Approximate Dynamic Programming with Neural Networks in Linear Discrete Action Spaces

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Abstract

Real-world problems of operations research are typically high-dimensional and combinatorial. Linear programs are generally used to formulate and efficiently solve these large decision problems. However, in multi-period decision problems, we must often compute expected downstream values corresponding to current decisions. When applying stochastic methods to approximate these values, linear programs become restrictive for designing value function approximations (VFAs). In particular, the manual design of a polynomial VFA is challenging. This paper presents an integrated approach for complex optimization problems, focusing on applications in the domain of operations research. It develops a hybrid solution method that combines linear programming and neural networks as part of approximate dynamic programming. Our proposed solution method embeds neural network VFAs into linear decision problems, combining the nonlinear expressive power of neural networks with the efficiency of solving linear programs. As a proof of concept, we perform numerical experiments on a transportation problem. The neural network VFAs consistently outperform polynomial VFAs, with limited design and tuning effort.

1 Introduction

Problems in operations research (OR) are generally concerned with allocating resources, aiming to maximize some reward function. Applications of OR are found in domains such as transportation, energy, and manufacturing. Although many effective solutions – particularly linear programs (LPs) – exist for static problems, solving dynamic problems over a time horizon remains challenging, as we need downstream values corresponding to current decisions. Estimating these values is often difficult within linear programming settings.

We address the integration of neural networks and linear programs in the context of Approximate Dynamic Programming (ADP). Spurred by increasing availability of both data and computing power, neural networks are successfully applied in many fields. Their potential applications have also been identified for ADP, yet their use is not widespread. This paper extends an effort in this direction, explicitly considering implementation for problems with large action spaces.

A key challenge of ADP is to reliably estimate the downstream value corresponding to actions, enabling to learn a policy that maximizes value over the full planning horizon. One research stream within ADP focuses on value function approximations (VFAs) to estimate downstream values. In this approach, we design a set of features (explanatory variables) and organize them as a polynomial function that represents the value of being in a given state and perform linear regression to learn weights associated to the features. Although polynomial VFAs often yield satisfactory results, designing the features is challenging. Particularly higher-level interactions are difficult to grasp for human designers.

The problem of features design is amplified by the large action spaces that are encountered in typical ADP settings. It is common for the action space growing too large to enumerate within reasonable time. Formulating the decision problem as a mathematical program – preferably a linear program for efficient solving – preserves optimality and often vastly enhances the magnitude of problems that can be handled. Even if the action space is not overly large, there may be reasons to use mathematical programming, such as higher speed or the availability of existing model formulations. However, mathematical programming poses additional challenges for VFAs. Assuming a linear program, the variables representing the features in the objective function must be linear as well. Although nonlinear features might be designed, they must be expressed as linear systems, often requiring complicated constructions of artificial variables. Complex polynomial VFAs are therefore difficult to embed in LPs.

The integration of neural networks within LPs for decision making addresses this challenge. Neural networks are able to learn complex nonlinear functions; theoretically, a single-layer network may learn any continuous function [Cybenko, 1989]. Because neural networks are not restricted by linearity, they may identify nonlinear structures between lower-level features, without explicitly defining these as features within the LP. The activation functions should be transformable into piecewise linear functions. Fortunately, most modern neural networks satisfy this condition.

In this paper, we design a hybrid approach to address ADP problems based on neural networks and LPs. The planning problem tested is a dynamic transport problem inspired by...
practice. To preserve focus on the methodological aspect of the paper, we will not discuss design choices in detail. The problem serves as a test case that is sufficiently rich and challenging to adequately test the solution method.

This paper contributes to the state of the art in the following ways. First, we design a hybrid approach for integrating neural networks and LPs to tackle ADP problems. Second, we provide insights into the performance of various neural network structures based on numerical experiments, specifically the quality and computational effort. Third, we show that neural network VFAs significantly improve upon current practice, which is based on polynomial VFAs.

