OPTIMAL SAMPLE SELECTION FOR BATCH-MODE REINFORCEMENT LEARNING

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Abstract: We introduce the *Optimal Sample Selection* (OSS) meta-algorithm for solving discrete-time Optimal Control problems. This meta-algorithm maps the problem of finding a near-optimal closed-loop policy to the identification of a small set of one-step system transitions, leading to high-quality policies when used as input of a batch-mode Reinforcement Learning (RL) algorithm. We detail a particular instance of this OSS meta-algorithm that uses tree-based Fitted Q-Iteration as a batch-mode RL algorithm and Cross Entropy search as a method for navigating efficiently in the space of sample sets. The results show that this particular instance of OSS algorithms is able to identify rapidly small sample sets leading to high-quality policies.

1 INTRODUCTION

Many problems in the fields of Finance, Engineering or Medicine can be cast as discrete-time Optimal Control problems. Such problems feature a dynamic system that evolves over several time steps and receives various rewards along the way, depending on how well it performs. Solving these problems consists in generating a sequence of appropriate control inputs, in order for the system to follow a trajectory providing an optimal cumulated reward. In the general case, this resolution rapidly becomes very challenging as the problem's size grows. Optimal Control problems have been studied by various communities (*e.g.*, Artificial Intelligence, Control Systems, Operations Research, or Machine Learning), each using different assumptions and formalisms to design algorithmic solutions.

Reinforcement Learning (RL) (Sutton and Barto, 1998) is a subfield of Machine Learning where one tries to infer a good closed-loop *control policy* from the sole knowledge of an observed set of one-step system transitions and their associated rewards. Such a set results from the sampling of the system's underlying dynamics and rewards. When this set of samples is given at once, as an input of the learning algorithm, one talks of *batch-mode* RL. In recent years, batch-mode RL algorithms, such as the tree-based Fitted Q-Iteration (FQI) (Ernst et al., 2005) or the Least Squares Policy Iteration (Lagoudakis and Parr, 2003a) algorithms, proved successful in tackling large Optimal Control problems. These methods relied on appropriate approximation architectures to efficiently generalize information throughout the state space. We now wish to understand how they could be used for solving large-scale problems when one has some freedom in the sample set input. In other words, we break free from the standard batch-mode RL hypothesis of a fixed, imposed sample set, and suppose that a generative model is available, providing an unconstrained way of picking new sample sets. Suppressing the constraint of a fixed, unquestionable input sample set, and allowing this input to be considered as a problem's variable, raises the question of identifying a set of one-step transitions which maximizes the learning algorithm's output, while keeping the number of such one-step transitions low, so as to extract good policies from the sample set in a reasonable amount of time.

An immediate approach at answering this question would be to collect experience uniformly and extensively over the problem's state-action space, as finely as necessary to provide a good representation of the system. But for large scale problems, as the dimension of this state-action space grows, such a sample set becomes so large that processing it becomes increasingly difficult (as reported in (Ernst, 2005) for instance). Hence, the problem we address in this context consists in identifying a training set of one-step transitions which both has a limited size, and maximizes the algorithm's output. For this purpose, we concentrate on the question of finding the input sample set of size N that will generate the best possible

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output policy, for a given batch-mode RL algorithm and a predefined sample set size N.

After recalling, in Section 2, the main notions of discrete-time Optimal Control and Reinforcement Learning, we formulate the search for an optimal fixed-size sample set as an optimization problem and discuss its properties in Section 3. This leads to the definition of the general *Optimal Sample Selection* (OSS) meta-algorithm for solving Optimal Control problems. Section 4 details a particular instance of OSS, using the tree-based FQI algorithm and Cross-Entropy search. Section 5 reports the method's results on the "car on the hill" domain, empirically illustrating the fact that small optimized sample sets can lead to high quality policies. Building on these optimization results, Section 6 discusses some more general properties of OSS methods, highlighting their strengths, weaknesses and perspectives. We particularly emphasize their potential for solving large scale Optimal Control problems. We finally summarize our contribution and conclude in Section 7.

2 OPTIMAL CONTROL AND REINFORCEMENT LEARNING

The framework of discrete-time Optimal Control (Bertsekas and Shreve, 1996) covers decision problems where one tries to control a system, characterized by its state $x \in X$, through the application of a sequence of discrete-time commands $(u_t)_{t\in\mathbb{N}}, u_t \in U$, in order to optimize a criterion based on the system's trajectory. Formally, such problems are described by a four-tuple $\langle X, U, f, r\rangle$, where X is the state space in which the system evolves, U is the set of all possible commands (or actions), f and r are respectively a transition and a reward model as illustrated on Figure 1. In the deterministic case, at time step t, if command u is applied while the system is in state x, a transition is triggered to the next state $x' = f(x,u)$. For this transition, a reward $r(x,u)$ is gained.

