u_t,k_t) \right\|^2 \right) \\
+ \sum_{t,t' \in \{0, \ldots, T-2\} \mid u_t = u_{t'}} & \quad \nu_{t,t'} \left( \left\| \hat{x}_{t+1} - \hat{x}_{t'+1} \right\|^2 - L^2_{f} \left\| \hat{x}_t - \hat{x}_{t'} \right\|^2 \right). 
\end{align*}
\]

- Polynomial complexity
Tightness of the bounds

- Comparison with the relaxation proposed in [1]:

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

\[
B_{CGRL}(\mathcal{F}, u_0, \ldots, u_{T-1}) \triangleq \max_{\bar{k}_{T-1} \in \{1, \ldots, n^{(u_{T-1})}\}} \max_{\bar{k}_0 \in \{1, \ldots, n^{(u_0)}\}} \left[ r^{(u_0), \bar{k}_0} - L_\rho \left( 1 + L_f + L_f^2 + \cdots + L_f^{T-2} \right) \left\| x^{(u_0), \bar{k}_0} - x_0 \right\| ight. \\
+ \cdots + \\
\left. + r^{(u_{T-2}), \bar{k}_{T-2}} - L_\rho \left( 1 + L_f \right) \left\| y^{(u_{T-3}), \bar{k}_{T-3}} - x^{(u_{T-2}), \bar{k}_{T-2}} \right\| \\
+ r^{(u_{T-1}), \bar{k}_{T-1}} - L_\rho \left\| y^{(u_{T-2}), \bar{k}_{T-2}} - x^{(u_{T-1}), \bar{k}_{T-1}} \right\| \right].
\]
Tightness of the bounds

• ITR versus [1]:

\textbf{Theorem 5.9.}

\[ B_{\text{CGRL}}(\mathcal{F}, u_0, \ldots, u_{T-1}) \leq B_{\text{ITR}}(\mathcal{F}, u_0, \ldots, u_{T-1}) \]

Sketch of proof:

– Compute the ITR relaxation with the constraints used by the CGRL bound
Tightness of the bounds

• Lagrangian relaxation versus ITR:

**Theorem 5.17.**

\[ B_{ITR}(F, u_0, \ldots, u_{T-1}) \leq B_{LD}(F, u_0, \ldots, u_{T-1}) \]

Sketch of proof:

– Strong duality holds for the Lagrangian relaxation of the ITR problem
Tightness of the bounds

- Synthesis:

\[
B_{\text{CGRL}}(\mathcal{F}, u_0, \ldots, u_{T-1}) \leq B_{\text{ITR}}(\mathcal{F}, u_0, \ldots, u_{T-1}) \\
\leq B_{\text{LD}}(\mathcal{F}, u_0, \ldots, u_{T-1}) \\
\leq B^*(\mathcal{F}, u_0, \ldots, u_{T-1}) \\
\leq J(u_0, \ldots, u_{T-1}).
\]

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

- Dynamics: \( \forall (x, u) \in X \times U, \quad f(x, u) = x + 3.1416 \times u \times 1_d \)

- Reward function: \( \forall (x, u) \in X \times U, \quad \rho(x, u) = \sum_{i=1}^d x(i) \)

- Initial state: \( x_0 = 0.5772 \times 1_d \)

- Decision space: \( U = \{0, 0.1\} \)

- Grid:
  \[ \forall u \in U, \mathcal{F}_{c_i}^{(u)} = \left\{ \left( \left( \begin{bmatrix} i_1 \\ i \\ i_2 \\ i \end{bmatrix}, u, \rho \left( \left( \begin{bmatrix} i_1 \\ i \\ i_2 \\ i \end{bmatrix}, u \right), f \left( \left( \begin{bmatrix} i_1 \\ i \\ i_2 \\ i \end{bmatrix}, u \right) \right) \right) \mid (i_1, i_2) \in \{1, \ldots, i\}^2 \right\} \]

- 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
Future work

Stochastic case

Exact solution

Infinite horizon

Computing policies


Hope to see you there!

http://sites.google.com/site/jfpda14/