2 Related work

Given the successful applications of neural networks in regression, their application on ADP problems seems natural. The idea is not novel; the seminal work of [Bertsekas and Tsitsiklis, 1995] already presents the use of feature vectors as input to neural networks as an established concept. Also [Powell, 2011] describe neural networks as a powerful tool for ADP algorithms. However, neural network VFAs have not yet been well-tested for large action spaces – where the neural network cannot be used to enumerate the downstream value for every action – we are not aware of previous studies addressing the integration of neural networks into decision-making LPs for this type of problems. We highlight some relevant works in ADP and reinforcement learning, discussing the most closely related applications of neural networks and linear programming.

We start with neural networks in ADP. [Bertsekas, 2008] discusses applying neural networks in ADP, coining the term neuro-dynamic programming. He broadly defines neural networks as essentially nonlinear VFAs, using either the full state or a smaller feature vector as input. Alternatively, neural networks may also be used as a pre-processing step to extract feature vectors from the state. According to [Powell, 2011], neural network VFAs have mainly been applied on classical engineering problems that typically have low-dimensional action spaces. [Schmidhuber, 2015] provides an survey of deep learning studies, including the use of neural networks in reinforcement learning. The neural networks are generally used to learn values associated to state-action pairs, i.e., as VFAs. No mention is made of embedding such VFAs in linear programs. [Van Heeswijk and La Poutré, 2018] study shallow neural network VFAs in a transportation context, but require full enumeration of the action space.

We proceed to discuss linear programming in ADP. [De Farias and Van Roy, 2003] study the linear programming approach for ADP, assuming linearly defined VFAs. [Powell, 2016] states that decision problems with tens of thousands dimensions can generally be solved with modern commercial solvers. However, when instances become too vast, also linear programming may require unsatisfactory computational times. [Dulac-Arnold et al., 2012] and [Pazis and Parr, 2011] propose factorization methods to divide the action space into linear subproblems, exponentially reducing the computational effort. The size of the state space is a limiting influence in their solution. In the transportation domain, [Pérez Rivera and Mes, 2017] and [Van Heeswijk et al., 2019] provide recent examples of polynomial VFAs integrated in linear programs.

3 Solution method

We briefly introduce the notation for Markov decision problems (MDPs) as used in this paper. MDP models are useful to mathematically model decision problems with stochastic and dynamic properties. In OR, many are combinatorial optimization problems. An MDP is a stochastic control process for which the objective is to maximize rewards (or minimize costs) over a discrete time horizon \( T \), with decision epochs \( t \in T \) separated by equidistant time intervals. A discounted MDP can be described by \((S, \mathcal{X}(S)), \mathbb{P}(S' | S, x), R(S, x, \rho)\), with \( S \) being the set of problem states, \( \mathcal{X}(S) \) being the set of feasible actions when in state \( S \in S \), \( \mathbb{P}(S' | S, x) \) being the transition probability of transitioning from state \( S \) to \( S' \in S' \subseteq S \) after taking action \( x \in \mathcal{X}(S) \), \( R(S, x) \) being the direct reward when taking action \( x \) in state \( S \), and \( \rho \in [0,1) \) is the discount rate applied to future rewards. The Bellman equation yields the maximum value corresponding to each state:

\[
V(S) = \max_{x \in \mathcal{X}(S)} \left( R(S, x) + \rho \sum_{S' \in S'} \mathbb{P}(S' | S, x) V(S') \right).
\]

Solving the Bellman equation for all states yields the optimal policy. Several techniques exist to accomplish this, yet for many realistic problems these are computationally intractable. The next section addresses this issue.

3.1 Approximate Dynamic Programming

Approximate Dynamic Programming (ADP) is a framework to learn policies for MDPs that are too large to solve exactly within reasonable time. This section provides a short and high-level overview. We refer to [Powell, 2011] for an extensive discussion on the topic. At its core, ADP uses Monte Carlo simulation to sample rewards and estimate the downstream values of state-action pairs, enabling to learn good policies without exhaustively exploring the MDP.

From a computational perspective, problems may arise in three areas of MDPs, namely the sizes of the state space (number of states), action space (number of actions per state) and outcome space (number of possible outcomes per action). Multiple solution approaches exist for each of these areas; we restrict ourselves to the ones used in this paper.