In the general case of stochastic Optimal Control, the (stationary) transition model is actually stochastic: $f(x,u)$ is a distribution over the possible next states x', and one writes $x' \sim f(x,u)$. The reward function then corresponds to the expected one-step reward for the considered state-action pair. For the sake of simplicity, we will consider deterministic problems in Sections 3 to 5 and will extend our approach to the stochastic case in Section 6.

A (stationary) *closed-loop controller*, or *decision policy*, for a discrete-time Optimal Control problem is a function $\mu : X \to U$ ($\mu \in \mathcal{F}(X,U)$), mapping each state x to an action u to undertake. The criterion J^μ we will consider in order to discriminate between policies and define optimality is the standard, infinite horizon, γ-discounted criterion. It maps each state x to the sum of the γ-discounted successive rewards obtained when applying policy μ from x, for an infinite number of steps: $\forall x \in X$,

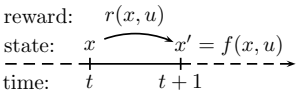


Figure 1: Transition and reward models of a discrete-time control problem.

$$J^\mu(x) = \sum_{t=0}^{\infty} \gamma^t r(x_t, \mu(x_t)) \text{ with } \begin{cases} x_0 = x \text{ and} \\ x_{t+1} = f(x_t, \mu(x_t)) \end{cases}$$

Then, a policy μ^* is said to be optimal if:

$$\forall x \in X, \mu \in \mathcal{F}(X,U),\ J^{\mu^*}(x) \geq J^\mu(x)$$

The J^μ function of a policy μ is called its value function. One writes J^* the value function of any optimal policy.

RL algorithms aim at finding the best control policy when the transition and reward models of the process are unknown. Instead, they rely on the collection of one-step transition *samples* from this underlying model. Each sample describes a one-step transition as a four-tuple (x,u,r,x'). These samples can be obtained either from interaction with the physical system or from a generative model. Hence, the standard input of any batch-mode RL algorithm is a set of samples $D = \{(x,u,r,x')\}$, approximating the transition and reward models, from which the algorithm infers a policy μ^*_D.

Since many applications of RL have very large or multi-dimensional, continuous state spaces, finding an exact representation of the optimal policy or value function is often a very difficult task. Consequently, there is a need for approximation methods that are able to solve the policy inference problem in a compact and efficient fashion (Buşoniu et al., 2010). In order to overcome this difficulty, different value function and policy approximation architectures have been proposed in the literature, such as combinations of linear features (Boyan, 1999), kernel methods (Ormoneit and Sen, 2002), forests of trees (Ernst et al., 2005) or classifiers (Lagoudakis and Parr, 2003b). All these methods have greatly contributed to extending the practical applicability of RL.

3 OPTIMIZING SAMPLE SETS

The general goal of batch-mode RL is, given a sample set D as input, to compute a policy μ^*_D which is as

Figure 2: Score of a sampling scheme.

close as possible to an optimal policy for the system the samples were gathered from. The RL literature provides a whole span of efficient methods to compute such a μ^*_D.

Consider the context where a generative model of the system is available. Such a model outputs a one-step transition (x,u,r,x') when presented with a state x and an action u. In many Optimal Control problems, such a model is often available. Since we have this generative model, the input sample set D is no longer imposed to us. The Optimal Control practitioner willing to exploit batch-mode RL methods then needs to answer the simple question of how to generate a good sample set, prior to running his favourite algorithm.

The generic question of collecting data for batch-mode RL algorithms has received little attention in the literature, as this problem is usually tackled from a problem-specific point of view (*e.g.*, (Neumann and Peters, 2009; Riedmiller, 2005; Ernst et al., 2006)). We investigate a way to tackle this problem from a *generic*, problem-independent, point of view.

3.1 Optimal Sample Selection

We consider the framework where the sample set's size is fixed and the batch-mode RL algorithm is chosen, and, in this context, we introduce a meta-algorithm[1] for generating good sample sets D.

Consider a sample set $D = \{(x,u,r,x')\}$ and let us introduce the set $\theta = \{(x,u)\}$ which we call the *sampling scheme* leading to D. Although, in the deterministic case, there is a complete equivalence between θ and D, this distinction will appear necessary when we extend this contribution to stochastic systems in Section 6. Suppose also that, for convenience, we ordered the different elements[2] in D and θ:

$$D = \left\{\left(x_i,u_i,r_i,x'_i\right)\right\}_{i\in[1;N]}$$
$$\theta = \{(x_i,u_i)\}_{i\in[1;N]}$$

Let $sample(\cdot)$ be the operator that computes D from θ, using the generative model. Let also $policy\_inference(\cdot)$ denote the batch-mode RL algorithm used, taking a set D as input, and outputting a policy μ^*_D, which is optimal (or quasi-optimal) with respect to an implicit, approximate problem, implied by D. Let us finally assume there exists a generic criterion $score(\mu)$, allowing to evaluate the actual quality of a policy μ, when applied to the domain at hand.

Then we propose to identify a good training set by formulating the following optimization problem (illustrated on Fig 2):

$$\theta^* \in \operatorname*{argmax}_{\theta\in(X\times U)^N} M(\theta) \quad (1)$$
$$M(\theta) = (score \circ policy\_inference \circ sample)(\theta)$$

Hence, given an Optimal Control problem's generative model, a batch-mode RL algorithm, and a size N of sample sets, we call *Optimal Sample Selection method of parameter N* (OSS(N)), an optimization method searching for this optimal sampling scheme θ^* and returning $\mu^* = policy\_inference(sample(\theta^*))$, as shown in Algorithm 1.

Algorithm 1: General layout of the OSS (N) meta-algorithm.

Input: Batch-mode RL alg. $policy\_inference(\cdot)$, ;
Policy evaluation method $score(\cdot)$,;
Generative model $sample(\cdot)$.;
Define $M(\theta)$ as in Equation (1). ;
Compute $\theta^* = \operatorname{argmax}_\theta M(\theta)$. ;
Return $policy\_inference(sample(\theta^*))$.

3.2 Creating Instances of OSS(N)

The performance and behaviour of an OSS(N) instance will depend on the choices made for $score(\cdot)$ and $policy\_inference(\cdot)$, but also on the value of N and on the optimization method used to solve problem 1. We provide hereafter some elements that may help make these choices.

Score Function. The score function should be chosen in order to guarantee that a policy which maximises this score is indeed a policy which, when used to control the real system, leads to high cumulated rewards. If the initial states from which the policy will have to drive the real system are known, a suitable choice for the $score(\cdot)$ function could be for example the average return of the policy over these initial states. These returns can be evaluated through Monte-Carlo simulations, using the generative model.

Batch-mode RL Algorithm. Most efficient batch-mode RL algorithms rely on value function or policy approximation architectures. A necessary condition for the OSS algorithm to work well is that there must

[1] We refer to it as "meta" because it considers a generic batch-mode RL algorithm among its inputs.

[2] For the sake of simplicity, in the remainder of the paper, we will make a slight notation abuse and will refer to θ indifferently as the set $\{(x,u)\}$ or as the vector of variables describing the elements of this set.

exist a sampling scheme leading to high-performance policies, which implies that these architectures need to be able to represent accurately (at least) the optimal policy. In general, this necessary condition is more likely to be verified if the RL algorithm relies on a rich, versatile approximation architecture. Note also that from one RL algorithm / approximation method to the other, the optimal sampling scheme θ^* might vary.

Choosing N. Picking N is a compromise between policy quality and computation time. Larger N increase the chance to find good policies, since the domain dynamics are captured more finely, but also result in increased computation burden. As Section 4 will illustrate, the main source of complexity of finding an optimal θ comes from the dependency of *policy_inference*$(\cdot)$'s complexity on N. Hence, looking for very small sample sets seems desirable. On the other hand, below a certain threshold on N, the search space $(X \times U)^N$ might not contain any element able to generate a policy leading to an optimal score. When N increases, there may exist more and more elements in this search space that lead to policies having near-optimal scores, and hence, finding such elements in the resolution of problem 1 can be easier. Therefore, the choice of N needs to balance the need for fine domains representation with the processing abilities of *policy_inference*$(\cdot)$. In very large domains, the former constraint will prevail.

Optimization Algorithm. Computing or evaluating the gradient $\frac{\partial M}{\partial \theta}$, or any subgradient of $M(\cdot)$ may reveal itself very difficult in the general case. In some very specific cases of RL algorithms, approximation architectures, and criteria used for M, an analytic formulation might be found, but we concentrate on the general case where such a gradient is not available. As a matter of consequence, we need to carefully choose the optimization method we will use in order to find θ^*. Since we cannot use any derivative of the M function, our resolution method needs to be of "order zero". These methods correspond to *gradient-free* optimization methods (such as EDA optimization, simulated annealing or genetic algorithms). However, such methods require numerous computations of $M(\cdot)$, each of them being costly in terms of calculation resources because each implies performing all the steps of the RL algorithm for which the problem is defined. While the reduced number of variables in θ helps leveraging this computational burden, experience dictates it cannot make it negligible. So this second constraint of M's evaluation cost must be carefully taken into account when choosing the optimization method.

4 OSS(N), TREE-BASED FQI AND CROSS-ENTROPY SEARCH

In this section, we define an instance of OSS(N) by using tree-based FQI as *policy_inference*$(\cdot)$, Monte-Carlo simulation as *score*$(\cdot)$, and Cross-Entropy search as the optimization technique.

A simple and efficient way of searching for a function's maximum — when computing its gradient is not possible — consists in transforming this deterministic problem into a so-called *associated stochastic problem*[3] (Kroese et al., 2006). Cross-Entropy (CE) search (Rubinstein and Kroese, 2004) is one of the methods that proved successful in this framework. The key idea of CE search, applied to our RL setting, is to let a distribution on $(X \times U)^N$ converge towards the best sample set, with respect to $M(\theta)$. Algorithm 2 presents, in a nutshell, the CE optimization-based OSS method applied to the computation of an optimal policy with the tree-based FQI[4] algorithm.