We start with the outcome space \( S' \subseteq S \). To identify the best action in any state, the Bellman equation requires computing \( V(S') \) for each \( S' \in S' \) where \( S' \) might be unique for each state-action pair. ADP circumvents this procedure by instead attaching a single value to a state-action pair. Thus, we replace the stochastic expression \( \sum_{S' \in S'} \mathbb{P}(S' | S, x) V(S') \) with a deterministic value function \( V(S, x) \). For each state-action pair, we only need to evaluate one downstream value rather than \( |S'| \) outcomes. This downstream value is estimated by repeated Monte Carlo sampling, i.e., we randomly draw outcome states \( S' \) and observe their values.
Next, we discuss the state space $\mathcal{S}$. In many optimization problems the state is a high-dimensional vector with numerous possible realizations. Computing the value for each individual state may therefore be intractable. Therefore, we replace the true value function with a value function approximation (VFA) $\bar{V}(S, x)$. The VFA is a function that returns an expected value given a set of features (explanatory variables) that capture the essential information in state-action pairs needed to estimate their value. The VFA design is further discussed in Section 3.2.

Finally, we address the action space $\mathcal{X}$. In combinatorial problems, this space quickly grows beyond the limits of enumeration. As we need thousands of observations to learn a good policy, each decision problem should typically be solvable within a few seconds. To avoid enumerating the full action space, the decision problem may be expressed as a mathematical program. In particular LPs are well-studied; modern solvers often solve such problems highly efficiently. Mathematical programs can be solved to optimality, while significantly upsizing the action space sizes that can be handled.

The outline of the ADP algorithm is now presented. We use $N$ iterations to learn the VFA; each iteration represents a discrete time step. At every iteration $n$, the action maximizes expected value given the prevailing VFA $\bar{V}_{n-1}()$, resulting in the following observed value:

$$\hat{v}_n = \max_{x_n \in \mathcal{X}(S_n)} \left( R(S_n, x_n) + \rho \bar{V}_{n-1}(S_n, x_n) \right).$$

The difference between expected value for the preceding state-action pair at $n - 1$ (i.e., $\bar{V}_{n-1}(S_{n-1}, x_{n-1})$) and the observation at $n$ (i.e., $\hat{v}_n$) updates the VFA, using an updating function $\check{V}_n() \leftarrow U(\bar{V}_{n-1}(), S_{n-1}, x_{n-1}, \hat{v}_n)$. Algorithm 1 shows the outline of the ADP algorithm to learn the VFA.

Algorithm 1 Basic ADP algorithm to learn the VFA.

1: initialize $V_0()$
2: $n \leftarrow 1$
3: $S_1 \leftarrow \mathcal{S}$
4: while $n \leq N$ do
5:     $x_n \leftarrow \arg \max_{x_n \in \mathcal{X}(S_n)} \left( R(S_n, x_n) + \rho \bar{V}_{n-1}(S_n, x_n) \right)$
6:     $\hat{v}_n \leftarrow R(S_n, x_n) + \rho \bar{V}_{n-1}(S_n, x_n)$
7:     $\check{V}_n() \leftarrow U(\bar{V}_{n-1}(), S_{n-1}, x_{n-1}, \hat{v}_n)$
8:     $S_n \leftarrow S^\prime$
9:     $S_{n+1} \leftarrow S^\prime$
10: $n \leftarrow n + 1$
11: end while
12: return $\check{V}_N()$

3.2 Polynomial VFA (PL-VFA)

This section addresses the VFA in more detail. As mentioned earlier, we operate on features that are extracted from state-action pairs. Let $\mathcal{F}$ be the set of indicators describing the features, with each indicator $f \in \mathcal{F}$ referring to some representative feature of a state-action pair. We define a contractive mapping $\phi$ that extracts features for any given state-action pair, i.e., $\phi : (S, x) \rightarrow \mathbb{R}^{|\mathcal{F}|}$, the corresponding vector of features is $[\phi_f]_{f \in \mathcal{F}}$. Formally, the VFA is described by $(\bar{V} \circ \phi) : \mathcal{S} \times \mathcal{X} \rightarrow \mathbb{R}$.