Algorithm 2: OSS(N) with FQI and CE search.

Input: *policy_inference*(D) = tree-based FQI$_{p_{FQI}}$, ;
score(μ) = Monte-Carlo evaluation of μ on a ; set of representative initial states,;
sample(θ) = the generative model.;
CE param.: initial distrib. d on $(X \times U)^N$, N_{TS}, ρ_{CE}. ;
repeat
  $T = \emptyset$;
  for $i = 1$ *to* N_{TS} **do**
    θ_i = draw a sampling scheme according to d ;
    $T \leftarrow T \cup \{\theta_i\}$;
  foreach *sampling scheme* $\theta_i \in T$ **do**
    $D = sample(\theta_i)$;
    $\mu_i^* = policy\_inference(D)$;
    $M(\theta_i) = score(\mu_i^*)$;
  S = sort $\{(\theta, M(\theta))\}$ according to $M(\theta)$. ;
  $M_{CE} = (1-\rho_{CE})$-quantile of S. ;
  S' = elements of T having scores above M_{CE}. ;
  $d \leftarrow$ maximum likelihood distribution over S'.
until *no more improvement in* M_{CE};
θ^* = draw a sampling scheme according to d ;
return *policy_inference*$(sample(\theta^*))$

[3]The deterministic optimization problem is transformed into a rare event estimation problem, which is then tackled using an adaptive density estimation algorithm.

[4]For the sake of simplicity, we do not recall the details on the tree-based FQI method and refer the interested reader to (Ernst et al., 2005) for that purpose. The few parameters this algorithm requires (number of iterations and tree-related parameters) are generically denoted p_{FQI} hereafter.

The algorithm starts with an initial distribution d over the $(X \times U)^N$ search space. A family T of N_{TS} small sample sets is drawn from d, and for each sample set, the optimal policy is computed and evaluated. This provides a set S of $(\theta, M(\theta))$ pairs, ordered by increasing value of $M(\theta)$. Then, according to the importance sampling method of CE-optimization, the ρ_{CE} best θ values are selected out of the initial S set; this provides the S' set and d is updated to fit the distribution of the sample vectors in S'.

In the particular case of continuous states and discrete actions, we chose to represent d as a product of Gaussian densities on the continuous X space (of dimension d_X), and Bernoulli distributions on the discrete U space (of size d_U). More specifically, d uses a Gaussian model for each of the Nd_X continuous variables of θ and a categorical distribution for each of the Nd_U actions (which boils down to a Bernoulli distribution when there are only two actions). We made the hypothesis that all continuous variables in θ were independent, hence the covariance matrix of the global Gaussian distribution on X^N is diagonal. Although this hypothesis can seem too naive, it still provided good results as Section 5 will illustrate.

The main advantage of such a simple distribution model over $(X \times U)^N$ is the simplicity of its update phase. According to the importance sampling foundations of CE optimization, each Gaussian and Bernoulli model in d is updated to fit the maximum likelihood distribution of its corresponding variable in S'. Updating the Gaussian distributions on the continuous variables of θ corresponds to finding the average and the standard deviation for the associated variable in S'. Similarly, updating the distributions over the discrete variables (the actions) corresponds to computing the new thresholds of the Bernoulli distributions, by counting the occurrences of each action in S'.

Similarly, N_{TS} (and ρ_{CE}) should be chosen by keeping in mind that $\rho_{CE} \cdot N_{TS}$ elements of S will be kept in order to update the distribution d. Hence, these $\rho_{CE} \cdot N_{TS}$ should be informative enough to approximate a sufficient statistics for the new value of d.

For domains where some previous information (about reachability for instance) is available, the initial value of d can be designed to incorporate such domain-specific, prior knowledge. Namely, in large domains, random or ε-greedy initial walks can help initialize d to non-zero values only in reachable regions of the $X \times U$ space.

The complexity of an iteration of the above OSS(N) instance can be analyzed as follows. The sampling phase is $O(NN_{TS})$ and, since we train N_{TS} policies on sets of N samples with tree-based FQI[5], the policy training part is $O(N_{TS}N\log(N))$. Finally, the density update phase is $O(N_{TS}N)$. So the overall time complexity of this OSS(N) algorithm is $O(N_{TS}N\log(N))$.

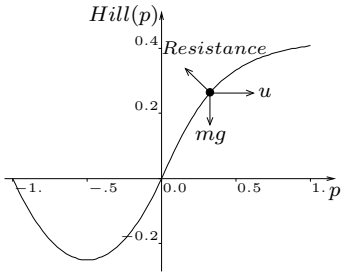


Figure 3: Car on the hill.

5 EXPERIMENTS

5.1 Experimental Protocol

The "Car on the Hill" Domain. In order to illustrate how the previous section's OSS(N) method performs in practice, and to visualize graphically the sample set's evolution in a two-dimensional state space, we report optimization results on the "car on the hill" domain. In this domain, an under-powered car tries to reach the top of a hill, in order to escape from a valley as illustrated on Figure 3. A positive reward is gained when the car exits from the right hand side of the domain. If the car goes too fast or exits from the left-hand side, it receives a negative feedback. Otherwise, zero rewards are obtained.

The action space is composed of the two "$\pm$4N" forces: $U = \{-4, 4\}$. The discrete-time dynamics are obtained from the integration of the car's law of motion, over time intervals of $0.1s$. We chose to use a γ factor of 0.95 as in (Ernst et al., 2005). With p the horizontal position of the car, $H(p)$ the hill's equation, and g the gravitational constant, the continuous time dynamics of the system are:

$$H(p) = \begin{cases} p^2 + p & \text{if } p < 0 \\ \frac{p}{\sqrt{1+5p^2}} & \text{if } p \geq 0 \end{cases}$$

$$\ddot{p} = \frac{u - gH'(p) - \dot{p}^2 H'(p)H''(p)}{1 + H'(p)^2}$$

The state space of the system is spanned by the two variables $(p, \dot{p})$ and is bounded: $X = [-1;1] \times [-3;3] \cup \{x_\infty\}$. The additional state x_∞ is an abstract

[5] Which has time complexity of $O(N\log(N))$.

absorbing state, entered only when the car's dynamics let it escape the domain's bounds (either in speed or position). The only non-zero rewards received in this domain are for the transition to x_∞:

$$r(x_t,u_t) = \begin{cases} 1 & \text{if } p_{t+1} > 1 \text{ and } |\dot{p}_{t+1}| \leq 3 \\ -1 & \text{if } p_{t+1} < -1 \text{ or } |\dot{p}_{t+1}| > 3 \\ 0 & \text{otherwise} \end{cases}$$

Initializing d. We initialized the distribution d by using a regular paving with N Gaussian elements in the state space and by drawing all actions at random (Bernoulli distribution with a 0.5 threshold), as illustrated in Figure 5(a), in order to promote sample diversity. Note however that many other choices for the initial d were possible, even the blind initialization of all Gaussian distributions to the same value.

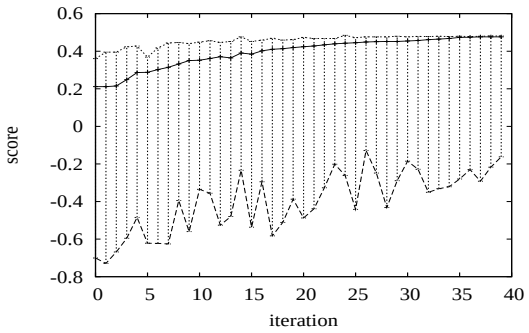
Choosing N, N_{TS} and ρ_{CE}. Recall that the first purpose of OSS is to use batch-mode RL algorithms in order to tackle large state-action spaces. We illustrate its properties on small domains, in order to show one can obtain optimal policies with small sample sets, but the real use of OSS(N) for RL practitioners lies in the case where the state-action space is too large to be uniformly partitioned and where N is strongly constrained by the available computational resources. In order to illustrate the ability of OSS to find efficient policies with few samples, we report experimental results with $N = 20$. Note that similar results were obtained with even lower values of N. We chose a value of 500 for N_{TS} with a ρ_{CE} of 0.1.

Parameters of Tree-based FQI. Tree-based FQI presents the advantage of requiring only few parameters to tune. In our case, each Q-function is represented with a mixture of 200 fully-developed extremely randomized trees and 30 iterations of FQI are performed to obtain an estimate of the Q^* function.

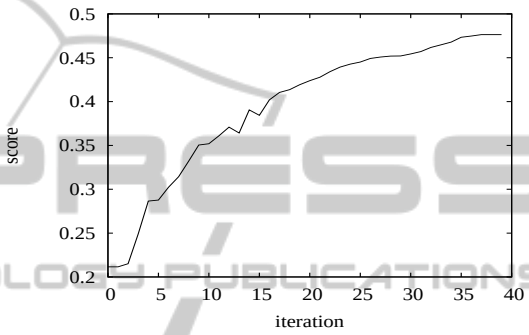
Scoring Function. We chose to evaluate a policy's quality by using a set of initial states corresponding to different initial values of p and to a null initial velocity. The policy's score is the average of the initial states' values, estimated by performing rollouts. These initial states are seven regularly dispatched positions on the hill, with zero velocity (the small bullets on the horizontal axis of Figures 5(a) to 5(i)).

5.2 Results

Figure 4 reports the evolution of the policy scores throughout the algorithm's iterations. The lowest curve represents the evolution of the worse sample



(a) M_{min}, M_{CE} and M_{max}.



(b) M_{CE}.