VFAs are commonly designed in polynomial form (PL-VFA). Let $w_f \in \mathbb{R}$ be a weight associated to feature $\phi_f \in \mathbb{R}$. Then, the polynomial VFA may be described by $\bar{V}(S, x) = \sum_{f \in \mathcal{F}} w_f \phi_f(S, x)$. PL-VFAs are popular for several reasons. Polynomials are able to approximate most functions, an appropriate polynomial in theory approaches the true value function arbitrarily close. Furthermore, although the features may be nonlinear, the expression itself is linear. It can therefore be incorporated into linear programming formulations. Techniques such as temporal-difference learning may be used to update the weights [Sutton and Barto, 2018].

Although polynomials might theoretically approximate the true value function, randomly defining a polynomial will likely not perform well [Powell, 2016]. A properly designed PL-VFA is aligned with the structure of the value function. This manual design of VFAs is a key challenge for successful implementations, requiring careful modeling and testing of individual value functions. This is where the linear formulation becomes restrictive, as features representing higher-order effects must be explicitly modeled. Additional problems arise when we resort to linear programming to handle large action spaces. It then becomes challenging to express non-linear features in linear form. Such conversions often require complicated structures involving many artificial variables.

To overcome the limitations of polynomial VFAs, the VFA may be expressed by neural networks. The nonlinear architecture of such networks allows to unravel complex structures, even when inputs are linear operands of state-action pairs. We further discuss neural network VFAs in the next section.

3.3 Neural network VFA (NN-VFA)

A general introduction to neural networks is provided by [Gurney, 2014], we only address the VFA design. In neural network VFAs (NN-VFAs), the feature vector $[\phi_f]_{f \in \mathcal{F}}$ is transformed by a weighted set of nonlinear activation functions (neurons), resulting into a single output value $\bar{V}(S, x)$. Compared to the PL-VFA, the main advantage is that the NN-VFA may learn higher-order effects that are not explicitly defined in the feature vector. We emphasize that the input quality remains crucial for the NN-VFA performance, but feature design is comparatively easier than for PL-VFAs.

The NN-VFA is composed of an input layer (the feature vector), a least one hidden layer containing neurons, and an output layer with a single node that returns the expected value for the given state-action pair [Van Heeswijk and La Poutré, 2018]. In a fully connected network, every neuron in the network connects to all neurons in the preceding layer. Each neuron receives the inner product of all neurons in the preceding layer and their corresponding output weights as input and transforms it into a single neuron value.

The NN-VFA contains $K \geq 1$ hidden layers; we use $K \triangleq \{1, \ldots, K\}$ to denote the set of hidden layers. The indicator $k = 0$ refers to the input layer that contains the features; layer $K + 1$ is the output layer. Furthermore, the index $d_k \in \mathbb{N}$ refers to a specific neuron in layer $k \in K$, with $D_k$
3.4 Integrating the NN-VFA in LPs

Piecewise linear functions. Integration of the NN-VFA in contemporary neural networks can be modeled by simple programs. However, most common activation functions in neural networks are nonlinear. Therefore, they cannot be directly computed within linear programs. To circumvent this, we deliberately do not put excessive effort into design and fine-tuning; the main goal of the NN-VFA is to reduce the manual design effort compared to the PL-VFA.

The experiments compare a PL-VFA to two neural network VFAs: the NN(1,20)-VFA (1 layer, 20 neurons) and the NN(3,20)-VFA (3 layers, 20 neurons per layer). Although a single-layer network theoretically suffices to learn a function, deep neural networks may model the same function with significantly fewer neurons [Delalleau and Bengio, 2011]. In fact, for many common functions, the required number of neurons decreases exponentially with the number of layers [Lin et al., 2017; Rolnick and Tegmark, 2018] suggest that, for many functions encountered in practical settings, relatively small networks suffice to accurately describe functions. Downsides of deeper networks are the longer training time and potential loss of information [Huang et al., 2016].

The experimental design is as follows. First, we compare convergence properties of VFAs. Second, we perform experiments on various neural network configurations and learning rates, giving insight into the behavior and robustness of the NN-VFA under varying conditions. Third, we report the computational times corresponding to various VFA configurations. Fourth, we evaluate the performance (i.e., the direct rewards) of the tested VFAs. We discuss offline performances over time – fixing the policy after every 10,000 training iterations – which is valuable when computational budgets are limited. We perform N = 100,000 training iterations and 10,000 performance iterations per offline policy.