Figure 4: Evolution of the scores throughout the iterations.

set's (among the set T) value M_{min}. The middle one is the evolution of M_{CE} and the top one corresponds to the value M_{max} of the best sample set of T. The most significant result of this figure is the steady evolution of the $(1-\rho_{CE})$-quantile M_{CE} since both M_{min} and M_{max} can be due to lucky outliers. As expected, all three scores increase with the number of iterations, with a larger variance for M_{max} and M_{min}. One can note the steady increase of M_{CE} towards the optimal value for this domain (0.49).

An interesting property can be noted if one allows for a slight modification of Algorithm 2. If, instead of returning $policy\_inference(sample(\theta))$ in the end, one stores offline the best policy obtained at each iteration, then, because M_{max}'s high variance allows it to reach some optimal values very early in the iterations, a close-to-optimal policy can be found much before M_{CE} converges to the optimal score. This adds very little overhead to the algorithm since it only requires one disk writing operation per iteration and can be beneficial in an *anytime* setting: the best policy is stored on disk and always available for retrieval if needed, and the probability of finding even better policies increases with the iterations (until asymptotic convergence of M_{CE}).

Figure 5 reports the graphical evolution of the Gaussian densities of d, describing where the crucial

samples concentrate in the state space. The triangles in these figures represent the samples the distributions are computed from. Hence, in a single figure, there are $\rho_{CE} \cdot N_{TS} \cdot N = 0.1 \cdot 500 \cdot 20 = 1000$ samples. A triangle oriented to the left (resp. right) stands for a -4 (resp. $+4$) action. Since we chose the naive model of uncorrelated variables, all the ellipses represented have their principal directions along the state space's axes. A richer covariance model might allow for a better sample set description at the cost of a more complex distribution parameter update phase.

The main conclusion one can draw from these results is that, by comparing the influence of different sample sets on the optimal policy computed by FQI, and by using a probability density-based optimization method, we were able to identify a distribution on the sampling scheme (Figure 5(i)) which induces very good policies with as little as 20 samples. In contrast, the original paper on tree-based FQI (Ernst et al., 2005) suggests that, in average, it is necessary to collect tens of thousands of samples via random walk in the state space, before an optimal policy can be found. The generalization of this experimental result indicates that instead of an ever-refining process for the sample set, batch-mode RL algorithms can take advantage of sample set optimization, through OSS(N) algorithms, in order to reach optimal policies with a low number of samples.

6 DISCUSSION

6.1 Time and Space Efficiency

When the state-action space's dimension becomes large, processing times for batch-mode RL algorithms increase dramatically, since the sample complexity of these algorithms is often worse than linear (*e.g.*, $O(Nlog(N))$ for tree-based FQI). At a certain point, it might become preferable to run N_{TS} sample collections and policy optimizations for small policies based on sample sets of size N, than one large computation on the very large equivalent sample set of size $N_{TS} \cdot N$ (if this computation is at all possible). More formally, this is supported by the complexity estimate of Section 4, which illustrates an $O(N_{TS}N\log(N))$ time per OSS iteration which can be advantageously compared to the $O(N_{TS}N\log(N_{TS}N))$ time complexity of applying tree-based FQI to the huge set of $N_{TS}N$ samples (recall N_{TS} is the large value here, N being fixed to a small value by the user).

On the space complexity side, both approaches require $O(N_{TS}N)$ space to store the trees and the sample sets. However, OSS can benefit easily from possible disk storage since all the sample sets are used independently and at different times. If one allows disk storage, then the space complexity of OSS boils down to $O(N)$ since an iteration of OSS(N) only requires keeping and processing one set of size N at once.

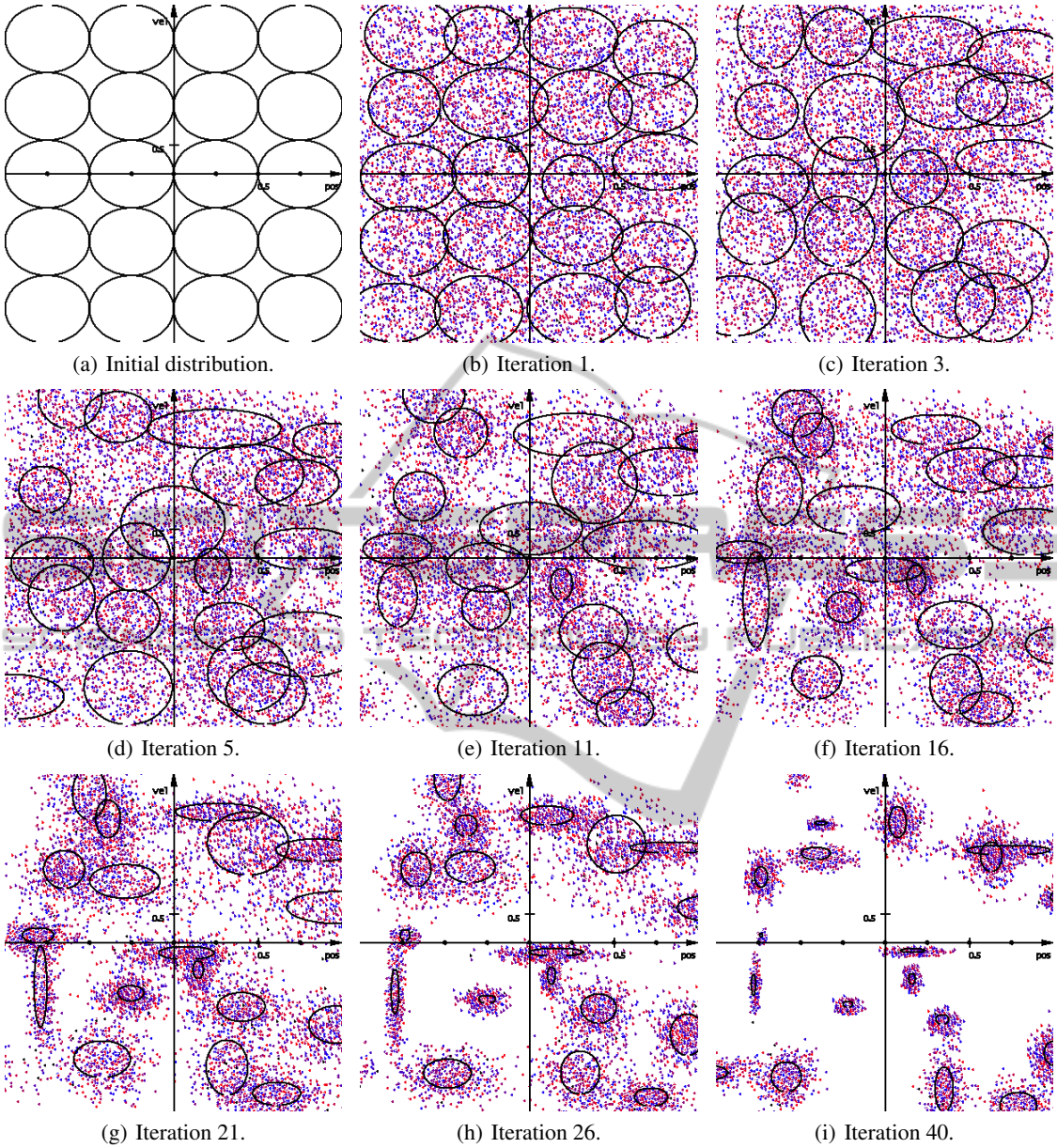
Furthermore, it is interesting to point out that computing the score of a given θ is fully independent of any other score computation. Hence OSS methods can be easily adapted to a setting of distributed computation on several small computers and can thus take advantage of parallel architectures, distributing the computational burden into small light-weight tasks.

6.2 Stochastic RL Algorithms

One of the possible *caveat* of using a forest of extremely randomized trees for the regressor in FQI is related to the possible variance in the results and the associated variance in policy quality. So far, all RL algorithms are implicitly supposed to be deterministic, *ie.* given a fixed sample set as input, they always output the same result. This is not true for extremely randomized trees. Their use in the general case of FQI is still relevant because the variance in the results tends to zero when the number of samples grows. But in our case, since we voluntarily kept the samples number very low, we witnessed a very large variance in the policies generated from a given set of 20 samples. To avoid such a variance, a simple option is to increase the number of trees in the forest, since the variance also tends to zero with a large number of trees. Although the 200 trees used per Q-function in the previous experiment were already a large forest compared to the one reported in (Ernst et al., 2005) (which only had 50 trees), we tried to run the OSS meta-algorithm on FQI with even larger numbers of trees (up to 1000) and observed the same behaviour as reported in Section 5.2. Obviously, when using a non-deterministic algorithm such as tree-based FQI, one cannot guarantee anymore that OSS will converge to a sample set providing the optimal policy every time, but instead, it will lead to a training set θ^* that provides the optimal policy *with high probability*. For the case where the variance in the results tends to zero (with a very large number of trees or with a deterministic algorithm such as LSPI), then this probability should tend to one.

It is also interesting to note that variance in the algorithm's output policies might actually be desirable, since it extends the set of policies which are "reachable" from an N-sized sample set. Then, by allowing the storage of the best found policies along the way, good policies can be found early in the search process (as Figure 4 illustrates).

These experiments highlighted an interesting (un-



(a) Initial distribution. (b) Iteration 1. (c) Iteration 3.

(d) Iteration 5. (e) Iteration 11. (f) Iteration 16.

(g) Iteration 21. (h) Iteration 26. (i) Iteration 40.

Figure 5: Evolution of the distribution density with the iterations.

expected) property of variance reduction for OSS(20). During the first iterations, if several policies are trained from a given sample set, we observe a large variance in the output[6]. However, as the iteration number grows and the distribution d concentrates on crucial samples, we observe both an increase in the expected value of $M(\theta)$ and a strong reduction in the output policy's variance: at iteration 40, when one trains several policies using a single sample set drawn from d, those policies both perform much better and are much closer to each other than the ones of iteration 1 were.