All procedures are coded in C++ and CPLEX 12.8 is used to solve the linear decision problems. The experiments were run on a 64-bit Linux machine with a 4x1.60GHz CPU and 8GB RAM.

4.1 Problem definition

This section outlines the transportation problem, which is based on the nomadic trucker problem [Powell et al., 2007]. It is characterized by a large discrete action space and a complex optimal policy. Let a strongly connected graph \( G = (V, E) \) represent a transport network. Vertex set \( V \) represents the potential origins and destinations of transport jobs. Edge set \( E \) specifies the undirected connections between vertices. Each edge has travel time 1. Edge lengths are \( L^2 \) distances between vertex pairs, used to compute travel costs. A capacitated agent roams the graph, traveling between directly connected vertices. At each decision epoch \( t \in T \), the agent decides (i) which jobs to load, (ii) which jobs to unload, (iii) which vertex to visit next (or to stay at the current vertex).

We sketch the corresponding MDP. The problem state \( S \) contains the information necessary for decision-making, namely the relevant properties of all transport jobs in the graph and the current location of the agent \( v(t) \in V \). Each job is defined by four properties, namely (i) the vertex \( v \in V \) at which the job is currently located, (ii) the destination vertex \( v^+ \in V \), (iii) the time remaining until the due date \( t^d \in T^+ \), and (iv) the assignment status \( a \in \{0, 1\} \) (\( a = 1 \) means the job is currently carried by the agent). Each unique combination of properties constitutes a job type \( [v, v^+, t^d, a] \); the number of jobs per type is denoted by \( I_{[v, v^+, t^d, a]} \). For the full system we define the vector \( I = \{I_{[v, v^+, t^d, a]}\}_{[v, v^+, t^d, a]} \). The
problem state is given by $S \triangleq [I, v^{loc}]$; the set containing all possible states is denoted by $S$.

We proceed to describe the action $x$. Let $V_{v^{loc}} \subseteq V$ be the set containing both $v^{loc}$ and the vertices adjacent to it. The variable $v^{next} \in V_{v^{loc}}$ describes the next destination of the agent. Furthermore, $\gamma = 0$ indicates that a job is unloaded and $\gamma = 1$ indicates that a job is loaded. The action is defined by $x(S) = [x_{v^{next}}, v^{next}, t^+, a, \gamma]$. The action space $\mathcal{X}(S)$ is bound to various constraints; due to space limitations the full LP model is omitted. The key constraints are that (i) the agent may only (un)load at its current location, (ii) jobs are always unloaded when at their destination vertex, (iii) the agent’s transport capacity may not be exceeded.

Next, we describe the reward function $R(S, x)$. The rewards consist of the following components: (i) a fixed reward for each successful delivery and (ii) a reward for bringing a job closer to its destination, proportional to the reduction in shortest path distance (an increase in distance yields a negative reward). We proceed to discuss the costs: (i) a fixed cost associated with each job that is (un)loaded, and (ii) a penalty for violating due dates. Jobs may be voluntarily unloaded when at their destination vertex, (iii) the agent’s transport capacity may not be exceeded.

For the experiments, we use an instance with $|V| = 5$, a maximum degree of 3, and up to 5 new jobs generated per vertex at each epoch, with accumulation possible up to 45 jobs. The agent may carry up to 20 jobs. The action space grows exponentially with the number of jobs, rendering enumeration infeasible even for this modest instance. An upper bound for the size of $|\mathcal{X}|$ is $\max(|\mathcal{X}|) = 2^{20} \cdot 2^{45} \cdot (3 + 1)$.

5 Numerical results

This section discusses the results of the experiments. Preliminary experiments on simplified problem settings with trivial policies indicate that all VFAs work correctly, converging to the true optimal value function, i.e., $\bar{V}(\cdot) \approx V(\cdot)$. Figure 1 shows a convergence example for the real problem instance. The PL-VFA converges fastest, but to considerably lower values than the NN-VFAs. Similarly, the NN(1,20)-VFA converges faster than the NN(3,20)-VFA, but to somewhat lower values.