[6]The statistical relevance of the S' set is still insured because the large number N_{TS} of sample sets averages out this variance for the update of d.

6.3 Dealing with Stochastic Problems

Algorithm 2 can be applied to stochastic problems without any change. However, the results need to be interpreted slightly differently. In stochastic domains, the equivalence between (x,u) and (x,u,r,x') does not hold anymore and, thus, one needs to emphasize the difference between the sets θ and D. As stated in Sec-

tion 3, θ defines a *sample collection scheme*. Then, finding the optimal θ consists in finding the sample collection scheme that will lead to the best *expected* policy, with respect to the transition model's distributions.

Indeed, in Section 3, we did not focus explicitly on the sample collection phase since a single θ always induced the same D set in the deterministic setting. But, in the stochastic case, one cannot make use of such a shortcut and one should note that we do not compute μ^*_θ anymore, but an optimal policy $\hat{\mu}^*_\theta$ for one possible training set D, drawn according to θ, among many others. This clarification raises the question of sampling several D from θ to assess the true value of $M(\theta)$. But, as for the variance reduction property of the previous section, we argue one does not need to do so and, instead, can rely on the large number of θ values drawn from d to average out the different possible D sets. This question remains open nevertheless and should be addressed in more detail in future research.

6.4 Related Work

In order to collect relevant sample sets for batch-mode RL algorithms, the naive approach of uniform grid sampling across the state-action space does not scale to high-dimensional domains since the RL algorithms become very slow (if able at all) at processing this exponentially increasing amount of data. We mentioned earlier the domain-specific approaches of (Neumann and Peters, 2009; Riedmiller, 2005; Ernst et al., 2006; Kalyanakrishnan and Stone, 2007). In the latter, the authors alternate a policy computation and a sample gathering phase, where the sample gathering is a carefully tuned ε-greedy exploration, with respect to the last computed policy, regularly reset to the start state. All the discovered samples are then added to the sample set and the optimal policy is recomputed. Such data collection schemes rely on Monte-Carlo exploration methods and present similarities with online-RL approaches, which provide reachability guarantees while incrementally extending the sample set. In general, these methods suffer from two defaults, which come in contrast with the OSS approach:

- They often require a lot of domain specific hand-tuning to be efficient.
- They keep on enriching the sample set, letting it grow up to a point where its size becomes again problematic for the batch-mode RL method.

The work of (Ernst, 2005) presents a method to select concise sets of samples for the same tree-based FQI algorithm than the present work. But their goal and approach was very different: instead of searching for the best possible fixed-size set of samples, they started with a very large constrained sample set and tried to extract a subset that would still provide policies with good performances, without requiring any extra sampling from a generative model. They based their approach on a Bellman error criterion and illustrated a pathological case where the subset found critically concentrates samples around Q-function discontinuities. It is also interesting to note that the reported original motivation of their paper confirms ours: their goal being to "lighten the computational burden of running the fitted Q-iteration algorithm on the whole set of four-tuples".

Finally, Cross Entropy methods, such as the one used in our experiment, have been quite widely used in recent years in the RL literature, for instance for the task of refining policies for Tetris (Szita and Lörincz, 2006), or for adapting feature functions for linear architectures (Menache et al., 2005), or to optimize fuzzy state space partitions for fuzzy Q-iteration (Buşoniu et al., 2008). An interesting parallel can be made between the latter approach and the present one: they define fuzzy partitions for the value function, implicitly identifying specific areas in the $X \times U$ space, similar to the areas of interest defined for samples by our density-based optimization method. Although CE search is not an imperative choice for OSS (other optimization methods are available), it seems to be well suited to handle the large dimensional, gradient-less optimization problems that arise in RL.

7 CONCLUSIONS

We introduced the *Optimal Sample Selection* meta-algorithm, in order to generate optimal policies for large sequential control problems. This approach consists in looking directly for a set of training examples that — given a batch-mode RL algorithm — will induce an optimal policy for the domain at hand. More specifically, an OSS(N) algorithm takes as input a generative model, a batch-mode RL algorithm, an evaluation procedure, then defines the search for an optimal set of N training examples as an optimization problem, and finally solves it using a stochastic optimization method. The instance of OSS we tested uses tree-based fitted Q-iteration as the batch-mode RL algorithm, evaluates a policy by generating trajectories to compute its average return over a set of initial states and optimizes the sample set by using Cross Entropy search. We studied this instance's properties under various simulation conditions. One remarkable property of OSS(N) is that a very small set of 20 carefully chosen samples was sufficient to generate a near-

optimal policy.

Based on these results and on other experiments not reported in this paper, we conjecture that for many Optimal Control problems, there exist sample sets of "acceptable size" which can lead to near-optimal policies when used as input of batch-mode RL algorithms and that finding these sets is computationally feasible. This leads us to believe that this OSS meta-algorithm may perform well, where other sampling/discretization-based resolution schemes in Optimal Control fail, due to limitations in the size of the sample sets that can be manipulated in a reasonable time by a computer.

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