The next experiment addresses learning rates, testing $\eta = \{0.001, 0.01, 0.1\}$. Figure 2 illustrates the convergence speeds per learning rate for the NN(1,20)-VFA; to aid the visual representation, we omit the other VFAs (which display comparable behavior). However, the NN(3,20)-VFA with $\eta = 0.1$ did not converge to a stable policy. In general, we find that deeper neural networks are less robust with respect to larger learning rates. Errors may be magnified when passing through multiple layers, returning extreme values. Furthermore, NN-VFAs with $\eta = 0.001$ do not converge within 100,000 iterations. We therefore use $\eta = 0.01$ onwards.

Next, we look at the effects of altering network configurations, varying the number of neurons per layer. The results are shown in Table 1. The results are fairly robust, with the exception of the NN(1,10)-VFA, which performs comparatively poorly. Balancing performance and speed, we use 20 neurons per layer for the remainder of the experiments.

We assess the computational time per iteration; roughly 99% of the computational budget is allocated to solving the LPs. On average, the polynomial VFA is solved in 0.02$s$ per iteration, the NN(1,20)-VFA takes 0.16$s$, and the NN(3,20)-VFA takes 0.39$s$. Due to the additional sets of variables and
Table 1: Policy performance $R(\cdot)$ for the NN(1,.-)-VFA and NN(3,.-)-VFA with various # neurons, normalized w.r.t. best VFAs.

| VFA            | # neurons per layer |
|----------------|---------------------|
|                | 10      | 15      | 20      | 25      | 30      |
| NN(1,.-)-VFA   | 0.66    | 0.91    | 1.00    | 0.92    | 0.98    |
| NN(3,.-)-VFA   | 0.92    | 0.99    | 0.99    | 0.98    | 1.00    |

Table 2: Computational time (in s) per iteration for various VFAs.

| VFA            | # neurons per layer |
|----------------|---------------------|
|                | 10      | 15      | 20      | 25      | 30      |
| PL-VFA         | 0.02    | -       | -       | -       | -       |
| NN(1,.-)-VFA   | 0.07    | 0.15    | 0.16    | 0.17    | 0.19    |
| NN(3,.-)-VFA   | 0.15    | 0.33    | 0.39    | 0.66    | 0.71    |

Table 3: Average policy performance $R(\cdot)$ after $N$ iterations, normalized w.r.t. PL-VFA.

| VFA            | Mean | St. dev. |
|----------------|------|----------|
| PL-VFA         | 1.00 | 1.25%    |
| NN(1,20)-VFA   | 1.10 | 1.65%    |
| NN(3,20)-VFA   | 1.19 | 0.72%    |

6 Conclusions

This paper introduces the integration of linear programs and value function approximations in the form of neural networks, geared towards solving high-dimensional and combinatorial problems in operations research. Our proposed hybrid method is rooted in the framework of approximate dynamic programming. Traditionally, large action spaces in OR problems are handled by formulating the decision problem as a linear program, yet it is difficult to properly define polynomial VFAs in this context.

The main contribution of the NN-VFA is the reduced effort of manual feature design, which is a crucial and precarious step in all solutions relying on VFAs. Unlike PL-VFAs, the NN-VFA is able to learn higher-order effects of simple input features without explicitly designing them, reducing the effort for manual feature design. This is particularly relevant when embedding VFAs in linear programs, in which the design of nonlinear features may be a cumbersome task.

We test our solution method on a representative transportation problem with a large discrete action space, a complex optimal policy, and a multi-component reward function. We compare NN-VFAs to the traditional PL-VFA, keeping all other factors equal. We observe significant improvements in performance. The findings are also robust with respect to neural network configurations; with various settings for training iterations, learning rates, neurons, and layers, the PL-VFA is consistently outperformed. NN-VFAs with multiple hidden layers yield the best and most stable policies, but also require more iterations to converge and more computational effort per iteration. We emphasize that this paper is an exploration of integrating LPs and NN-VFAs; additional research on different problems is needed to draw more general conclusions about the NN-VFA. In our opinion, the obtained results warrant such further studies.

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